Notes- Workshop on Computer-Aided Design and Simulation of Waste Treatment Systems

Training Manual
EPS 6-WP-74-1

Water Pollution Control Directorate
January, 1974

ENVIRONMENTAL PROTECTION SERVICE REPORT SERIES

Training Manuals present information that is used primarily for training purposes.

Other categories in the EPS series include such groups as Regulations, Codes, and Protocols; Policy and Planning; Economic and Technical Review; Technology Development; Surveillance; Briefs and Submissions to Public Inquiries; and Environmental Impact and Assessment.

Inquiries pertaining to Environmental Protection Service Reports should be directed to the Environmental Protection Service, Department of the Environment, Ottawa K1A OH3, Ontario, Canada.

Canadian Printco Limited
Montreal
03KT. KE204-4-PO64

NOTES
WORKSHOP ON COMPUTER-AIDED DESIGN AND SIMULATION OF WASTE TREATMENT SYSTEMS

by

B & P Silveston,
Engineers,
Kitchener, Ontario

for the

Water Pollution Control Directorate
Environmental Protection Service
ENVIRONMENT CANADA

Report No. EPS 6-WP-74-1

January, 1974

REVIEW NOTICE

This manual has been reviewed by the Water Pollution Control Directorate, Environmental Protection Service, and approved for publication. Approval does not necessarily reflect the views and policies of the Environmental Protection Service. Mention of trade names or commercial products does not constitute endorsement for use.

INFORMATION CANADA
Cat. No. En43-6/74-1

PREFACE

At the present time - almost 30 years into the age of computers, it is vacuous to argue for the use of computers by engineers. The relevant question is which jobs are worthwhile programming for a computer.

In the waste management field extensive use is being made of computers for large scale systems studies such as the well known Delaware River study done about 10 years ago in the United States or for studies of dam storage and release policies with respect to water flow for waste dilution. Studies of this type, however, have been performed by university research groups, Government agencies or just a few highly specialized consultants. Computers have not been applied to the more mundane tasks of planning local waste treatment systems or to treatment plant design to any significant extent in either the U.S. or in Canada.

The potential for computer application to performance, planning and design studies of waste treatment systems is substantial. Why the application has not been made rests upon the argument that no two design or planning situations are the same, so that these activities are "non repetitive". Also cited are: the high level of uncertainty in design which negates any attempt at sophistication; the judgement and experience which enters into design; computer cost; and, the need for "computer specialists", whereas in most consulting organizations and municipal staffs almost every man must be a "generalist".

These reasons were valid until just a few years ago. The rapid advance in applications software now make it possible to handle "non routine" waste treatment systems almost as easily as "routine" ones. Computer-aided design does not overcome the problem of uncertainty. However, with this approach,explicit allowance can be made for uncertainty. Design "risks" can be quantitized. The software packages that we will consider in these Notes have been so organized that the judgement and experience of senior staff can be brought to bear on design or analysis problems almost as easily as they can using conventional engineering procedures. The software has been developed so that it can be used and even modified by a "generalist" having only an undergraduate's

background in computing. Computing costs have become surprisingly reasonable.

Computing terminals connected to large central machines cost in the order of $150/month. Charges for actual computing time vary considerably depending on the priority requested. Use of the type of programs discussed in the Notes will require only 5 to 15 seconds of computing time/run (at a cost of between $2 to $6). A design job might require in the order of 10 to 20 runs to test different arrangements and types of units. Thus, the direct computing cost for a design will be in the order of $20 to $120. Cost alone is not the real justification for adopting computer-aided procedures. The justification is that a substantially better job can be done at little extra cost.

We believe that computers should find use in waste treatment planning and design studies and we are confident that widespread use in Canada is just a few years away. One day, we expect, it will be difficult to imagine how waste treatment planning studies could have been done without computer simulation or how design studies could have been carried on without computer assistance. We hope that these Notes and the Workshop which the Notes are intended for will contribute to the early realization of our expectation.

PREFACE

Aujourd'hui, quelque trente ans après la naissance de l'ordinateur, point n'est besoin de prêcher en faveur de son emploi par les ingénieurs. Il s'agit maintenant de savoir déterminer quelles tâches justifient une programmation.

Dans le domaine de la gestion des déchets, on fait un emploi intensif des ordinateurs pour les études de systèmes à grands échelle tel la fameuse étude de la Delaware, effectuée aux Etas-Unis il y a une dizaine d'années, ou pour l'étude de programmes de gestion des barrages-réservoirs quant au débit d'eau nécessaire à la dilution des résidus. Ces études n'ont toutefois été réalisées que par des groupes de recherche universitaires, par des organismes gouvernementaux, et par une poignée de conseillers hautement spécialisés. Aux Etats-Unit comme au Canada, les ordinateurs n'ont pas été appliqués d'une façon sérieuse aux tâches plus routinières que constituent la planification de systèmes de traitement des déchets locaux ou la conception d'usines de traitement.

L'application de l'ordinateur, aux études de performance, de planification et de conception de systèmes de traitement des résidus offre de grandes possibilités. Si l'application n'a pas été faite, c'est parce qu'on soutient que jamais deux situations de conception ou de planification ne correspondent exactement, et que ces démarches ne sont pas répétitives. Parmi les autres arguments invoqués, on trouve: la profonde incertitude dans laquelle se déroule la conception, ce qui hante toute recherche de perfectionnement; le jugement et l'expérience qui entrent en ligne de compte; les coûts associés aux ordinateurs; et finalement le besoin d'informaticiens, vu le fait que presque tout le personnel de la plupart des organismes de consultation et du personnel des municipalités se doit d'être généraliste.

Ces raisons étaient encore acceptables il y a quelques années à peine. Mais les progrès rapides enregistrés dans les périphériques d'application permettent aujourd'hui de manier les systèmes de traitement non-routiniers aussi rapidement que les systèmes routiniers. Quoique la conception automatisée n'élimine pas le problème de l'incertitude, elle nous permet d'en tenir compte avec précision.

Les "risques" de conception peuvent ainsi être quantifiés. Les ensembles de programmes que nous étudierons dans ces Notes ont été organisés de sorte que la jugement et l'expérience du personnel expérimenté puissent être amenés à résoudre des problèmes de conception ou d'analyse presque aussi facilement qu'à l'aide de méthodes classiques. Les périphériques ont été déterminées de façon qu'elles puissent être utilisées et même modifiées par un "généraliste" ne possédant que la connaissance en informatique d'un étudiant sous-gradué. De plus, les coûts de calcul sont maintenant très abordables.

Les postes de calcul reliés aux ordinateurs centraux géants ne coûtent environ que $150 par mois. Les taux de la durée effective de calcul varient considérablement selon les priorités. L'emploi des types de programmes étudiés dans ces Notes n'exigera qu'une durée de calcul de 5 à 15 secondes (soit un coût de $2 à $6). Un programme de conception peut nécessiter entre 10 et 20 essais pour vérifier divers arrangements et types d'unités. Le coût effectif des calculs pour un programme de conception donné se situerait donc entre $20 et $120. Le coût n'est alors par la seule véritable raison d'adopter les méthodes automatisées. La raison majeure qui justifie l'emploi de l'ordinateur est qu'un travail de qualité sensiblement supérieure peut être effectué à un coût à peine plus élevé.

Nous sommes d'avis que l'ordinateur devrait être employé dans les études de planification et de conception de système de traitement des résidus et confiants d'être témoins d'un emploi généralisé de l'ordinateur au Canada d'ici quelques années. Nous croyons qu'un jour il sera difficile d'imaginer comment les études de planification de traitement des résidus auraient pu, déjà, s'effectuer sans la simulation mathématique ou comment les études de conception aurient pu être réalisées sans l'aide de l'ordinateur.

Nous espérons que ces Notes et l'Atelier auquel elles sont destinées contribueront à la réalisation prochaine de nos espoirs.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

TABLE OF SYMBOLS AND NOTATION

(A Bracketted number, e.g. (10), following the definition indicates the chapter in which the symbol is used primarily)

Symbols

A		Area
	A_s	Surface area
	A_x	Cross section area
	A_p	Specific surface area of packing (ft^{-1}, m^{-1}) (10)
	A_{filt}	Filter surface area (13)
A		Chemical Species (7)
		Arbitary coefficient
A^-		Ionized Volatile acid (11)
A_{Alk}		Alkalinity (conc'n)
a		Specific surface area, interfacial area (cm^{-1}, ft^{-1})
		Arbitrary coefficient
a_{ij}		Arbitrary element of a matrix (7)
B		Birth rate in population balance relation (7)
		Arbitrary coefficient
		Chemical species (7)
BHP		Brake horse power
BOD		Biological oxygen demend (conc'n)
	BOD_5	5 day BOD measurement
	BOD_{ult}	Ultimate BOD measurement
b		Endogenous respiration rate coefficient
b'		Rate coefficient for the formation of non biodegradable material in endogenous respiration (9)
C		Concentration
	C_{g_o}	Gas phase or equicalent gas phase concentration
	C_g	Gas concentration in liquid phase corresponding to atmospheric or ideal conditions
	C_L	Concentration in the liquid phase
C		Cost (7)
	C_T	Total cost (7)
C		Arbitrary coefficient
C_{O_2}		Oxygenation capacity (9)

C_D		Drag coefficient (8)
CH_4		Methane (11)
Cl_2		Chlorine (conc'n) (12)
CO_2		Carbon dioxide (11)
COD		Chemical oxygen demand (conc'n)
c		Concentration (7)
		Specific heat (13)
		Arbitrary coefficient
c_p		Heat capacity
D		Death rate in population balance relation (7)
		Dispersion coefficient (9)
		Arbitrary coefficient
DBOD		Dissolved BOD (conc'n) (6)
DO		Sissolved oxygen (conc'n)
DOC		Dissolved organic carbon (6)
DP		Design parameter
d		Depth
d		Diameter
	d_{imp}	Impeller diameter (9)
	d_{disc}	Disc diameter (10)
	d_p	Particle or drop diameter
	d_{set}	Clarifier diameter (8)
E		Activation energy
E(t)		Residence time distribution
EN		Equipment parameter matrix
F		Food
	F/X	Food to organism ratio or organic loading (9)
f		Friction factor for flood flow
		Function
f		Fraction or ratio
	f_B	Ratio of SBOD to suspended solids
	f_E	Raction of sludge solids in overflow
	f_C	Weight fraction of carbon in sludge (13)
	f_{cair}	Fraction of cooling air sent to combustion zone (13)
	f_c	Fraction of chemcials added recovered in sludge (13)

	f_{H_2}	Weight fraction of hydrogen in sludge (13)
	f_I	Inorganic fraction of the suspended solids (9)
	f_j	Fraction of total flow assigned to the jth line (12)
	f_n	Fraction of flow going to the nth stage (9)
	f_{Alk}	Alkalinity correction factor (11)
	f_{nb}	Non biodegradable fraction of suspended solids (9)
	f_{O_2}	Weight fraction of oxygen in sludge (13)
	i	Fraction of oxygen in bubbles reaching top surface in an aerator (9)
	f_p	Weight fraction of phosphorous in sludge (9)
	f_N	Weight fraction of nitrogen in sludge (13)
	f_R	Fraction of suspended solids removed
	f_S	Fraction of BOD removed
	f_{Su}	Weight fraction of sulfur in sludge (13)
	f_{Sub}	Fraction of filter drum submerged (13)
	f_*	Fraction of BOD as suspended matter (9)
G		Sludge age
g		Gravitational constant
g_c		Force-mass conversion factor
H		Fluid head (12)
		Liquid holdup in packing (10)
		Henry's law constant (9)
H^+		Hydrogen ion concentration
HA		Unionized volatile acid (conc'n) (11)
HCO_3^-		Bicarbonate alkalinity (conc'n) (11)
HP		Horsepower
h		Height, depth
	h_{pool}	Pool depth in centrifuge (13)
h_r		Combined radiation and convection heat transfer coefficient (11)
ΔH_r		Heat of reaction (7)
ΔH_c		Heat of combustion of sludge (13)
ΔH_{fuel}		Heat of combustion of fuel (13)
$f\ell$		Humidity
	$f\ell_o$	Humidity corresponding to saturation at temperature T_o

I		Index
i		Index
J		Index
J		Mass transfer flux
	J_T	Turbulent mass transfer flux (8)
	J_u	Solids flux in thickening (8)
j		Index
K		Equilibrium constant
	K_a	Ionization constant for a volatile acid (11)
	K_w	Dissociation constant for water (11)
K		Arbitrary coefficient
k		Kinetic rate constant
	k_m	Saturation constant in Monod eqn.
	k_A	Area dependent rate constant (10)
	k_S	Rate constant for substrate removal (9)
	k_{tp}	Rate constant for cell growth in two phase model (9)
	k_i	Rate constant for ionization (11)
	k_{20}	Rate constant at 20^oC
k		Ratio of specific heats (7)
		Arbitrary coefficient
$\bar{k}$		Conductivity (7)
k		Mass transfer coefficient
	ka	Volumetric mass transfer coefficient
L		Length, depth
	L_e	Equivalent length (12)
L_o		BOD loading as lbs BOD_5/day/lb MLVSS (9)
M		Suspended solids, MLSS (conc'n)
	M_B	Biodegradable suspended solids (9)
	M_b	Suspended solids conc'n at top of sludge blanket (8)
	M_I	Inorganic suspended solids (conc'n)
	M_{nb}	Nonbiodegradable suspended solids (conc'n) (9)
MLSS		Mixed liquor suspended solids
MLASS		Mixed liquor active suspended solids
MLVSS		Mixed liquor volatile suspended solids
MW		Molecular weight
m		Arbitrary Exponent

N		Nitrogen (conc'n)
	N_{AM}	Ammonia (conc'n)
	N_{ON}	Organic nitrogen (conc'n)
N		Dimensionless number
	N_{Pe}	Peclet number
	N_{Fr}	Froude number (9)
n		Arbitrary exponent
n		Integer
	n_s	Number of stages in cascade (9)
	n_{dBC}	Number of discs in tank (10)
P		Phosphorus or phosphate (conc'n)
P(v)		Cumulative weight fraction of particles with settling velocities greater than v (8)
P_{crit}		Cumulative weight fraction of particles with settling velocities greater than V_o (8)
P_f		Weight fraction of suspended solids remaining after zone settling (8)
P		Arbitrary exponent
P		Pressure
	P_{atm}	Atmospheric pressure
	P_{O_2}	Oxygen Partial pressure
	P_W	Water partial pressure, vapor pressure
p(v)		Frequency or density distribution function of particles with settling velocity between v and v + dv (8)
pH		Hydrogen ion conc'n (as log)
Δp		Pressure difference over filter (13)
Q		Volumetric flow rate
	Q_o	Overflow rate (8)
	Q_{Air}	Air flow rate (9)
	Q_{cair}	Air flow rate for shaft cooling (13)
	Q_{CH_4}	Methane flow rate (11)
	Q_r	Recycle flow rate
	Q_W	Waste water flow rate
		Sludge wasting flow rate (9)
q		Specific flow rate

	q_{Air}	Air flow rate per unit volume of aerator (9)
	q_{filt}	Filtrate flow rate per unit area of filter (13)
q		Heat load, heat transfer rate
	q_{req}	Heat required (13)
	q_{sup}	Heat supplied (13)
R		Kinetic rate of change
	R_{AM}	Rate of ammonia consumption (9)
	R_M	Rate of increase of suspended solids (9)
		Rate of growth of methanogenic organisms (11)
	R_{O_2}	Rate of oxygen consumption (9)
	R_S	Rate of substrate consumption
	R_X	Rate of cell growth
R		Gas constant
R		Adjacency matrix (6)
	R*	Boolean sum of matrices (6)
	R^T	Transpose of matrix (6)
r		Recycle or recirculation ratio
		Ratio of return sludge flow to waste flow (9)
		Radius
r_E		Wash water ratio
r_s		Fouling coefficient in heat exchanger (11)
		Mass transfer rate
S		Substrate or BOD (conc'n)
	S*	Soluble substrate (conc'n)
	S_*	Suspended substrate (conc'n)
	S_b	Substrate concentration at end of constant rate period (9)
	S_e	Effluent substrate (conc'n)
	S_{ir}	Equivalent concentration of BOD removed by sorption on sludge (9)
	S_o	Entering or initial substrate concentration
	S_∞	Equilibrium substrate concentration due to endogenous respiration
SBOD		Suspended BOD (conc'n)
SOC		Suspended organic carbon (conc'n)
SN		Stream matrix

STRMI		Input stream matrix for a process unit
STRMØ		Output stream matrix for a process unit
SVI		Sludge volume index
T		Temperature
	T_{amb}	Air or ambiant temperature (13)
	T_{ash}	Ash temperature leaving incinerator (13)
	T_{cair}	Cooling air temperature leaving shaft (13)
	T_{fg}	Flue gas temperature (13)
	T_o	Reference or initial temperature
TOC		Total organic carbon (conc'n) (6)
TSS		Total suspended solids (conc'n)
t		Time
	$\bar{t}$	Mean residence time
	t_c	Cycle time (13)
	t_d	Cake drying time (13)
	t_f	Cake forming time (13)
	t_p	Time for peak signal to appear (8)
ΔT_{lm}		Mean temperature driving force in heat exchanger (11)
U		Overall heat transfer coefficient (11)
u		Fluid velocity
V		Volume
	V_{filt}	Volume of filtrate collected (13)
VA		Volatile acid (conc'n)
VSS		Volatile suspended solids (conc'n)
v		Paricle velocity
	v_{fl}	Flotation velocity
	v_b	Settling velocity at top of sludge blanket (8)
	v_d	Settling velocity of discrete particles (8)
	v_o	Critical settling velocity (8)
		Overflow rate
	v_{sc}	Scour velocity
	v_t	Terminal settling velocity (8)
	v_z	Settling velocity of zone (8)
v		Arbitrary independent variable

v_{sat}		Specific volume of saturated air (13)
W		Width
		Work
W		Weight flow of solids or gases
		Wastes generated in preliminary treatment (12)
		Waste removal rate (13)
	W_c	Weight rate of chemicals addition
W'		Power
w		Mass of solids deposited per unit area of filter (13)
		Arbitrary independent variable
w'		Weight of gas component produced per unit
		weight of fuel (13)
X		Distance (7)
X		Cell or active cells (conc'n)
	X_N	Nitrifying cells (conc'n)
	X_M	Methanogenic cells (conc'n) (11)
x		Arbitrary independent variable
		Arbitrary exponent
		Shell or wall thickness (11)
Y		Yield coefficient
	Y_X	Cell yield coefficient
	Y_{CH_4}	Yield coefficient for methane
	Y_N	Yield coefficient for nitrifying bacteria
Y		Arbitrary dependent variable (7)
y		Vertical position variable
		Arbitrary dependent variable
		Arbitrary exponent
y_E		Density ratio of sludge before and after elutriation
Z		Charge difference (total cation conc'n - total anion
		conc'n) (11)
z		Axial position variable
		Arbitrary independent variable
		Arbitrary exponent

Greek Symbols

α	Surface resistance to mass transfer (9)

		Arbitrary coefficient
		Root of quadratic equation (7)
		Specific cake resistance (13)
β		Term in equation (7)
		Arbitrary coefficient
		Root of quadratic equation (7)
γ		Random variable or age (7)
		Model parameter (8)
		Fraction of wash water recovered (13)
Δ		Difference
ϵ		Void or fluid fraction
η		Efficiency
		Aeration efficiency
	η^o	Aeration efficiency in clean water (9)
	η_{dig}	Digester efficiency (11)
η		Dimensionless position variable
θ		Dimensionless time
		Temperature correction factor
λ		Thermal conductivity (11)
		Ratio of settling velocity to critical
		Velocity (8)
μ		Specific cell growth rate
	μ	Maximum growth rate in Monod equation
	μ_M	Maximum growth rate for methanogenic bacteria
	μ_N	Maximum growth rate for nitrifying bacteria
μ		Viscosity
ξ		Dimensionless position variable
ρ		Density
	ρ_W	Water density
	ρ_*	Density of solids in cake (13)
σ		Standard deviation
	σ^2	Variance
τ		Detention or holdup time
	τ_{bl}	Holdup in sludge blancket (8)
	τ_H	Holdup in packing (10)

ϕ		Arbitrary function
	$\phi(t)$	Weighing coefficient (8)
ϕ		Ratio or fraction
	ϕ_r	Ratio of liquid volume to solid volume for a settling particle (8)
	ϕ_{decomp}	Fraction of decomposition of chemical compounds in incineration (13)
	ϕ_{rain}	Ratio of inches of rain to inches of water drained from sludge (13)
ϕ		Angle of inclination
Ψ		Dimensionless term
Ψ_{CH_4}		Methane yield (11)
Ψ		Fraction or weight fraction
	Ψ_{moist}	Weight fraction of water (moisture) in sludge (13)
	Ψ_{filt}	Weight fraction of solids retained on filter or solids retention factor (13)
	Ψ_{VS}	Weight fraction of volatile matter in sludge (13)
	Ψ_{Xair}	Fraction of excess air (13)
ω		Rotational speed (rpm)
	ω_{disc}	Disc rpm (10)
	ω_{imp}	Impeller rpm (9)

Subscripts

A	Area
Air, air	Air
AM	Ammonia
Alk	Alkalinity
a	Area
act	Activated sludge
amb	Ambiant or air
aq	Aqueous
atm	Atmospheric
ash	Ash
B	Biodegradable
Bar	Bar screen

b	Top of sludge blanket
bl	Sludge blanket
C	Carbon
CH_4	Methane
Cl_2	Chlorine
CO_2	Crabon dioxide
Channel	Channel
Chlor	Chlorinator
c	Chemicals, constant, cycle
cair	Cooling air
comp	Compression
crit	critical
D	Debris solids (non biodegradable)
dig	Digester
disc	Disc contactor
e	Effluent, exit, outlet, equivalent
el	Elutriator
fg	Flue gas
filt	Vacuum Filter
float, fl	Flotation, flotation tank
fuel	Auxiliary fuel
g	Gas
grit	Grit Chamber
H,H_2	Hydrogen
H	Holdup
H_2O	Water vapor
I	Inorganic, inert
i	Inactive, i^{th} item, inside, ionization
imp	Impeller
ir	Irreversible
j	J^{th} item
kin	Kinematic
L	Liquid
M	Methanogenic bacteria
max	Maximum
mech	Mechanical

min	Minimum
mix	Mixing, mixture
moist	Moisture, water
N	Nitrogen, nitrosomonas bacteria, nutrient
NB, nb	Non biodegradable
n	Stage
O, o	Overflow
O_2	Oxygen
ON	Organic nitrogen
0	Inlet, initial, outside, reference condition
opt	Optimum
P	Phosphorus, phosphate
P	Particle, packing
pump	Pump
pool	Pool
R	Removed
r	Recycle
rain	Rain
req	Required
rock	Rock
S	Substrate, BOD
Su	Sulfur
s	Surface, stage
sat	Saturated
set	Clarifier
skim	Pre aeration tank
stat	Static
suction	Suction
scrub	Scrubber
sup	Supplied
T	Total
t	Terminal
tric	Trickling filter
u	Underflow, bottoms, sludge
ult	Ultimate

VA	Volatile acid
VS	Volatile solids
W,w	Water
X	Cells, active cells
xair	Excess air
y	Vertical position, direction
z	Axial Position, direction
1	Inlet
2	Outlet
20	$20^{\circ}C$
∞	infinite, equilibrium
+	Upper surface of infinitesimally thin film
-	Under surface of infinitesimally thin film
*	Suspended, solid

Superscripts

o	Base, uncorrected, high dilution
T	Transpose (of matrix)
*	Soluble, dissolved, Boolean sum (of matrix)

Other Notation

__ as in $\underline{N}$	Vector, matrix
R (bold type)	Matrix
__ as in $\bar{N}$	Mean, average
',' (primes)	Coefficient or varable is similar to unprimed quantity, but has a different value and perhaps different units

1 INTRODUCTION

The objectives of the Workshop will be dealt with in this chapter. Organization, including how the lectures and Workshop sessions will be conducted, will also be discussed. We will indicate the individual work - as projects - you should undertake, and how to make the best use of these Notes and other materials furnished during the course.

1.1 Objectives

The Workshop is intended, first of all, to introduce you to the "art" of mathematical simulation and computer-aided design of waste treatment systems. For participants whose functions are primarily managerial, course content and your active participation in a working group should give you an appreciation of the power and the utility of these computer-oriented techniques. You should also obtain insight into possible applications of these techniques within your organization.

For engineers who intend to use the techniques personally, the Workshop proposes to achieve a level of understanding and competence that will enable you to undertake computer-aided design and system simulation confidently. At the end of the course, you should be able to use the SEPSIM Executive and the existing model library on systems you are working on. You should be able to modify a process model or even to program your own models within SEPSIM. Perhaps some of you may be capable of developing your own design and/or simulation systems.

The Workshop also has the aim of introducing you to the rapidly developing research literature on computer-aided design and management techniques. Unfortunately, the literature on applications of these techniques to real problems is quite sparse.

1.2 Organization of the Workshop

The objectives we have set for the Workshop cannot be accomplished by just reading or attending lectures. Your personal involvement in applying the techniques is essential. This is why we have chosen a "workshop" format for our course.

Contact with ideas, techniques and conventions will be made through the lectures and these Notes. Understanding and confidence will

come about through the application of the course material to real simulation and design problems.

The Workshop will consist of lectures - two each day - which will discuss the basic concepts in simulation and design and introduce the specialized techniques which have been developed as well as the conventions which have become accepted. All the lecture material will be drawn from these Notes. Moreover, the Notes contain the details and the background information which cannot be fitted into the lectures.

The second component of the Workshop will be the working sessions. Again, there will be two of these per day with an evening session, if required. Your full participation in the sessions is essential if you are to gain full benefit, and also if the course is to be useful to others.

The working group will undertake a task in simulation or design the same day it is dealt with by the lectures or in the reading. This will provide immediate reinforcement of reading and lecture material.

1.3 Workshop Sessions

Computer simulation and design should not be treated as "push-button" operations. There is quite a bit of work required before you push the button and, of course, the computer cannot interpret for you the significance of the computer print-out. There is, as Figure 1-1 shows, a cooperative relationship between you and the computer.

Your information input into the computer must be through a specialized "language" compatable with the Executive routine used for design or simulation. A well designed Executive routine talks back fortunately in the standard engineering language. In this course, the "language" we will use is specific to the SEPSIM Executive. Nonetheless, there is much similarity between the "languages" used by the various routines so that once you can work with the SEPSIM version, others can be acquired easily.

The SEPSIM "language" is not difficult to learn. It is a FORTRAN type "language" supplemented simply by ways of encoding information

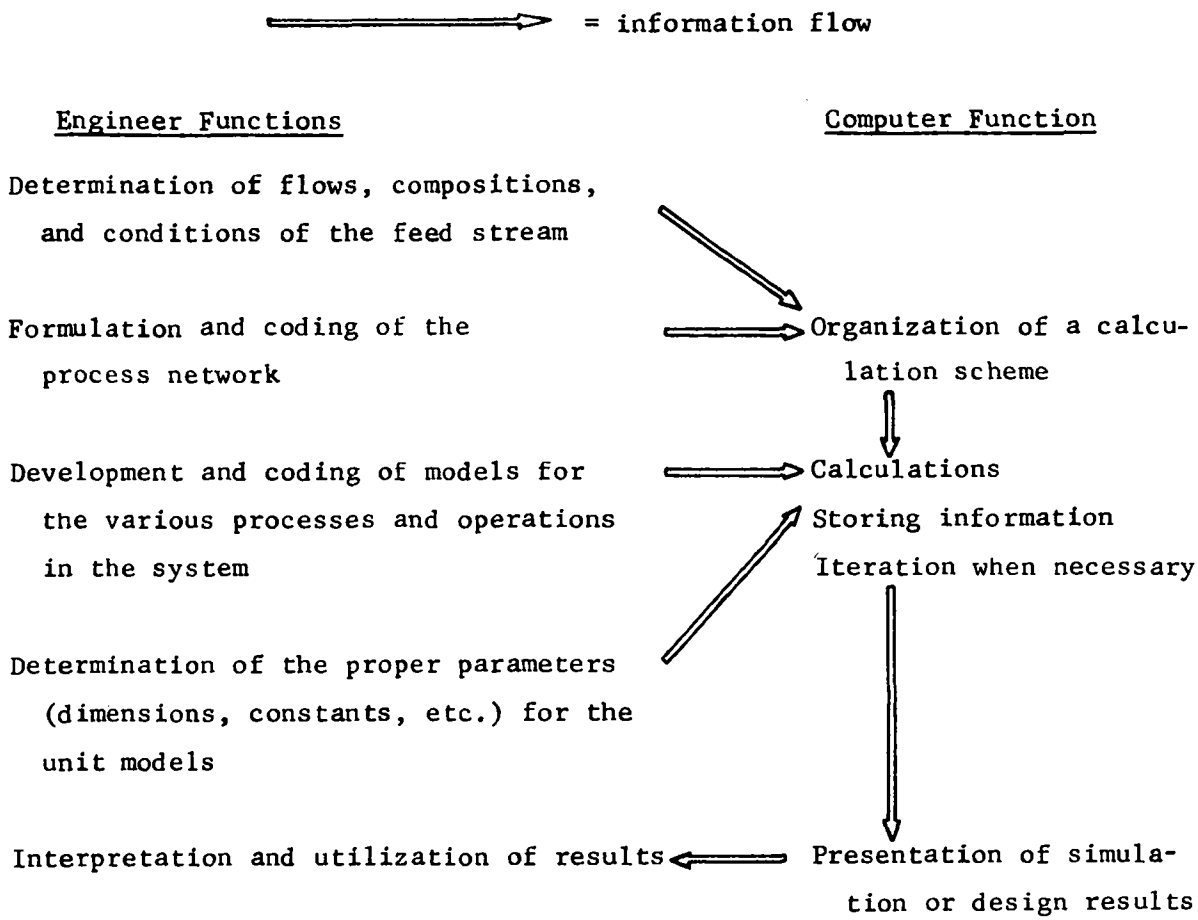


FIGURE 1-1. SCHEMATIC DIAGRAM OF THE COMPUTER-ENGINEER RELATIONSHIP IN SIMULATION AND DESIGN.*

*This figure adopted with permission from Crowe et al., "Chemical Plant Simulation", Prentice Hall (Englewood Cliffs, N.J., 1971).

and operating directions for the program. In the Workshop sessions you will learn to communicate with the computer in the SEPSIM "language".

An important aim of the Workshop sessions will be to provide you with an exercise in writing mathematical models for various process units in a waste treatment plant. You will see that this is hardly the formidable task it appears to be.

Workshop sessions will provide direct "hands on" experience for the tasks required in simulation and computer aided design. These tasks are:

(i) Preparation of a simulation model for a process unit; e.g., a primary settler

(ii) Preparation of a design model for a process unit as in (i)

(iii) Flow network analysis and encoding for simulation or design

(iv) Selection of a stream content list (information vector)

(v) Data organization for simulation or computer-aided design

(vi) Running of a simulation or a single design case

(vii) Program modification

Working groups will be organized to undertake either the simulation of the mean performance of an operating Canadian treatment plant; the design of a plant expansion; or the design of a completely new plant using the tools to be developed in the course. Each group will consist of five to six members and will be assisted by one of the instructors or a special assistant. Instructors and assistants will act as group supervisors. They will also provide individual assistance in the modelling task and group assistance in other organizing and programming tasks. They will be with the group throughout the workshop sessions.

Of the tasks listed above, only (i) and (ii), and possibly (vii) are to be done individually. The other tasks are much less time-consuming. They can be undertaken by the group together or by smaller sub-groups so as to provide most group members with experience.

To keep the length of the Workshop within reason, the time you will have to work on a model and to prepare data for a computer run will

be limited. The models you use therefore will be rather primitive. It is important that a strong contribution be made by each participant if the workshop sessions are to be successful.

1.4 Materials to be Furnished

As appendices to these Notes, the Workshop materials include a "User's Manual for SEPSIM" and a similar manual for the TESTER program. The manuals are primarily intended for use after the course, but you may wish to refer to them during the Workshop sessions.

Both user's manuals contain detailed instructions for the preparation of data for submission to a batch terminal. They discuss details of the output format which may be helpful in interpreting computer printout. The SEPSIM manual contains an explanation of how the SEPSIM Executive functions. A listing of the executive is in this manual. A listing of TESTER is contained in the second manual.

The manuals contain the software you will need to mount a simulation system for your company. It is, however, rather tedious to convert a listing into a program. A less costly action would be to obtain a tape copy or a card deck. If you are interested, arrangements for decks and tapes can be made through Professor P. L. Silveston, Department of Chemical Engineering, University of Waterloo, Waterloo, Ontario, N2L 3G1.

1.5 Use of the Notes

These Notes are intended to be a primary source of the ideas, principles and methods used in simulation and computer-aided design. All the lecture material, including the slides, is presented herein. Moreover, the Notes offer a more detailed treatment of many of the principles and methods, as well as some discussions on the backgrounds of some of the concepts. The Notes are also intended to serve as a reference for your further efforts in this area once the course has been completed.

Directions for many of the tasks in the Workshop sessions will be found in these Notes. Examples illustrating model development and such things as network encoding are provided. You will find that theoretical and to a lesser extent performance data are supplied in chapters 7 to 13 for the more frequently encountered unit operations and

processes in waste treatment.

It would be to your advantage to read through the pertinent section of the Notes before a topic is introduced in the lecture. It will in fact be necessary for you to read sections of these Notes before undertaking Workshop tasks such as writing process models, encoding networks, etc.

2 USE OF COMPUTERS IN PROCESS ANALYSIS AND DESIGN

Our purpose in this chapter is to demonstrate the usefulness of computer-aided process design and simulation by describing a few of their recent applications. Our examples will be taken from the chemical industry rather than waste treatment simply because much more has been written about chemical applications. We shall examine briefly the variety of computer programs which have been developed for design and/or simulation. Finally, we shall suggest promising applications of these techniques to waste treatment systems.

2.1 Some Definitions

In this Workshop, we are dealing essentially with the discipline called variously process analysis, operations research or systems engineering. In this discipline, problems or systems are placed in mathematical form - that is, a model is constructed - and the behaviour of the system or its cost is studied by manipulating the mathematical model. Through study of the model then, we can find what equipment is required to do a job. This is referred to as "design". Alternatively, through simulation, we can see how a system will behave as the inputs change or when its operation is varied. Simulation and computer-aided design are the forms that operations research take for different types of problems.

Let's define "simulation" first. It is currently an "in" word with many meanings. However, we will use it to mean the representation of a system - specifically, the behaviour of a system - by a model.

"Model" is easier to describe than define. Figure 2-1 tabulates commonly encountered models and classifies them in groups according to the increasing level of their abstractness. It is evident from the figure that the cost of using the model decreases sharply as abstractness increases. The figure suggests why mathematical models are used whenever possible. We will deal only with mathematical models in the Workshop.

A mathematical model is easier to illustrate than to describe. Take the expression,

$$y = x + f(x, w, v, z)$$

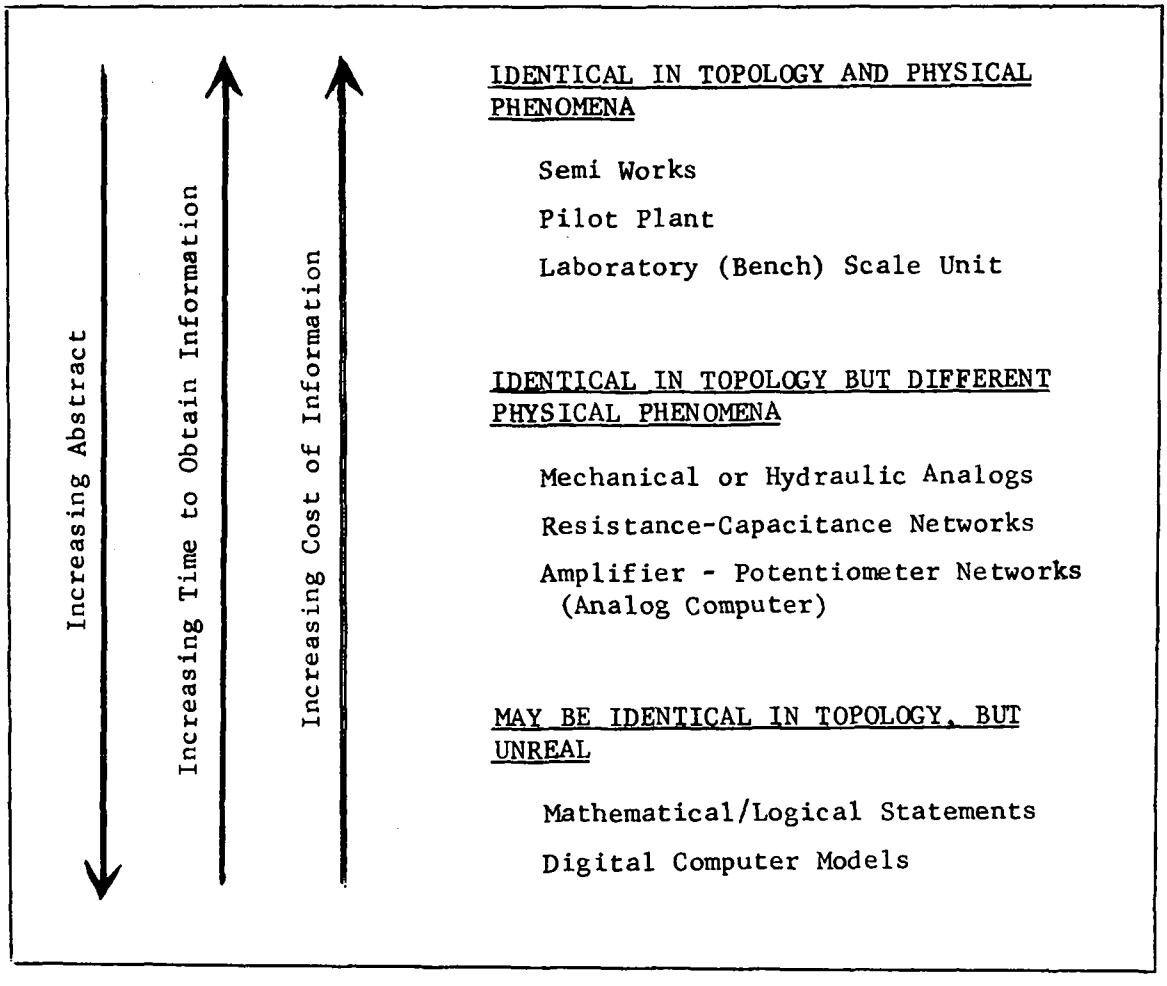


FIGURE 2-1. CLASSES AND CHARACTERISTICS OF PROCESS MODELS

This statement could be a model by itself or just part of a model. If y = the number of E. coli per cc. leaving a chlorine contact basin, x = the number of these bacteria entering; and w, v and z are, for example, the chlorine dosing rate, the detention time and the temperature, then the statement would be translated into English as: The E. coli population after chlorination will depend upon the number entering and the operation of the contact basin. The mathematical statement is also quantitative. The function $f(x, w, v, y)$ says exactly how the parameters w, v, z govern the exit population.

Parameters are properties (such as temperature, volume of a

basin, or impeller speed) which can be assigned a numerical value. In models, they will usually appear as constants, either coefficients or exponents, in an equation.

For a system there will normally be a model for each component of the system. The models are tied to one another through a network representing the flow lines (pipes, power lines, etc.) which connect the components or units in the real system. Consequently, in simulation, we study the real system by manipulating a collection of models and their embracing network.

In simulation, the inputs and the design are known and we seek the output. In design, on the other hand, we know the outputs and the inputs and seek the system. Only a few of the many possible systems are usually considered in design, and in waste treatment the choice is reduced further by regulatory agencies and, to some extent, tradition. Since the network is often fixed thereby, the design problem simply becomes one of finding the sizes and operating conditions for the process units making up the system.

Computer-aided design differs from design in general only through the "tools" used. Mathematical representations of the process units are used, and the parameters of these models are determined so that the system will achieve the specified outputs. The "best" collection of parameters in the "best" network gives the system design.

2.2 Brief Historical Background

The first major application of mathematical modelling of systems to solve operating problems or improve design was during World War II. Strategic problems such as the moving of equipment and materials, and tactical problems such as designing fire-control systems were solved through modelling. Simulation and other aspects of systems analysis have continued to play an important role in all phases of military planning.

Applications in the early 50's were mainly to transport and business problems. For example, modelling was used to determine the quantities of stock a manufacturer should keep on hand, and the best production schedules for multiple styles and sizes of articles. Oil

refiners used various types of modelling and simulation procedures to organize their tanker shipments and to determine the size of the fleets they should maintain.

By the end of the 50's, work had started on applying modelling and simulation techniques to process systems where material is converted physically and/or chemically from one form to another. The intent of much of this early work was to see if the operation of existing process systems could be improved.

Interest in computer simulation and eventually in computer-aided design had reached a sufficient level by the middle of the last decade, that students were being introduced to the techniques as part of their graduate and, in some cases, undergraduate training. In 1965, chemical engineering undergraduates at McMaster University undertook the simulation of a sulfuric acid plant as part of their undergraduate program. Currently, most chemical engineering departments in North America have a simulation program which they use on occasion for student project studies. The PACER executive program, developed at Purdue University between 1961 and 1963 was in use at twenty-five academic institutions by 1968.

Application of the techniques to waste treatment system began in the 60's. A few papers[1,2,3] in the Sanitary Engineering literature discussed the behaviour and the design of river-treatment plant systems. Application to the treatment plant proper was underway in 1966 in both the U.S.A. and Canada. In 1968, students at the University of Waterloo undertook the modelling and simulation of six municipal treatment plants in Southern Ontario[4], while R. Smith and co-workers at the Cincinnati Water Research Laboratory[5,6] described a computer-based system they had developed to size and cost a conventional activated sludge waste treatment system.

---

(1) Lynn, W. R., J.A. Logan, and A. Charnes, J.W.P.C.F., 34, 565 (1962).

(2) Galler, W.S., and H.B. Gotaas, J. San. Eng. Div., A.S.C.E., 92 (SA1), 163 (1966).

(3) McBeath, B.C., and R. Eliassen, J. San. Eng. Div., A.S.C.E., 92 (SA2), 147 (1966).

L. T. Fan and colleagues at Kansas State University published in 1972 the first of series of papers on the application of computer-aided design to waste treatment systems[7]. There appears to have been a surge of interest in applications to waste treatment systems in the last few years. A few of the publications which have appeared are listed below in the footnote[8-12]. The interest has centered primarily in University or Government Laboratories, however. There seem to be no applications to "real" problems.

---

[4] Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control, 69, No. 6, pp. 686-693 (1970).

[5] Smith, R., "Preliminary Design and Simulation of Conventional Waste Water Renovation Systems Using the Digital Computer", Water Pollution Control Research Series Publication, WP-20-9, Ohio Basin Region, F.W.P.C.A., Cincinnati, Ohio, May 1968.

[6] Smith, R., Eilers, R.G., and Hall, E.E., "Executive Digital Computer Program for Preliminary Design of Waste Water Treatment Systems", Water Pollution Control Research Series Publication, WP-20-14, F.W.P.C.A., Ohio Basin Region, Cincinnati, Ohio, August 1968.

[7] Chen, G.K., Fan L.T., Erickson, L.E., "Computer Software for Waste Water Treatment Plant Design", J.W.P.C.F., 44, 746-762 (1972).

[8] Silveston, P.L., "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research, 6 (1972).

[9] Hoffman, T.W., Woods, D.R., Murphy, K.L. and Norman, J.D., "The Strategy and an Example of Simulation as Applied to a Petroleum Refinery Waste Treatment Process", J.W.P.C.F., in print (1973).

[10] Naito, M., T. Takamatsu, and L.T. Fan, Water Research, 3, 433 (1969).

[11] Matsumoto, J., and M. Onuma, J. Jap. Sew. Works Assn., 5, (46), 37 (1968).

[12] Evenson, D.E., G. T. Orlob, and J.R. Monser, Ind. Water Engrg., 6 (2), 16 (1969).

2.3 Examples of Recent Applications

Computer-based simulation and process design are now used routinely by the major petroleum refiners, such as Shell, Mobil, and Humble, as well as major petrochemical and chemical producers such as Du Pont, Monsanto, Dow, and I.C.I. Pulp producers in the U.S. have reported the use of simulation, and apparently some of the international extractive metallurgy companies are employing it as well.

Wide use of computer-based techniques by the industrial colossi have forced engineering consultants and contractors who provide services to these companies to adopt these methods. Organizations such as Catalytic Construction Co., M.W. Kellogg, Lummus, Bechtel, Chiyoda (Japan) and Fluor employ computers for their process design studies.

Industrial corporations have been rather secretive about how they are using computer techniques. A few publications, however, have indicated the broad outline of their application. The Fortier, Louisiana Complex Ammonia plant of American Cyanamid was simulated in the early 60's to see if production could be increased without additional investment or to minimize the capital required for plant expansion[13].

The Fortier plant begins with a waste stream containing hydrogen, and dry air. The hydrogen stream is reacted catalytically with steam to increase its hydrogen content and then partially condensed to yield almost pure hydrogen. High purity nitrogen is obtained from air by low temperature fractionation. Both gases are combined and react at high pressures to form ammonia. Figure 2-2 shows a simplified flow sheet of the process. The flow sheet is appreciably more complex than those encountered in waste treatment, while the catalytic reactions which occur are about as difficult to model as biological oxidation.

A 10% increase in production was achieved through the simulation study without any major new investment. This surprising increase resulted from changing plant operation so as to eliminate mismatching of

---

[13] Armstrong, G.M., and Olson, L.R., "Improving a Chemical Plant via Process Simulation", Chemical Engineering, September 3, 1962, pp. 135-142.

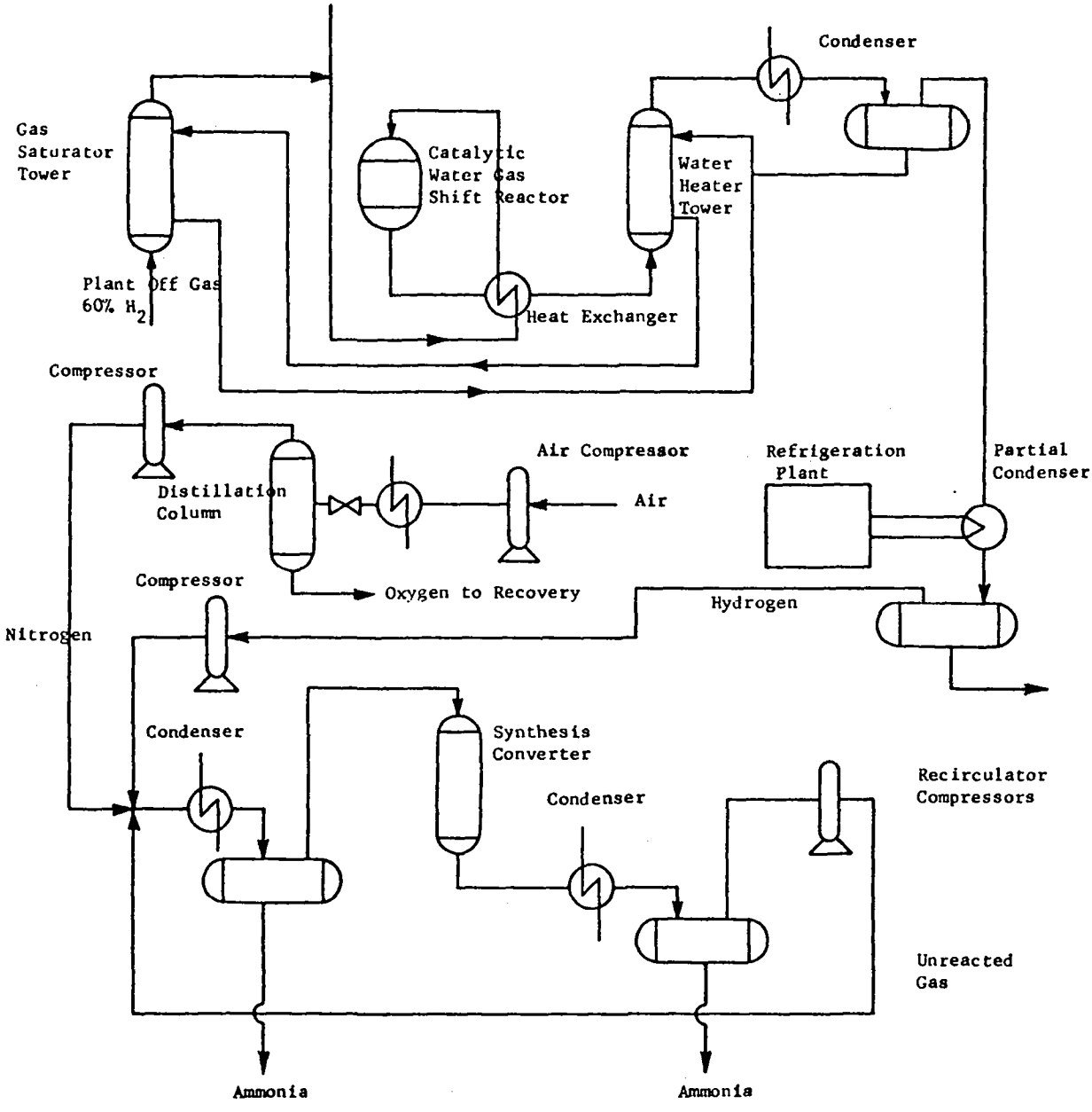


FIGURE 2-2. SCHEMATIC FLOWSHEET OF THE FORTIER (LOUISIANA) AMMONIA PLANT

different units in the plant. Mismatching occurred originally because of differing design safety factors which caused the capacity of one unit to be larger or smaller than that of another unit.

When simulation was used to study expansion of the Fortier plant, it was found that a 50% increase in production could be obtained at an investment which was 25% less than that which would have been estimated using conventional design techniques. Much of the increased production came from adding superchargers to the nitrogen and hydrogen compressor. This was possible because the two catalytic reactors in the system were overdesigned and therefore they had spare capacity. An analogous situation in waste treatment would be increasing the h.p. of surface aerators in an activated sludge unit as an alternative to building an additional train with aerators of the same horsepower.

In another application[14], I.C.I. used simulation to suggest the best operating conditions to permit a methanol synthesis plant to use an improved catalyst which lowered operating pressure, and to replace reciprocating compressors with centrifugal machines. The conditions found in the simulation study indicated a five fold increase in profitability would result from the plant changes. The study also established which operating conditions were sufficiently important to be controlled either by an operator or by automatic process control.

Diamond Shamrock Corporation has used computer-aided design to investigate alternative processes for chemicals manufacture. The evaluation of processes to produce cyclohexane from a benzene feedstock is one application which was discussed in an article[15] a few years ago. In their procedure a computer program first produced a material balance for the entire plant from specified plant inputs and outputs. The material flows calculated were supplied along with design parameters to another part of the computer program which then produced operating conditions, preliminary size of equipment, materials of construction and cost for each

---

[14] Shah, M.J., and Stillman, R.E., "Computer Control and Optimization of a Large Methanol Plant", Ind. Eng. Chem. 62, No. 12, pp. 59-75 (1970).

[15] Klumpar, I.V., "Process Predesign by Computer", Chem. Eng., September 22, 1969, pp. 114-122.

unit of the plant. Unit costs were combined to give the cost of the process. A comparison of costs then indicated the "best" process for cyclohexane production. In waste treatment this type of problem arises in comparing different modes of activated sludge operation or an oxidation pond against a small activated sludge plant.

As our final example, we will discuss briefly a computer-aided design study of ethane and propane recovery from natural gas recently completed by a Canadian engineering organization[16]. One of their clients wanted to determine if it was economically feasible to recover light hydrocarbon liquids (ethane and propane) from his natural gas wells and what the recovery would cost. Preliminary designs of two different processes were prepared and studied. One was a conventional process (Figure 2-3) employing oil absorption, while the other process (Figure 2-4) was a new proposal employing a turbo expander which condensed some of the high pressure natural gas feed by refrigeration and expansion in a turbine. A computer-aided design program developed specifically for hydrocarbon systems by the ChemShare Corp. (Houston, Texas) was used to prepare the process designs for both processes. The computer printout provided sufficient information to calculate capital and operating costs. On this basis, the competing processes were compared.

The designs for both processes are sensitive to the operating conditions. Consequently a realistic comparison of the processes can be made only when each process operates under optimal conditions. In the systems shown in Figures 2-3 and 2-4, a multitude of choices are available for the operating conditions; however, the design will be more sensitive to some choices than others. For example, the design for the lean oil absorption system is particularly sensitive to the temperature in the absorption tower. On the other hand, the turbo expander system design is strongly affected by the pressure in the fractionating tower. With computer-aided design, a search can be undertaken to find the optimal conditions for each process. A like search without a computer normally would be far too time-consuming. Figure 2-5 shows the variation of the

---

[16] Cullen, P.D., "The Turbo-Expander Process: A Critical Analysis", Engineering Report, Dept. of Chem. Eng., Univ. of Waterloo, Waterloo, Ontario (1972).

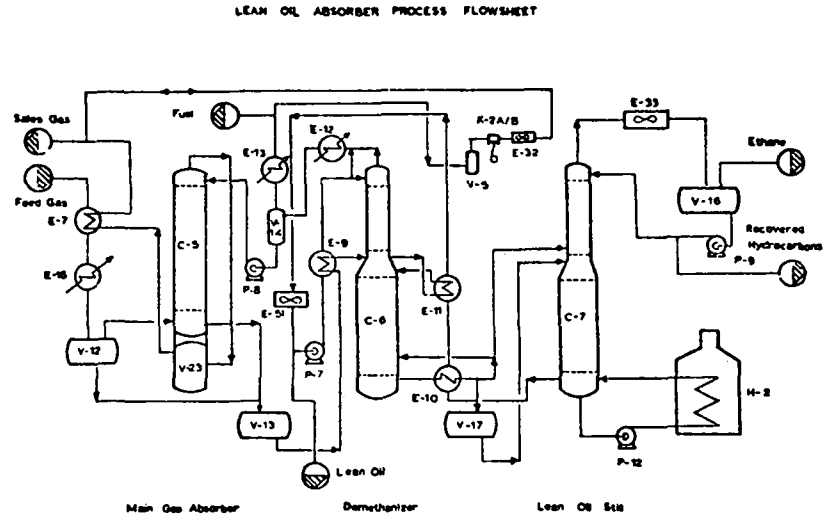


FIGURE 2-3. CONVENTIONAL PROCESS FOR RECOVERING LIGHT HYDROCARBONS FROM NATURAL GAS

(E- = Heat Exchangers, Air Coolers or Condensers;
V- = Drums; C- = Columns; P- = Pumps; K- = Compressors)

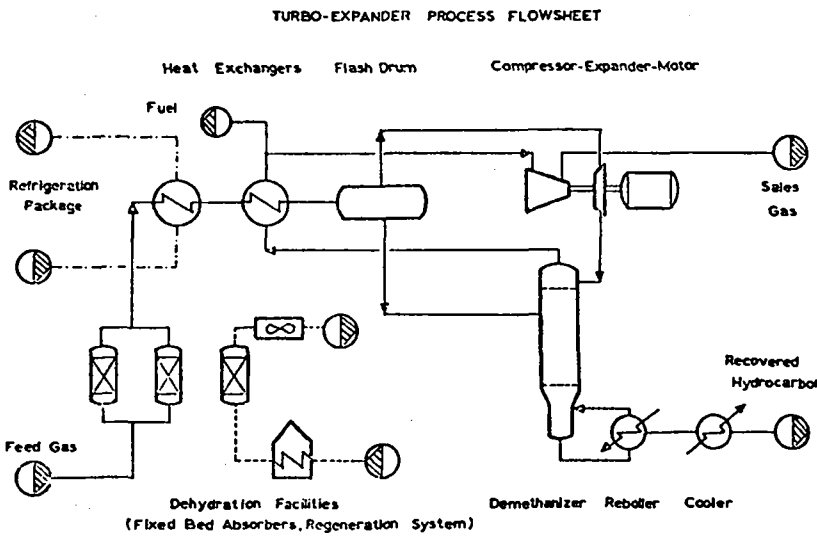


FIGURE 2-4. PROPOSED TURBO EXPANDER PROCESS FOR RECOVERING LIGHT HYDROCARBONS FROM NATURAL GAS

TURBO-EXPANDER PROCESS EQUIPMENT SIZES & INSTALLED COSTS

BASIS (i) Demethanizer pressures of 250, 350 and 500 psia considered.
(ii) Equipment sizes as provided by computer output.
(iii) Installed costs given as at mid - 1972 and based on article "Data & Techniques for Preliminary Capital Cost Estimating" K.M. Guthrie, Chemical Engineering, 1969.

EQUIPMENT ITEM	FRACTIONATOR OPERATING PRESSURE					
	250 PSIA		350 PSIA		500 PSIA	
	EQUIPMENT SIZE	COSTS ($)	EQUIPMENT SIZE	COST ($)	EQUIPMENT SIZE	COST ($)
1. FEED DRIERS						
3 Vessels	7'6" Øx30' - 1000psig	560,835		-		-
Regeneration Furnace	8MM BTU/Hr.	79,100		-		-
Regeneration Cooler	7600 ft^2 - 150 psig	19,000		-		-
2. REFRIGERATION PACKAGE	12MM BTU/Hr.	716,300		-		-
3. FLASH DRUM	6' Øx24' - 1000 psig	63,300		-		-
TOTAL PRESSURE INDEPENDENT ITEMS		1,438,500		1,438,500		1,438,500
4. FEED GAS HEAT EXCHANGER	2,733ft.^{2} - 1000 psig	106,000	5,443ft.^{2} - 1000 psig	166,000	10,372ft.^{2} - 1000 psig	232,000
5. EXPANDER	1201 HP		957 HP		661 HP	
6. COMPRESSOR	5025 HP	2,083,000	4184 HP	1,553,000	2544 HP	1,023,000
7. MOTOR	4624 HP		3227 HP		1883 HP	
8. DEMETHANIZER	4'6" Øx50' - 275 psig	101,900	3'6" Øx50' - 400 psig	81,900	2' Øx50' - 550 psig	50,500
9. DEMETHANIZER TRAYS	20 Valve Trays	4,300	20 Valve Trays	3,200	20 Valve Trays	1,500
10. DEMETHANIZER REBOILER	163ft.^{2} - 275 psig	20,200	93ft.^{2} - 400 psig	13,900	80ft.^{2} - 550 psig	16,900
TOTAL		3,753,900		3,256,500		2,762,400
CONTINGENCY (18%)		675,700		586,200		497,200
GRAND TOTAL		4,429,600		3,842,700		3,259,600

FIGURE 2-5. RESULTS OF A COMPUTER-AIDED DESIGN STUDY OF THE EFFECT OF ONE OPERATING CONDITION ON THE DESIGN

design (see demethanizer or compressor) and the costs with tower pressure for the turbo-expander process. Although operation at 250 psi entailed the highest capital cost, hydrocarbon recovery was also highest and the cost per lb. recovered was lowest. These latter numbers are not shown in Figure 2-5. Indeed, it was found that the cost per lb. was lower than that achievable in the lean oil absorption process. Operation at 500 psia, on the other hand, results in a cost per lb. recovered which was higher than that for lean oil absorption.

To obtain the design information summarized in Figure 2-5, a coded flow sheet must be provided; the models to be used for each process unit in the flow sheet must be known; the composition and conditions of all streams entering the system as well as any compositions or conditions which are fixed within the process must be supplied. Furthermore some of the design parameters must be fed into the program. A design parameter could be the tower pressure (Figure 2-3). Figure 2-6 shows the coded input for the turbo expander process, while Figure 2-7 shows a portion of the input for the streams in the process.

LIQUID HYDROCARBON RECOVER-TURBO-EXPANDER

'PROCESS VECTORS'

..... EQUIPMENT			STREAM NUMBERS			
NUMBER	MODULE	NAME				
2	HXER	HX-1	8	16	-9	-4
3	ADBF	FL-1	4	-6	-5	0
4	PUMP	PP-1	6	-7	0	0
5	VALV	VL-1	5	-15	0	0
6	DVDR	DV-1	9	-10	-12	0
7	PUMP	PP-2	10	-11	0	0
8	HXER	HX-2	13	-14	0	0
11	CAD1	ST-1	7	15	-8	-13
12	HXER	HX-3	2	17	-16	-18

FIGURE 2-6. PROCESS NETWORK OF FIGURE 2-4, ENCODED FOR THE CHEMSHARE CORP. DESIGN PROGRAM

HXER = Heat Exchanger
ADBF = Flash Drum
VALV = Throttling Valve
PUMP = Compressor or Turbo Expander
CADI = Demethanizer Column

INPUT DATA

LIQUID HYDROCARBON RECOVERY-TURBO-EXPANDER

STREAM NUMBER		2	4	5	6
EQUIP CONXION		IN -HX-3 (0)-(12)	HX-1-FL-1 (2)-(3)	FL-1-VL-1 (3)-(5)	FL-1-PP-1 (3)-(4)
VAPOR FRACTION		1.000	.000	.000	.000
TEMPERATURE, F		113.000	.000	.000	.000
PRESSURE, PSIA		950.000	.000	.000	.000
ENTHALPY, MBTU/HR		1626.991	.000	.000	.000
GPM-FT3/MIN	T-P	.0000	.0000	.0000	.0000
Z-FACTOR	T-P	.0000	.0000	.0000	.0000
GPM - MCFH	STP	.0000	.0000	.0000	.0000
COMPOSITION, LB-MOLES/HOUR					
METHANE		7167.900	.000	.000	.000
ETHANE		737.300	.000	.000	.000
PROPANE		258.900	.000	.000	.000
I-BUTANE		48.500	.000	.000	.000
N-BUTANE		91.000	.000	.000	.000
I-PENTANE		18.700	.000	.000	.000
N-PENTANE		13.500	.000	.000	.000
N-HEXANE		8.500	.000	.000	.000
N-HEPTANE		1.300	.000	.000	.000
N-OCTANE		.300	.000	.000	.000
N-NONANE		.100	.000	.000	.000
NITROGEN		32.500	.000	.000	.000
TOTAL		8378.500	.000	.000	.000

FIGURE 2-7. PORTION OF INPUT DATA TO THE COMPUTER GIVING COMPOSITION AND CONDITION OF THE FEED STREAM

A portion of the computer output is shown in Figure 2-8. For the compressor, the h.p. of the machine, outlet temperature, number of stages and the gas requirement of the turbine driver are all shown. This information usually will be sufficient to obtain the cost or select a unit from a manufacturer's trade literature. Figure 2-9 shows the information on streams in the process provided by this computer routine.

2.4 Simulation and Design Systems Available

An indication of the widespread interest in the techniques we are discussing in the Workshop is the large number of executive computing programs which have been written for process simulation or design. We will discuss executive programs, how they operate and why they are so popular in the next chapter. For the moment, executive programs are computer routines which organize calculations required for simulation or design,

FINAL RESULTS

LIQUID HYDROCARBON RECOVERY-TURBO-EXPANDER

STREAM SUMMARY

STREAM NUMBER	2	4	5	6
EQUIP CONXION	IN -HX-3 (0)-(12)	HX-1-FL-1 (2)-(3)	FL-1-VL-1 (3)-(5)	FL-1-PP-1 (3)-(4)
VAPOR FRACTION	1.000	.914	.000	1.000
TEMPERATURE, F	113.000	-16.627	-16.627	-16.627
PRESSURE, PSIA	950.000	940.000	940.000	940.000
ENTHALPY, MBTU/HR	1626.991	-14301.137	-3847.892	-10453.229
GPM-FT3/MIN T-P	.0000	.0000	106.0	443.7
Z-FACTOR T-P	.0000	.0000	.2341	.6866
GPM - MCFH STP	.0000	3171.	103.6	2900.
COMPOSITION, LB-MOLES/HOUR				
METHANE	7167.900	7167.900	352.665	6815.232
ETHANE	737.300	737.300	135.162	602.139
PROPANE	258.900	258.900	107.117	151.784
I-BUTANE	48.500	48.500	27.648	20.852
N-BUTANE	91.000	91.000	59.639	31.362
I-PENTANE	18.700	18.700	14.286	4.414
N-PENTANE	13.500	13.500	11.030	2.470
N-HEXANE	8.500	8.500	7.732	.768
N-HEPTANE	1.300	1.300	1.239	.061
N-OCTANE	.300	.300	.293	.007
N-NONANE	.100	.100	.099	.001
NITROGEN	32.500	32.500	.578	31.922
TOTAL	8378.500	8378.500	717.487	7661.013

FIGURE 2-8. PORTION OF COMPUTER OUTPUT GIVING COMPOSITION AND CONDITION OF EACH STREAM IN THE PROCESS (Compare with Input in Figure 2-7)

***PUMPS/COMPRESSOR ***

EQUIPMENT NO.	4	7
EXTERNAL NAME	PP-1	PP-2
COMP. STAGES	1.0000	2.0000
WORK CAPACITY (HP.)	10000.0000	10000.0000
OUTLET PRES.	250.0000	930.0000
POWER TYPE : (+)=STEAM, (0)=ELEC., (-1)=FUEL GAS, (-100)=ENTROPY CALC.	-100.0000	-100.0000
H-OUTLET STEAM (BTU/LB)	.0000	.0000
POLYTROPIC COEF OR EFFICIENCY FOR ENTROPY CALC. MACHINE	.6800	.6500
INTSTAGE OUT T,DF	.0000	130.0000
FUEL USAGE (MSCF/HR)	.0000	49273.0200
WATER USAGE (GAL/HR)	.0000	-12008.8345
STEAM USAGE (M LBS/HR)	.0000	.0000
KW USAGE	.0000	.0000
WORK REQ (HP)	-1387.6178	5525.7858

WORK IS NEGATIVE FOR EXPANDER

FIGURE 2-9. PORTION OF COMPUTER OUTPUT GIVING DESIGN PARAMETERS FOR THE COMPRESSOR AND TURBO EXPANDER REQUIRED (See Figure 2-7)

manage the actual calculations and decide when they can be terminated when iterative procedures are used. These programs also provide printout of the computer results. The actual calculations are usually performed by subroutines. Normally, a distinct subroutine will be needed for each type of process unit. Additional specialized subroutines provide various services such as cost calculations, accelerating iterative calculations, debugging assistance and calculation of physical properties. The collection of subroutines is referred to as a library.

Table 2-1[17] provides a roster of computer programs. These are arranged by the type of organization which owns or developed the program. Since 1969, the date of the Table, a number of additional programs have appeared. An updated version of CHESS known as DESIGN or CAPS (for Chemshare Automatic Process Simulation) is owned by the ChemShare Corp. of Houston, Texas. It is available through Computer Sciences Canada Ltd. on a fee basis. SEPSIM, which we will use in the Workshop, is not included in the Table. Missing as well is the ASOP (Activated Sludge Process Optimization Program) developed by Fan and Associates at Kansas State University[18].

Virtually all of the programs listed in the Table 2-1 are general executive programs capable of handling a wide variety of process networks. In most cases, a library of subroutines has been developed for each; it is these libraries which limit applicability. For example, CAPS or DESIGN are limited by their library to hydrocarbon processes as might be encountered in a petroleum refinery or a natural gas plant. FLOWTRAN has a somewhat more general library, but it is nonetheless limited to petrochemical processes. SEPSIM, on the other hand, has a library which limits it to waste treatment systems.

Programs of service and consulting organizations will in some cases be available through the support services of computer manufacturers. Thus, CHIPS UOS should be available to IBM users. As mentioned above,

---

(17) Wilhelm, D.J., "Scale-Up, A Status Report", Chemical Age of India, 21, No. 2, p. 162 (1970).

(18) Fan, L.T., Chan, G.K.C., and Erickson, L.E., J.W.P.C.F. 44, No. 5, p. 746 (1972).

TABLE 2-1. DIGITAL COMPUTER PROGRAMMES FOR COMPUTER-AIDED DESIGN, ANALYSIS, AND OPTIMIZATION OF INTEGRATED CHEMICAL PROCESS SYSTEMS ON WHICH SOME INFORMATION IS AVAILABLE.

Name of Program		Organization where developed	Status
INDUSTRY			
CHEOPS	Chemical Engineering Optimization System	Shell Development Co. Emeryville, California. USA	Proprietary-for-sale
CHEVRON System	General Heat & Material Balancing System	Chevron Research Co. Richmond, California, USA	Proprietary, but now somewhat obsolete
Computer Programming System for the Economic Evaluation of New Chemicals & Chemical Processes		Merck & Co., Inc., USA	Proprietary
Flowtran		Monsanto Co., USA	Proprietary
GPPS	Generalized Process Flow Simulator	Sun Oil Co., USA	Proprietary-for license
Lummus General Process Simulator (56)		Lummus Co., USA	Proprietary
NETWORK 67		Imperial Chemical Industries. Ltd., U.K.	Proprietary
PEDLAN	Process Engineering Design Language	Mobil Oil Co., USA	Proprietary
PIPE	Process Integrated Performance Evaluation	American Cyanamid Co., USA	Proprietary
PROCESS	Process Oriented Chemical Engineering Simulation System	Pure Oil Division, Union Oil Co., of California	Proprietary
PROJECT SCREENING PROGRAM		W. R. Grace & Co., USA	Proprietary
SCOPE (66)	Sizing and Costing of Process Equipment	Diamond Shamrock Co. U.S.A.	Proprietary-for Sale
SERVICE & CONSULTING COMPANIES			
CHem E Simulator		Petrochem Consultants, Houston, Texas, USA	For License
CHESS	Chemical Engineering System Simulator	University of Houston, USA	For License
CHIPS	Chemical Engineering Information Processing System	Service Bureau Corp. (Subsidiary of IBM) Palo Alto, California, USA	Proprietary-for Sale
COPS	Catalytic Optimum Profit Sequencing	Catalytic Construction Co., USA	Proprietary
Executive Computer Program for the Design of Wastewater Treatment Systems		U.S. Dept. of the Interior, Cincinnati, Ohio, USA. Water Treatment Laboratory	Available
FLEXIBLE FLOWSHEET		M. W. Kellogg Co., New York, N. Y. USA Kellogg International Corpn. London, England	Proprietary
PACER-245	Process and Case Evaluator Routine	Originally Developed at Purdue University & Dartmouth College, USA. Later expanded by Digital Systems Corp., Hanover, New Hampshire U.S.A.	For License at $ 90,000
PECOS		Bechtel Co., San Francisco, Calif., USA	Proprietary
UOS	Unit Operations	Developed by Bonner & Moore Associates, Inc., Houston, Texas, USA for IBM's Service Bureau Corporation	Proprietary

Table 2-1 cont'd....2-17

TABLE 2-1 CONTINUED

Name of Program		Organization where developed	Status
EDUCATIONAL INSTITUTIONS			
Chemical Engineering Calculating System		University of Michigan & Univ. Pennsylvania, USA	Under development
CHESS*	Chemical Engineering System Simulator	University of Houston, Houston, Texas, USA	for sale to Academic Institutions
CPC	Chemical Plant Calculating System	University of Cambridge, England	Uncertain
DISCOSSA		Oregon State University, USA	Uncertain
DYNSYS	Dynamic Systems Simulator	McMaster University, Canada	Under Development
GEMCS*	General Engineering & Management Computer System	McMaster University, Canada	Available from the Ch.E. Dept., McMaster Univ.
LINSYS*	Linear Systems Simulator	McMaster University, Canada	Available from the Ch.E. Dept., McMaster Univ.
MACSIM		McMaster University, Canada	Operational (Availability uncertain)
MAEBE	Material & Energy Balance Execution	University of Tennessee USA	Available (1st generation material energy balance program)
PACER*	Process & Case Evaluator Routine	Simplified Version in use at Dartmouth College, USA	Available from Digital Systems Corp., USA
SLED	Simplified Language for Engineering Design	University of Michigan, Ann Arbor, Michigan, USA	Uncertain
SPEED-UP	Simulaion Program for the Economic Evaluation and Design of Unsteady State Processes	Imperial College London, England.	Still under development

Table taken from reference (17). Permission for use requested.

CAPS/DESIGN is available in Canada on a license + per use fee basis. Both SEPSIM and the Executive Program of the Cincinnati Water Laboratory (Table 2-1) are available without fee. The university programs at the end of the Table are usually offered to universities at a nominal cost, but a fee is charged for commercial use. The GEMCS system is an exception. It is available through the GEC and CDC Computer Support Systems.

Before leaving this section, it would be well to mention two areas of program development. The first area encompasses specialized programs to choose the process networks. Programs of this sort would have their main application in choosing treatment for industrial wastes. The second area is that of specialized executive programs for dynamic simulation of processes. Programs of this sort would be useful for modelling start-up of treatment plants, or examining plant behaviour after sharp changes in flow or waste loading. A number of programs are already available. These are listed in Table 2-2.

TABLE 2-2. EXECUTIVE PROGRAMS FOR DYNAMIC SIMULATION OF PROCESS SYSTEMS

PROGRAM NAME	ORGANIZATION WHERE DEVELOPED	TYPE
DYFLO	E.L. Du Pont de Nemours	Executive, Library of Process Model, Integration Subroutines
SPEED UP	Imperial College, U.K.	"
DYNSYS	McMaster University	"
DSUSIUM	Ohio State University	"
PRODYC	University of Houston	Executive, Library of Process Models, Routine which converts System to CSMP input
REMUS	University of Pennsylvania	Executive, Library of Process Models and Integration Subroutines
CSMP	IBM	Program for Solution of Systems of Differential Equations
MIMIC	Univac, CDC	"

2.5 User Opinions

In their promotional literature, developers of programs available for license cite samples without naming users that demonstrate large savings. The ammonia plant simulation study mentioned earlier did claim very significant savings. However, when programs were first being developed in the early sixties, it was rumoured that they cost more to develop than they actually generated in savings. The programs developed by the large industrial organizations were indeed expensive. The cost of development is suggested by the purchase price of the PACER-245 program (Table 2-1) which was $90,000 a few years ago. The promise of simulation and computer-aided design, however, is manifested by the large number of systems shown in Table 2-1 and the continued development of new software systems.

2.6 Potential Applications in Waste Treatment

Although some use of Smith's executive program for preliminary design of waste treatment plants[5] appears to have been made by U.S. consultants, simulation and design studies of waste treatment systems has been largely confined to universities up to now. University activity has been largely to develop and test models and software systems. No "real" applications can be cited so therefore, we will examine in this final section what we believe will be the attractive applications of these computer techniques.

Applications of simulation are listed in Table 2-3. Leaving aside design for the moment, perhaps the most important applications for consultants and regional or provincial Sanitary Engineers are entries A to D in the table. A supervisory function of Sanitary Engineers in local or provincial governments is to monitor the performance of their plants and compare their performance to the design specifications. Simulation is an attractive tool for this function. Thus, it would be useful to have a model for each plant against which the plant performance could be compared.

A second function - improving plant performance - is also well suited to simulation. The technique is called parameter variation or sensitivity analysis. Simulation runs are conducted varying one at a

TABLE 2-3. APPLICATIONS OF SIMULATION

A	Analysis for 'bottlenecks' to locate process units which are limiting plant performances and/or capacity.
B	Determination of the effect of feed stream composition changes, use of different chemical reagents, or changes in product specifications on plant performance and/or capacity.
C	Prediction of conditions under which plant will become "overloaded".
D	Prediction of the effect of plant modification on performance or capacity.
E	Investigations to develop data for costing individual products in multiproduct plants or for pricing decisions.
F	Study of dynamic behaviour of systems for process control purposes.
G	Investigations of system stability to possible disturbances.
H	Training of operators and other plant personnel.
I	Engineering study of plant operation under extremes of conditions which cannot be examined in prototype, or pilot scale installations.
J	Sensitivity analysis to find where research is needed to improve system or system models

time the parameters characterizing the size or operation of each unit in the plant. In this way, the sensitivity of the plant performance or capacity to the size and operation of each process unit can be established. Units which have inordinately large effects on performance or capacity are referred to as "bottlenecks". Elimination of "bottlenecks" is usually the least expensive way to expand a plant.

Both supervisory groups and consultants often are faced with predicting the effect of extending a sewer system or introducing industrial wastes on their treatment plant. Simulation can provide this information. Although an experienced engineer can estimate the maximum capacity of a treatment plant, his estimates are educated guesses. By contrast, a simulation which describes the current operation of a plant is a much more reliable means of estimating the throughput at which the plant will be overloaded.

A plant simulation provides a convenient and low-cost way of determining the effects of plant modification through the introduction of new equipment, resulting in, say, increased aeration, or a new reagent such as a flocculating agent on plant performance or capacity. This needs little elaboration.

Going to E in Table 2-3, simulation can also aid the assessment of just sewer charges. Should charges be on a volume basis? If not, how should different waste and waste loads be handled? Since a sensitive simulation will show the effects of flow, load and even composition on performance, it provides a tool for estimating what changes in operation, chemicals usage will be required to handle individual industrial wastes or wastes from an area. The resulting extra costs and a share of the capital investment surely are the proper bases for sewer charges.

Process control probably will become more important as effluent controls become stricter and treatment process becomes more chemically oriented. Simulation plays an important part in the design of control systems. Specifications for a control system, points for making measurements, and streams to be controlled all depend on the dynamic behaviour of a process. Dynamic simulation of the process and control systems often is necessary to determine the stability of the controlled system. Steady-

state simulation, which we consider in this Workshop, has a role. It can indicate the important variables to control.

Sensitivity analysis, as described above, is also a valuable tool for R & D management. For example, parameter variation simulations of conventional treatment processes operating on high BOD industrial wastes will disclose which process units or which parameters of individual models have the greatest effect on performance. It goes without further elaboration that these units or model parameters should be given the most emphasis in laboratory work or pilot plant studies. Simulation is a powerful tool for analyzing and planning experimental research.

Computer-aided design is attractive fundamentally, because it lends itself so well to optimization. The choice of process units, e.g., sedimentation vs. flotation, and their linking in a process network can be tested in a series of case studies to determine the best performance in terms of capital, operating or annual cost. Optimization of a design deals with the sizing of equipment for a specific process flow sheet and feed. To carry this out, we would run the design program through a series of case studies or imbed it in an optimization routine. The object in either procedure would be to choose equipment sizes which minimize annual or capital cost.

Optimization of an operating plant is also possible. This operation may be undertaken either directly on the plant or via simulation. The latter is frequently convenient because information is available faster, and operating changes in the wrong direction will not be catastrophic. What is done in this application is that changes in model parameters are introduced which reflect operating changes, and their effect on performance is evaluated. This activity is essentially "bottleneck removal" listed as A in Table 2-3.

The real "payout" of computer techniques for waste treatment will be in optimization. We can close this chapter best by pointing out that optimization is only meaningful if we employ reliable models. Simulation, thus, has a key function. Only through simulation can we test the reliability of models.

3 CHAPTER 3 - CHOICE OF APPROACH

In the previous chapter, we used the impressive number of executive simulation and design programs in Table 2-1 to suggest the wide acceptance of computer centered analysis and design in the process industries. This table implies, however, that simulation and computer-aided design is only carried out through executive programs. Actually various approaches are open. On one extreme, each computer program may be tailored to a specific plant or design situation; while on the other extreme, a fully modular computing system can be employed in which the plant or design is just a case. In between are various levels of executive systems. For example, the network of the treatment plant could be included in the program, but the models for the process units employed could be called as separate subroutines. The choice of approach often influences the choice of models; but more important it may have a large effect on the time and cost of simulation or design.

This chapter examines the choice of approach and introduces our discussion of process analysis and the SEPSIM Executive Program in subsequent chapters. Before taking up the choice of approach, we will discuss briefly data handling problems and the components of process systems. Simulation will be the main vehicle of discussion in this chapter.

3.1 Calculation and Bookkeeping Problem

Computer oriented simulation of processes are more thorough than desk top studies. The computer permits the user to keep track of all the species of interest (BOD, suspended solids, dissolved organic nitrogen, etc.) at any point in a waste treatment plant. The calculations that are required to do this, however, and the information storage and handling needed grow quickly with the number of units in the plant and the complexity of the process network.

In the WATCRAP-PACER studies of Ontario sewage plants[1], for example, up to 17 components were kept track of. With usually 8 process units, this meant that a system of at least 136 algebraic equations had to be solved. With 13 streams in the process network, 221 variables had to be manipulated and stored. The bookkeeping and calculational problem was even more formidable in the McMaster sulfuric acid plant study.

According to Shannon et al.[2], 42 units and 70 streams were involved, requiring the solution of 500 simultaneous equations and keeping track of about 1000 variables.

3.2 Components of a Process System

We have talked about process units and defined what we mean by a "network" in Chapter 2. Now we will look at both "concepts" as part of a process system. Waste treatment is a typical process system in so far as identifiable changes in flows and compositions occur and that these changes can be associated with separate and distinct pieces of equipment. For simulation and design, a process system is composed of:

1. a network of streams connecting the process units;
2. a collection of process units which 'operate' to change the flows and compositions transmitted by streams;
3. feed streams which are known and invariate for each simulation or design case, and;
4. output streams whose flows and compositions are of primary interest in simulation, but whose compositions are partially specified in design.

Breakdown and classification proceeds further. The collection of process units may in turn be divided into groups of unit operations or processes such as biological reactors or clarifiers. Subdivision eventually leads us to units which have the same model structure.

Process systems are inherently modular.

3.3 Simulation Incorporating the Process Network

We might term this approach a 'do-it-yourself' procedure. No executive program is employed to set up the calculations, organize storage of data or perform input/output operations. Significantly, the process network is not treated as data, but is built into the program as 'CONTINUE' and 'GO TO' statements. The program must also contain models for the process units, a convergence testing procedure if recycle occurs, provide

---

[1] Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants using the WATCRAP-PACER System", Water Pollution Control, 69, No. 6, 686-693 (1970)

[2] Shannon, P.T. et al., "Computer Simulation of a Sulfuric Acid Plant", Chem. Eg., Progress 62, June, 49, (1966)

input/output and a suitable exit plus error message package.

We can suggest the broad structure of simulation by this approach through an example. Figure 3-1 shows the fluid side of a waste treatment process employing a trickling filter. It is a relatively simple recycle system. Figure 3-2 sketches a computer flow diagram of a simulation for this process. A program of this type can be made more versatile by introducing as much information about the system as possible through data statements.

"Stream vector" in Figure 3-2 refers to the information content of streams or the variables list. The term simply indicates that the list is structured like a vector. We do not undertake vector operations with the list. The circled number refers to the stream marked in the same way in Figure 3-1. We will discuss the "stream vector" further in Chapter 5.

Calculations indicated in portions of the computer flow diagram (Figure 3-2) use models discussed in subsequent chapters.

The procedure suggested by the diagram is known as successive substitution. The feedback path in Figure 3-2 is first assumed to contain no information. In the second pass the flow and composition of stream (8) is no longer zero so the flow and composition entering unit 1 change. If the equations which make up the models are free from discontinuities, such as poles and zeroes, the procedure converges to the proper values for all streams. Fortunately, discontinuities in the range of variables normally encountered is rare. We exit from the recycle loop and proceed further after the desired degree of convergence in an outlet of the loop is attained. There is no need to test each of the stream vectors for convergence.

Since FORTRAN (or ALGOL) statements must be written for each calculation and for each of the information organizing and storage operations, preparing a simulation program for a large process plant can become exceedingly time consuming. Thus, the approach under discussion is suited to small, relatively simple simulations. It offers the advantages of compactness so that simulation can be undertaken on computers with a small

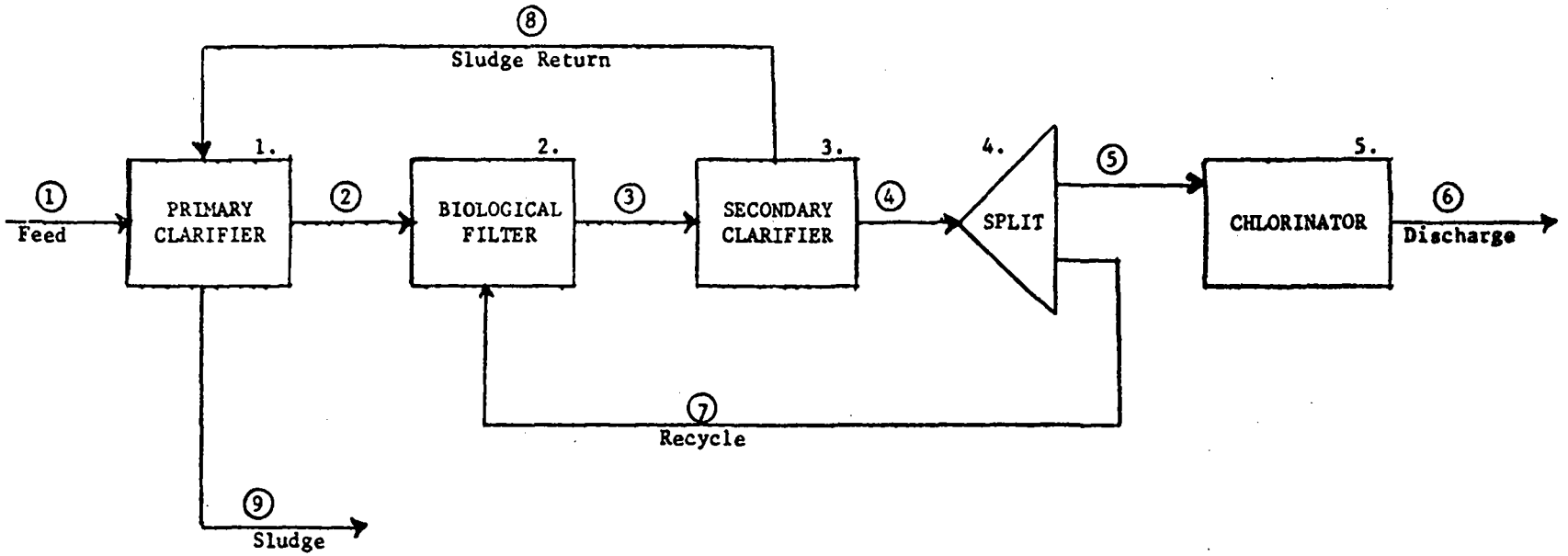


FIGURE 3-1. FLUID SIDE OF A TRICKLING FILTER WASTE TREATMENT PROCESS

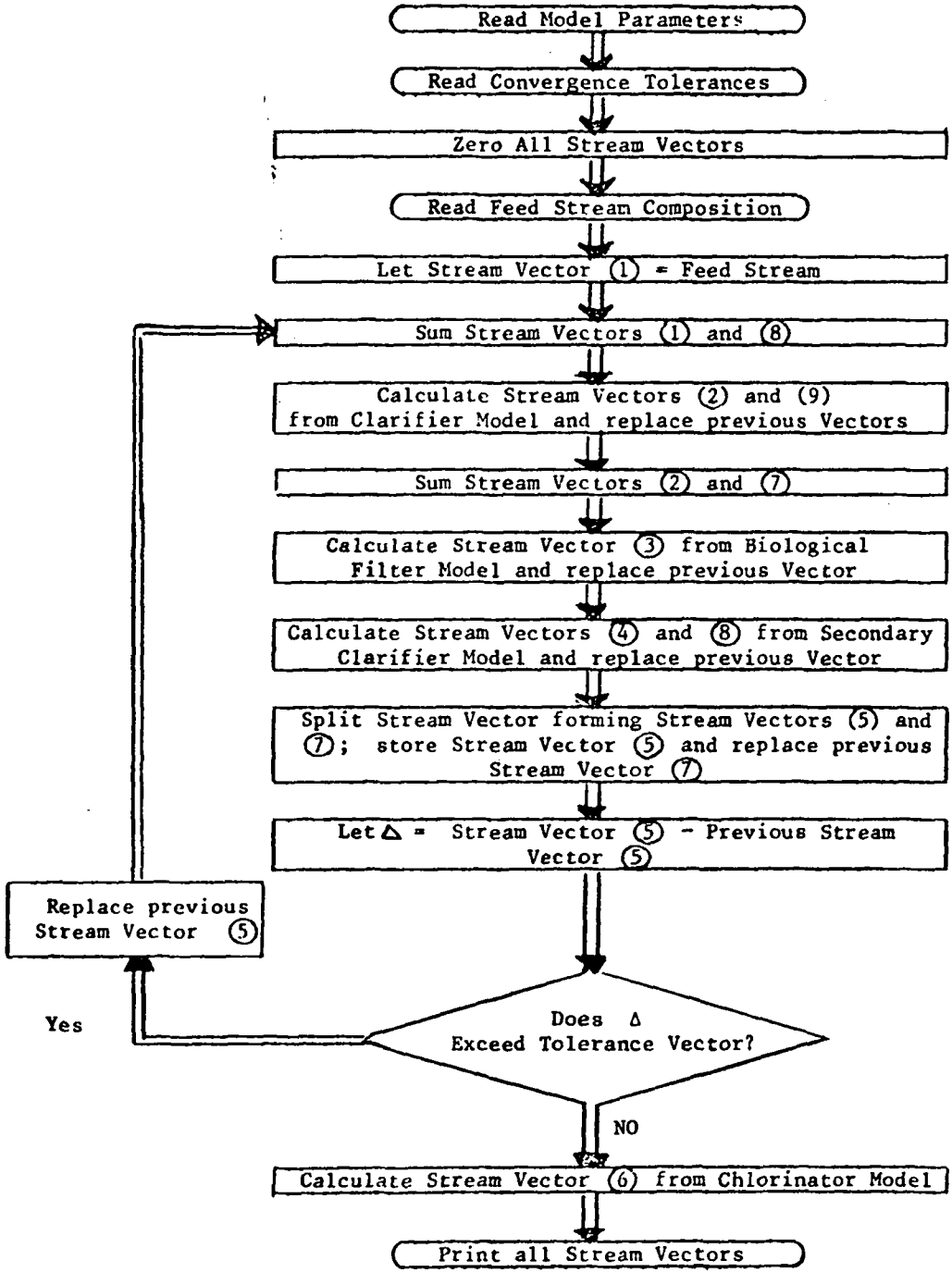


FIGURE 3-2. LOGICAL FLOW CHART FOR SIMULATION OF WASTE TREATMENT SYSTEM EXAMPLE

fast core capacity. Furthermore, it can make use of highly specific models, such as statistical models, which would not be general enough for executive programs. Its job time should be shorter than for runs using executive programs. Disadvantages are that it is cumbersome and time consuming to allow for changes in the process flow sheet or for updating of models. Any modification of the program requires moderate programming skill.

Although waste treatment plants contain a large number of individual pieces of equipment, many units are in parallel and for simulation purposes they can be modelled as just one unit. The 12 mgd Kitchener W.T.P. contains 27 units handling sewage, apart from pumps. Duplication is such that this plant can be simulated with at most 8 models. Waste treatment systems are small enough and their networks are sufficiently simple that the direct approach cannot be rejected out of hand. Smith's first design program[3] used this approach. Unfortunately, the program listing runs over 14 pages so it is too lengthy to reproduce here as an example.

3.4 Executive Simulation Programs

An essential characteristic of executive programs is that the process flow sheet is part of the job data. This permits a program to handle a wide variety of systems. Executive programs organize the computations by "preparing" a logical flow diagram like Figure 3-2 from the process flow sheet. They may contain algorithms for finding efficient calculation orders and suitable starting points for iterative calculations. Input and output (I/O) operations, of course, are handled by the executives. They may also check input data for error. Bookkeeping (storage of calculated results) and testing for convergence when iterative calculations arise are other standard functions of executive programs.

Figure 3-3[1] illustrates the function of a typical executive program. Notice that there are two types of inputs. The first, shown on

---

[3] Smith, R., "Preliminary Design and Simulation of Conventional Waste Water Renovation Systems Using the Digital Computer" Water Pollution Control Research Series, WP-20-9, F.W.P.C.A., U.S.D.I. (Washington, 1968)

the left in the figure consists of data for a simulation: flows and compositions of all feed streams, guesses for other streams (although this is not essential); values of parameters in models; a computer compatible description of the process network, and operating instructions for the computer. The second input at the top of the figure is a collection of models which provide the executive with the equations it needs to calculate the compositions and flows in all streams in the system. The latter, of course, is the output in a simulation.

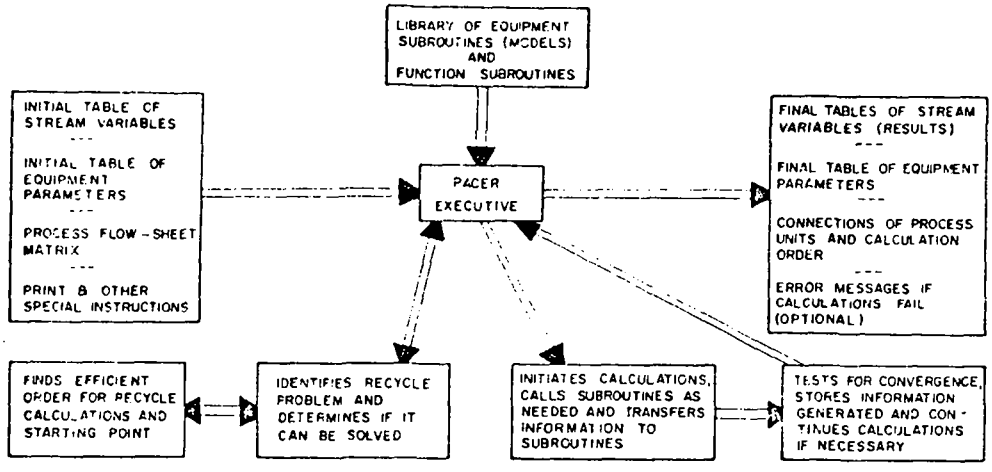


FIGURE 3-3. OPERATION OF THE PACER EXECUTIVE*

Figure 3-3 shows two other groups of operations initiated and managed by the executive. On the lower right the figure shows the calculation of outputs through calling of library subroutines which furnish the equations, and the testing for convergence in iterative procedures. On the left, we see functions of some executive: 1) the analysis of the process network to determine if iterative calculations are necessary, and 2) organization of a reasonably efficient procedure for these calculations. The SEPSIM executive which we will employ in this Workshop does not have this capability. Of the executive programs in Table 2-1 for which details are available, MACSIM, CHESS and MAEBE share this analysis or "decomposition" capability with the PACER executive.

*Figure taken from reference (1) with the kind permission of the Journal.

The advantages of the executive program approach to simulation are their versatility, their modular structure which permits relatively easy updating of model or program, and their ease of use. The SEPSIM executive, for example, can be used in case studies by simply varying some of the input data. It may be used for design as well as simulation. Executive programs are suited to large systems with many streams and process units which would be impractical to handle without an executive. Finally, once the coding of the input data has been mastered, executives such as SEPSIM can be used by personnel relatively unskilled in programming.

Executive programs generally suffer from their large size. PACER, for example, requires between 120 and 140 K of core. Thus, without reprogramming for overlaying they cannot be run on small computers. A modest drawback is that most executive programs require a special language beyond FORTRAN or ALGOL and this must be learned before models can be written for use with an executive.

3.5 Choice of Approach for Design

Certainly one of the salient attractions of computer-aided design is that it provides an opportunity for optimization of the system chosen. Optimization of recycle systems, where models are nonlinear generally will be handled by search methods. The search proceeds in principle by designing the plant a large number of times so as to identify gradients or surface features of the dependent variable or objective function. Computer time required for searches can be quite large so that it is important to perform the calculations as efficiently as possible. Executive programs because of their versatility may not provide the most efficient calculation procedure. Whereas for simulation, executive programs are preferable in all but a few cases, the choice between a specific program and the use of an executive program remains a question for design.

L. T. Fan and co-workers[4] have developed an optimization program which employs an executive program of the type discussed in the pre-

---

[4] Fan, L.T., Erickson, L.E. and Chen, G.K.C., "Computer Optimization of Biological Waste Water Treatment Processes", in WATER - 1971, Chem. Eng. Progress Symp. Series, (1973)

vious section.

3.6 Executive Programs for Waste Treatment Plant Simulation and Design

Simulation and computer-aided design of wastes treatment systems, we pointed out in Chapter 2, has been largely confined to universities. Much of the university work has been conducted using executive programs. We will examine these programs in the remainder of this chapter, but since we have not looked into details of how executive programs operate our discussion must be rather superficial. Work without the aid of executives has been confined largely to computer-aided design of serial systems.

Table 3-1 summarizes the executive programs that have been used for waste treatment plant studies. The first four are essentially general purpose simulation executive programs which have been adapted for waste treatment systems by formulating a specialized library of subroutines. All are quite similar in operation. PACER and MACSIM contain a network analysis or decomposition routine which as we discussed in the previous section locates recycle loops in the flow sheet and organizes the iterative calculations needed with these loops. In both executives, this portion can be bypassed if the user wishes to specify a calculation scheme. GEMCS contains an optional subroutine ORDER to perform the network analysis. SEPSIM, on the other hand, has no analysis capability. It was specifically developed for waste treatment systems which have simple enough networks so that the calculation order can be established by inspection. We will discuss the SEPSIM executive in some detail in Chapter 6.

The E.P.A. executive is intended for design only. It can handle most networks. Iterative calculations still arise because design of a unit is based on just one or two variables while other variables change over the unit. The other variables are handled as in a simulation. The presence of recycle loops in the system, therefore, leads to iterative calculations. The procedure used to organize iterative calculations and, indeed, control the execution of the design is the same as in SEPSIM. We will discuss it, therefore, when we examine SEPSIM. Costs for each unit are calculated as part of the library subroutine for the unit. A separate

TABLE 3-1. EXECUTIVE PROGRAMS USED FOR WASTE TREATMENT STUDIES

Executive	Type of Application	Plant	Reference
PACER	Simulation	Municipal Sewage Treatment Plants in Kitchener and Oshawa, Ontario	(1), (5)
SEPSIM	Simulation	Municipal Sewage Treatment Plants in Kitchener, Toronto, Brantford, Galt and Preston, Ontario	(6), (7), (8), (9)
GEMCS, MACSIM	Simulation	Waste Treatment System of a BP Refinery, Chemicals Waste Treating Facilities in B.C. (Dowpac Trickling Filter) Arbitrary Waste Treatment System	(10), (11), (12)
E.P.A. Executive	Preliminary Design and Cost Estimating	Sensitivity Studies, Municipal Treatment Plant in Boulder, Colorado	(13), (14)
ESTHER	Design/Simulation	Sensitivity Studies	(15)
ASOP	Optimal Design	Sensitivity Studies	(4), (16)

(5) Singh, D.P., "Steady State Simulation of the Kitchener Waste Water Treatment Plant", M.A.Sc. Thesis, Dept. of Chem. Eng., Univ. of Waterloo (1970)

(6) Silveston, P.L., "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research, 6, (1972)

(7) Silveston, P.L., "Computer Simulation of Waste Treatment Plants", ACS/CIC Symposium "Pollution Problems of Our Environment", Joint ACS/CIC Conference, Toronto, May 1970

subroutine COST determines capital and operating costs, amortization, etc.

Figure 3-4 is a flow sheet of a rather complicated process handled by the E.P.A. executive. The process symbols are defined below the figure.

In a rather curious study[14], the E.P.A. executive was used to simulate the Boulder, Colorado W.T.P. by comparing the actual equipment sizes with those calculated by the program. The study served to show that the parameters recommended in the publications[3,13] describing the models, are not satisfactory for that plant. Adjusting the parameters heuristically improves the size agreement considerably. Waterloo studies using the Smith models rewritten for simulation confirm Goering's observation[8,9].

---

[8] Silveston, P.L., "Computer Simulation of Waste Water Treatment Plants", Proc. 1st PACHEC Meeting, Kyoto, Japan (1972)

[9] Peeling, D.A., "Simulation of Waste Treatment Plants Using SEPSIM", Engineering Report, Dept. of Chem. Eng., University of Waterloo (1972)

[10] Hoffman, T.W., Woods, D.R., Murphy, K.L., Norman, J.D., "The Strategy and an Example of Simulation as Applied to a Petroleum Refinery Waste Treatment Process", in print (1973)

[11] Curry, E.V., "Computer Simulation of a Biological Waste Treatment Facility", Engineering Report, Dept. of Chemical Engineering, University of Waterloo (1971)

[12] Tan, P.G.C., M. Eng. Thesis, Dept. of Chemical Engineering, McMaster University, Hamilton, Ontario (1972)

[13] Smith, R., Eilers, R.G., Hall, E.D., "Executive Digital Computer Program for Preliminary Design of Waste Water Treatment Systems", Water Pollution Control Series WP-20-14, F.W.P.C.A., U.S.D.I. (Washington, D.C., 1968)

[14] Goering, S.W., "A Computer Model of the Sewage Treatment Process of Boulder, Colorado", M.Sc. Thesis, Dept. of Chemical Engineering, University of Colorado (1972)

[15] Chen, G.K., Fan L.T., Erickson, L.E., "Computer Software for Waste Water Treatment Plant Design", J.W.P.C.F., 44, 746-762 (1972)

[16] Fan, L.T., Mishra, P.N., Chen, G.K.C., Erickson, L.E., "Application of Systems Analysis Techniques in Biological Waste Treatment", 4th Int. Fermentation Symp., Kyoto Japan (1972)

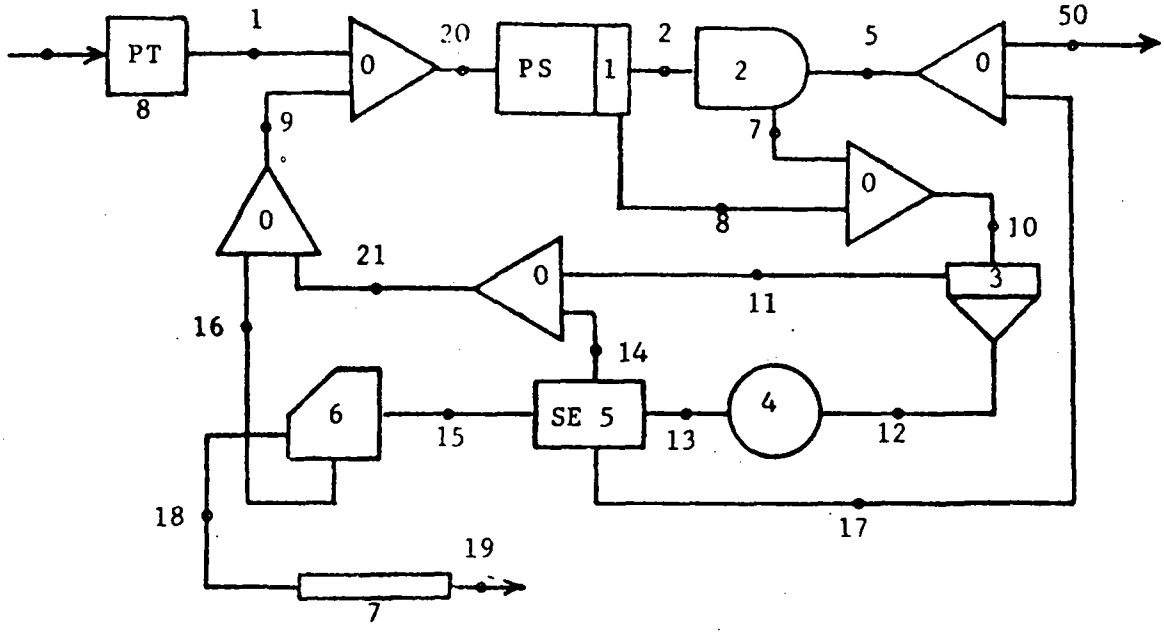


FIGURE 3-4. a) FLOW SHEET OF PROCESS HANDLED BY E.P.A. EXECUTIVE PROGRAM*

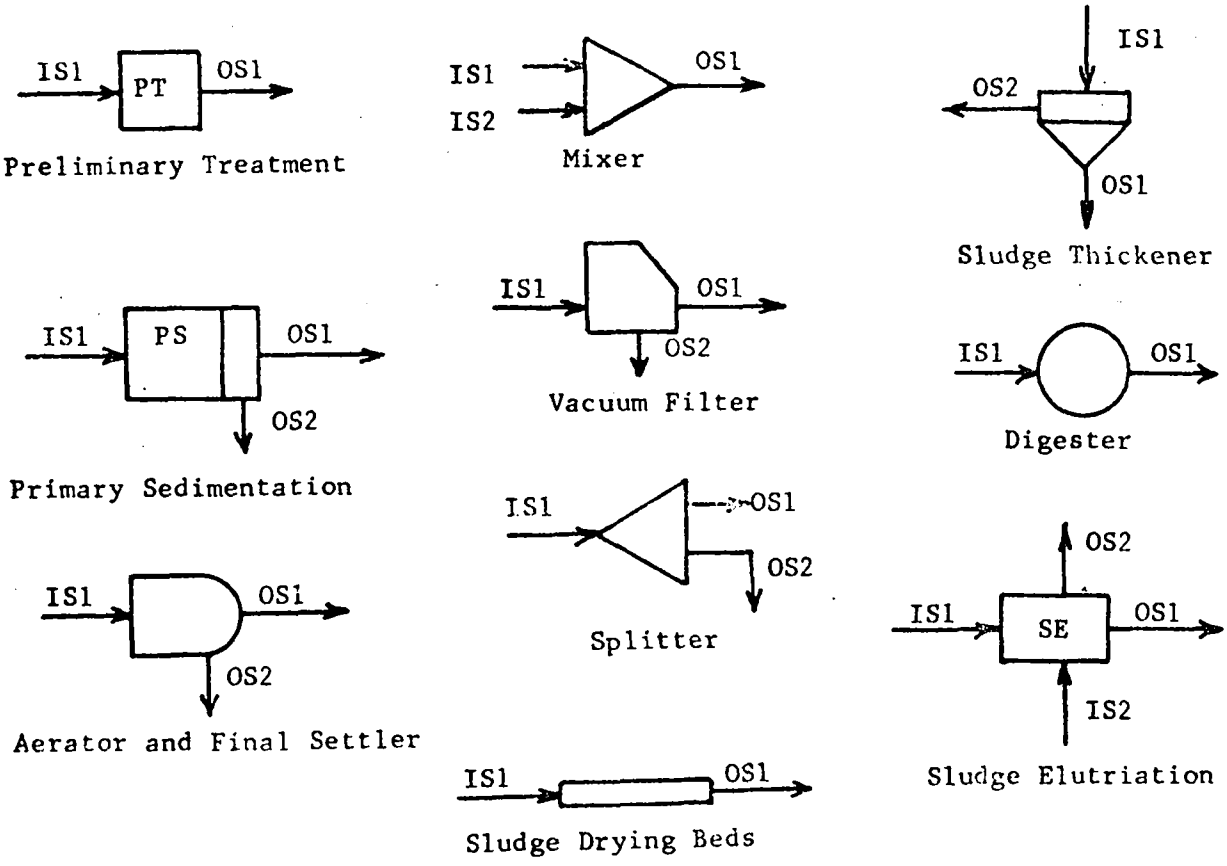
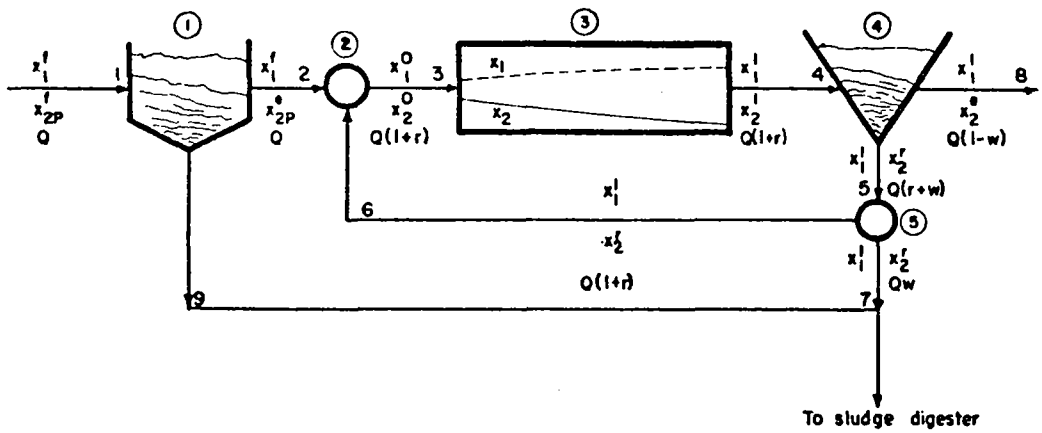


FIGURE 3-4. b) PROCESS SYMBOLS IN FLOW SHEET

*Figure taken from Reference (13).

The ESTHER and ASOP Executives can be discussed together. ASOP is a version of ESTHER which includes a pattern search routine. Thus, it is capable of choosing a set of design parameters (equipment sizes, for example) which will optimize an objective function chosen by the user. ESTHER is a combined design-simulation program which through a user specified control value selects either a simulation or design mode. The design mode operates like Smith's E.P.A. executive in that it chooses equipment sizes for a given effluent quality. Both modes use a simple sub executive called SPCHEN which calculates the output for each unit in the process system. SPCHEN operates differently from SEPSIM and the other executives discussed in this section. Whereas these executives use the flow sheet as encoded in the process matrix to order the calculations, SPCHEN uses the matrix only to establish the input and output streams for each unit. The units are calculated in a sequence following the flow direction irregardless of recycle. In principle ESTHER-SPCHEN can handle a variety of waste treatment systems. The 1972 version, however, is written specifically for an activated sludge system shown as Figure 3-5 below.



Treatment process sequence. (Circled numbers indicate process unit in simulation program, and other numbers denote stream numbers. Stream numbers: 1. raw waste, 6. return sludge, 7. waste sludge, 8. effluent. Process numbers: 1. primary clarifier, 2. mixer, 3. aerator, 4. final clarifier, and 5. splitter).

FIGURE 3-5. ACTIVATED SLUDGE SYSTEM CONSIDERED IN THE ESTHER-SPCHEN EXECUTIVE*

*Figure taken from reference (5) with permission of the Journal.

This system contains just one recycle loop.

The SPCHEN sub executive is unusual also because alternate model subroutines are written as part of the executive. This may be seen in Figure 3-6. SPCHEN contains two models for the primary and secondary clarifier and three models for the activated sludge units to represent different degrees of mixing (see Chapter 9). The user controls the choice of models.

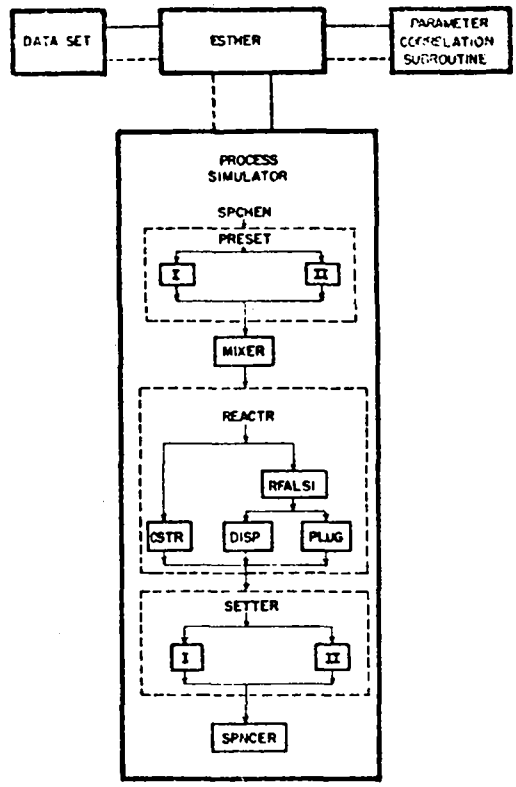


FIGURE 3-6. GENERAL FLOW DIAGRAM FOR THE ESTHER-SPCHEN SIMULATION PROGRAM*

In our "classification" of approaches at the beginning of the chapter, SPCHEN lies in between the extremes of specific simulation programs and fully modular executives.

ESTHER meets our designation of an executive more fully since it controls SPCHEN and contains the I/O operations. Its operation is indicated

*Figure taken from reference (5) with permission of the Journal.

by Figure 3-7.

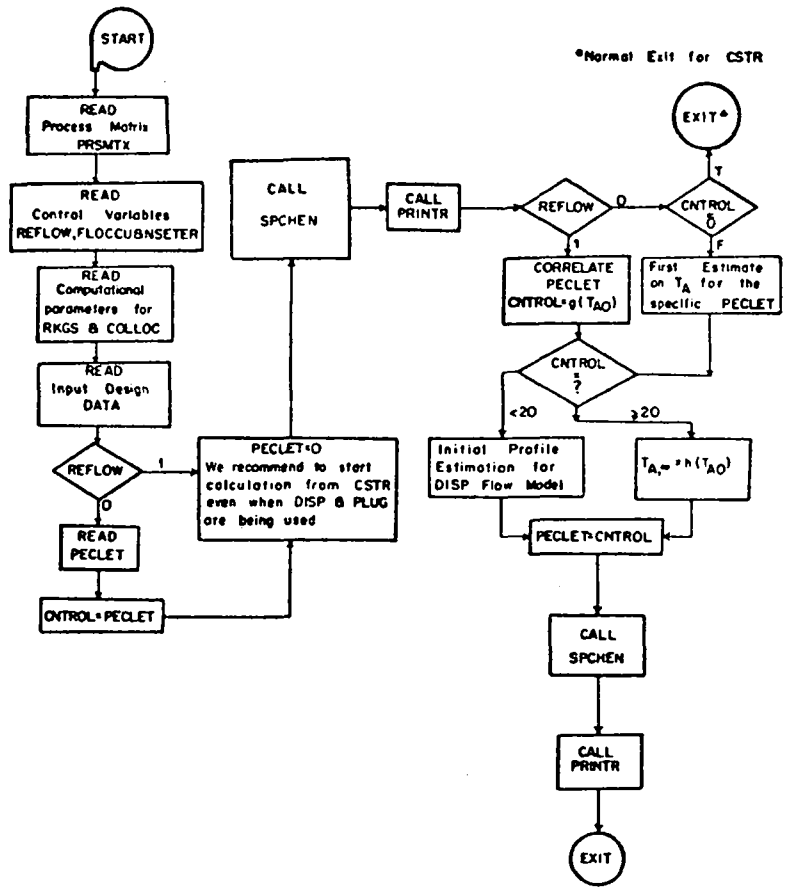


FIGURE 3-7. FLOW DIAGRAM FOR ESTHER

4 PROCESS SYSTEMS ANALYSIS

In the previous chapter, we referred frequently to iterative calculations. We will examine when and why such calculations occur in this chapter. We will consider as well translation of a process flow sheet so it can be read and used by the computer. The last part of the chapter deals with network decomposition and relatively sophisticated ways of determining how to handle calculations for complex recycle systems. It is not necessary for the workshop, but it can be read if you are interested in this subject.

The material in this chapter has been adapted from or at least inspired by two books, "Chemical Plant Simulation"[1] and "Process Analysis and Simulation"[2]. For further discussion of network analysis and representation of networks for computers, these two fine texts should be examined.

4.1 Calculation Problems with Recycle Processes

The central problems of process systems analysis are representing the flow network in a form amenable to computer manipulation, setting up a calculational procedure to efficiently evaluate system variables and choosing the variables. We will examine the first two problems in this chapter, and the third in the succeeding chapter.

To illustrate the discussions, we will make use of a process simulated in the WATCRAP Project[3], which is shown in Figure 4-1. Streams (7), (8), (12), and (13) in the figure are recycle streams. However, streams (12) from the digester and (13) from the filter are small and have little effect on plant performance. These streams can be neglected so that the plant can be represented by the fluid side with respect to water. Figure 4-2 shows the fluid side.

[1] C.M. Crowe et al., "Chemical Plant Simulation", Prentice-Hall (Englewood Cliffs, N.J., 1971)

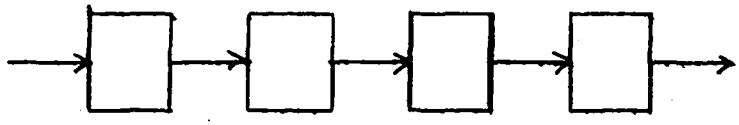
[2] D.M. Himmelblau & K.B. Bischoff, "Process Analysis and Simulation", Wiley (New York, 1968)

[3] P.L. Silveston, "Digital Computer Simulation of Waste Treatment Plants using the WATCRAP-PACER System", J. Water Pollution Control (London) 69, No. 6, 686 (1970)

For the purpose of organizing a design or simulation, process flow sheets (Figures 4-1 and 4-2) can be viewed as information networks. These networks consist of directed flows or "signals" between process units, single input "signals", and one or more output "signals". In Figures 4-1 and 4-2 the major output "signal" is stream (6). Usually this "signal" must be represented closely in simulation. In design, this signal may act as a constraint or as a design parameter.

Process units in the network act as "signal" modifiers. They can be thought of as operators which alter the information content of the stream. Each bit of information reaching the process unit is either altered or passed through unchanged. Take the clarifier, it operates on bits corresponding to suspended matter transferring, figuratively speaking, the bit from one stream (feed (1)) to another (sludge underflow (9)). Bits corresponding to the soluble matter are unchanged by the clarifier operator. Clearly, it is important in modelling to identify the information content of streams in the network.

Let us now look at the problem of ordering calculations. Figure 4-2 will be used as an example. Calculations are straightforward for a chained multistaged system. If streams (7) and (8) were stripped from Figure 4-2 it becomes a chained system. We begin, then, with the feed



Chained, Multistaged System

stream. Neglecting stream (8), the input to process unit 1 is known and the output streams (2) and (9) may be calculated if a model for the unit is available. With stream (7) deleted, the input to unit 2 (stream (2)) now is known so its output could be determined and so on stepwise through the process. There is no calculation problem with branched systems or by pass (feed forward) loops, illustrated below, since at each stage we know all the input streams.

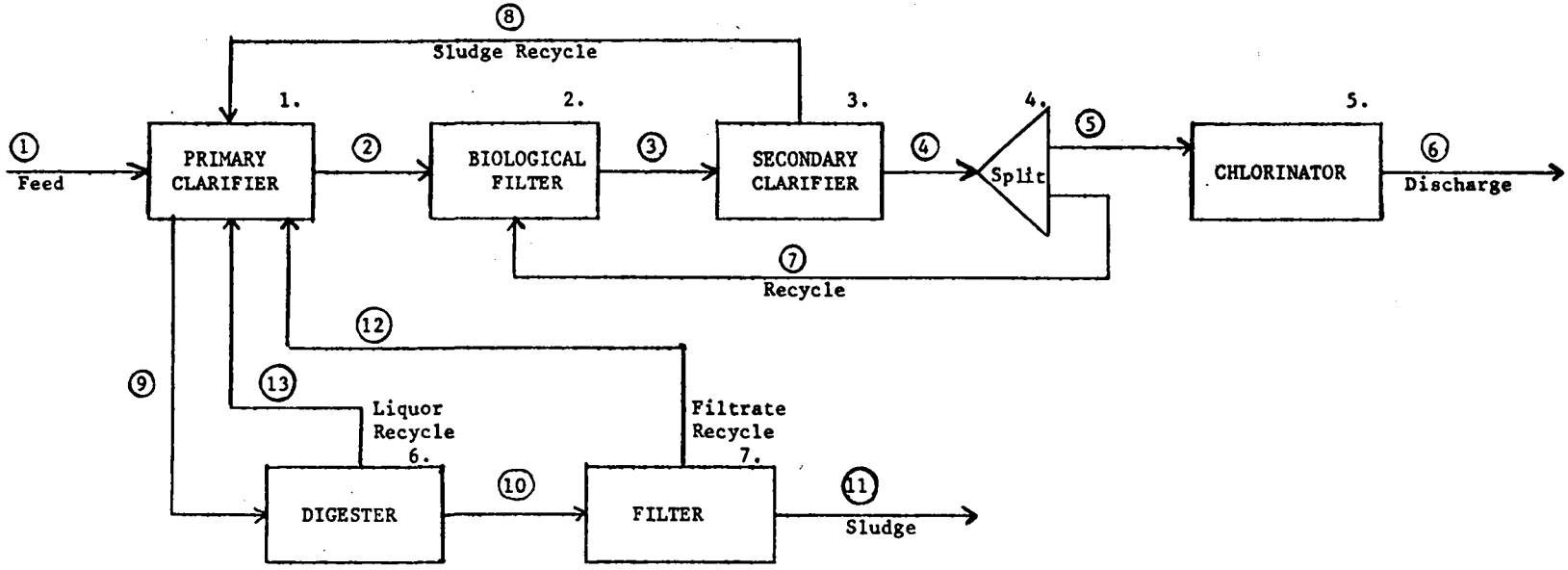


FIGURE 4-1. TYPICAL WASTE TREATMENT PROCESS

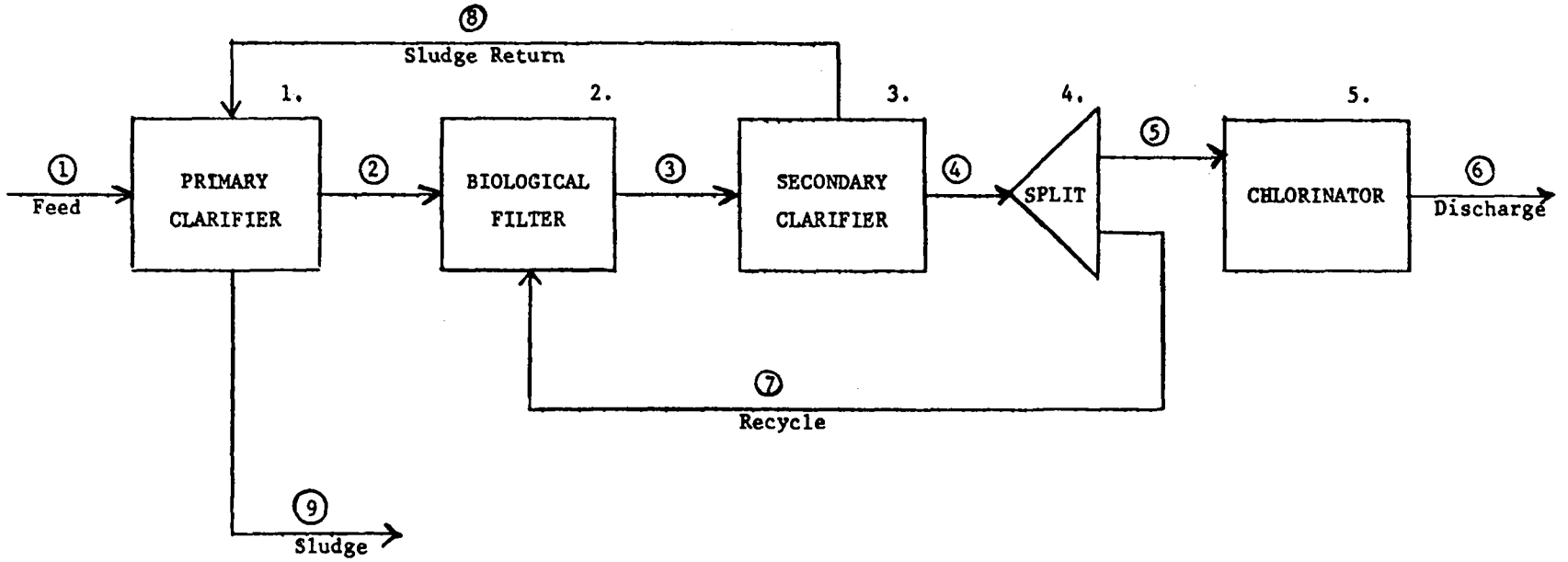
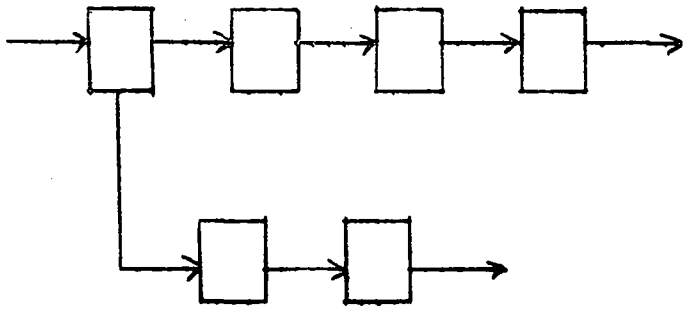
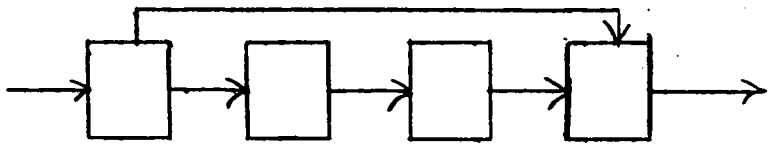


FIGURE 4-2. FLUID SIDE OF WASTE TREATMENT PROCESS

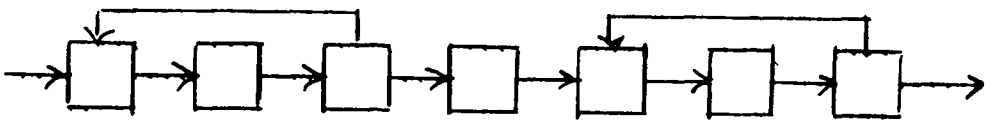


Branched Chain System



Chained System with Bypass

Recycle (feed back) causes the calculation problem. When a recycle stream feeds a process unit then all the inputs are not known. For example, we are unable to determine streams (2) and (9) for unit 1 because we do not know what is in stream (8). In order to calculate these outputs we would have to specify stream (8). The problem arises again for unit 2 and if we want to calculate stream (3), we must specify stream (7). To convert this recycle system to an easily handled chain system, we must specify two streams. This is referred to as a second order recycle system. Order of a recycle process is defined as the minimum number of streams which must be simultaneously specified to reduce the system to a chain system. In Figure 4-2 we can distinguish two "nested" loops - one involving units 1, 2 and 3 and the other units 2,3 and 4 - which form a "grand" loop containing units 1 to 4. In order to handle the "grand" loop, we must specify 2 streams. However, if the interior loops were not crossed (i.e. they did not contain common members) as illustrated below, we could assume the first recycle stream known and calculate the first portion of the resulting chain. Then, we could assume the second known and repeat the operation. By our definition this is the first order



System With Two First Order Recycle Loops

recycle process even though there are two recycle loops.

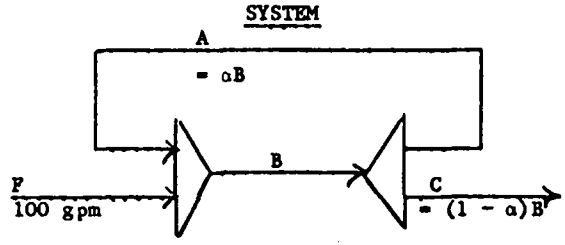
Two techniques are available for input-output calculations in the presence of recycle loops. If the operators of the unit processes in Figure 4-2 are linear or can be linearized, we can describe the system by a set of linear algebraic equations. The set can be solved by various methods; perhaps the most familiar is the use of Cramer's Rule. The second technique which is suitable for either linear or non-linear operators is the method of successive substitution. The variables in streams (7) and (8) initially are set to zero. Streams (2), (3), (4) and (7) and (8) may now be calculated sequentially. With streams (7) and (8) known from the first stepwise calculation, the procedure can be repeated successively until values of all variables no longer change in each iteration. Once convergence has occurred, streams which are not part of a recycle loop, e.g. streams (5), (6) and (9) may be calculated. There is no point in including them in the iteration steps since they are not input streams. Similarly unit 5, need not be included in the set of linear equations. Stream (6) can easily be obtained once (5) is known. Eliminating unit 5 reduces the size of the determinants in a Cramer's Rule solution and thereby the amount of computing time required. This should illustrate the importance of locating recycle loops and suitably ordering calculations.

Figure 4-3 taken from Crowe et al.[2] compares the analytical solution to successive substitution for a very simple two stage linear recycle process. Analytical solutions are preferable when possible. Unfortunately, many real systems have strongly non-linear process units so that these solutions are not possible.

Figure 4-3 gives the progress of the iterations for two recycle fractions. This simple example shows that when the recycle flow is smaller or equal to the feed convergence occurs rapidly, but when feed is

SUCCESSIVE SUBSTITUTION

ITERATION	B	A
1	100	100
2	$100(1 + \alpha)$	$100(1 + \alpha)$
$\alpha 3$	$100(1 + \alpha + \alpha^2)$	$100(\alpha + \alpha + \alpha^2)$
.	.	.
.	.	.
n	$100(1 + \alpha + .. + \alpha^{n-1})$	$100(\alpha + .. \alpha^n)$
	$100\frac{(1 + \alpha)(1 - \alpha^n)}{(1 - \alpha)}$	$100\ (\frac{1 - \alpha^n}{1 - \alpha})$



ANALYTICAL SOLUTION
(for linear operations)

Stage 1: $100 + A = B$

Stage 2: $A = \alpha B$

Solving: $A = 100\ \frac{\alpha}{1 - \alpha}$

For $\alpha = 0.33$ (Moderate Recycle)
$A = 50$

For $\alpha = 0.9$ (High Recycle)
$A = 900$

CONVERGENCE DEPENDS ON MAGNITUDE OF RECYCLE

Moderate Recycle Ratio $\alpha = 0.33$		High Recycle Ratio $\alpha = 0.90$	
ITERATION	FLOW IN A	ITERATION	FLOW IN A
0	0	0	0
1	33.3	1	90
2	43.3	2	171
3	48.1'	3	244
4	49.4	4	310
:	:	5	369
:	:	6	422
:	:	7	470
∞	50.0	:	:
		:	:
		∞	900

FIGURE 4-3. SUCCESSIVE SUBSTITUTION vs. ANALYTICAL SOLUTION*

*Figure taken from reference 2 with the kind permission of the publishers.

very much smaller (1/9 in the second case) convergence is slow. Serious convergence problems can arise in process simulations in this way. Fortunately, convergence promoters can be built into executive programs for simulation to overcome this difficulty.

4.2 Representation of Process Systems

Process systems are traditionally depicted in various types of flow diagrams. These can be fairly elaborate ones in which each piece of equipment is represented by a graphic facsimile, they can be schematic sketches using standard symbols, or just block diagrams as Figures 4-1 and 4-2. In all of these forms, connecting lines represent actual conduits or pipes in the system and all major pieces of equipment appear in the diagram. A flow sheet such as Figure 4-1 with the compositions and flows of all streams and sizes of all equipment shown on the diagram or tabulated in attachments is a compact and complete form of process representation. Engineers obtain virtually all of their process information from flow sheets. Unfortunately, however, a digital computer is not yet able to interpret a flow sheet.

The first requirement for submitting system information to a computer is to code the streams and process units with either letters or numbers. Number coding is more convenient and we have used this in Figures 4-1 and 4-2. The second requirement is to key the process units to their models so that when a model is needed for input output calculations, the proper model is called up.

The process matrix is perhaps the simplest numerical representation of a process system. It is a table rather than a matrix, but we use that term because other system representations can be manipulated as matrices. The table consists of a list of the process units appearing in a flow sheet. Each row of the table contains the number of a unit given on the flow sheet, the model name, and the numbers of the input and output streams for the unit. In some executives (PACER, CAPS, GEMCS), a single array of associated streams are used in which input stream numbers are positive and output stream numbers are negative. For convenience the streams and process units are usually numbered following the main flow of material through the process. Table 4-1 gives a process matrix for Figure 4-1. The model names are those used in the SEPSIM and WATCRAP-PACER lib-

TABLE 4-1. PROCESS MATRIX FOR A WASTE TREATMENT PROCESS (Figure 4-1)

		Associated Streams	
Equipment No.	Model Name	Input	Output
1	PRISTL	1, 8, 12, 13, 0	2, 9, 0, 0, 0
2	TRFLTR	2, 6, 0, 0, 0	3, 0, 0, 0, 0
3	SECSET	3, 0, 0, 0, 0	4, 8, 0, 0, 0
4	MIXER3	4, 0, 0, 0, 0	5, 7, 0, 0, 0
5	CHLOR	5, 0, 0, 0, 0	6, 0, 0, 0, 0
6	DIGSTR	9, 0, 0, 0, 0	10, 13, 0, 0, 0
7	VACFL	10, 0, 0, 0, 0	12, 11, 0, 0, 0

raries.

Advantages of the process matrix are that it can be readily written and it is easy to check and to modify.

When, as is so often the case, two or more streams enter or leave a process unit, there must be a way of relating the ordering of these streams in the subroutine model stored in the computer and in the process matrix. For example, a settler has overflow and underflow output streams. In a settler model such as PRISTL, we may choose to let the overflow be the first output stream and the underflow be the second stream. In the process matrix, used by SEPSIM, PACER, GEMCS, CAPS, for example, the first output stream in the list of associated streams must be the overflow and the second output stream must be the underflow stream.

The process matrix is the only form of numerical representation which contains this stream ordering information. Likewise it is the only form which relates model name to a process unit number. If other forms of system representation are used, these two pieces of information must be supplied separately to the computer.

The process matrix, however, submerges the structure of the network. Figure 4-1 has 4 recycle loops, but this would be difficult to discern from Table 4-1.

While the process matrix compactly summarizes information for each process unit, the stream connection matrix shows the function of each stream. It is simply a table of the streams in a flow sheet showing their source unit and their destination. Zeros are used to indicate sources or destinations outside the flow diagram. Therefore zeros indicate feed and product streams. Table 4-2 is the Matrix for Figure 4-1.

TABLE 4-2. STREAM CONNECTION MATRIX FOR A WASTE TREATMENT PROCESS (Figure 4-1)

Stream No.	Source Unit	Destination Unit
1	0	1
2	1	2
3	2	3
4	3	4
5	4	5
6	5	0
7	4	2
8	3	1
9	1	6
10	6	7
11	7	0
12	7	1
13	6	1

If streams and units are numbered in ascending order following the main flow of information, as was the case for Figure 4-1, the matrix can indicate recycle streams. These are streams which go from a high number to a low one. Streams (7), (8), (12) and (13) are thus recycle streams.

Although this is useful for locating recycle streams, the table does not easily yield the size of different recycle loops.

An alternative to the above matrix is the incidence matrix which is shown in Table 4-3 for Figure 4-1.

TABLE 4-3. INCIDENCE MATRIX FOR A WASTE TREATMENT PROCESS (Figure 4-1)

Unit Number	Stream Number												
	1	2	3	4	5	6	7	8	9	10	11	12	13
1	+1	-1						+1	-1			+1	+1
2		+1	-1				+1						
3			+1	-1				-1					
4				+1	-1		-1						
5					+1	-1							
6									+1	-1			-1
7										+1	-1	-1	

A positive value (+1) in the incidence matrix means the stream feeds the unit whereas a negative value (-1) means it leaves. Summing each column of the matrix indicates the function of the stream. If the sum is zero the stream connects two units; while if the sum is + 1 we have a feed stream or if it is - 1, an output stream. Summing + and - on rows gives the number of input and output streams for each stage.

If stream and unit numbers ascend following the main information flow, the structure of the network becomes discernible. For example, in the chain region, units 1 to 5, the entries fall along the diagonal with a -ive entry over a +ive entry in each column. Where the signs are reversed, we have a recycle stream (this is the same as going from a higher number to a lower one in the stream connection matrix). Thus, streams (7), (8), (12) and (13) appear as recycle streams. Stream (9) shows the same sign order as the chain portion. Consequently it repre-

sents a branch or feed forward loop.

4.3 Adjacency Matrix

The adjacency matrix, **R**, (or associated, relation, or structural matrix) is a particularly useful way of describing a network. It is capable of finding recycle loops and generally decomposing the system into sub-assemblies, such as chain sections or recycle loops, that can be handled separately. The matrix contains unit numbers but suppresses stream numbers as may be seen in Table 4-4 which is once again based on Figure 4-1.

TABLE 4-4. ADJACENCY MATRIX FOR A WASTE TREATMENT PROCESS (Figure 4-1)

		To						
		1	2	3	4	5	6	7
	1	0	1	0	0	0	1	0
	2	0	0	1	0	0	0	0
	3	1	0	0	1	0	0	0
From:	4	0	1	0	0	1	0	0
	5	0	0	0	0	0	0	0
	6	1	0	0	0	0	0	1
	7	1	0	0	0	0	0	0

The number of units in the information flow diagram designate both the rows and the columns of this square matrix. Information flow between units are indicated by a value of unity at the element formed by the row corresponding to the number of the unit from which the stream came, and column corresponding to the number of the unit to which the stream goes. Thus, the matrix shows the direct connections of units in the network. This type of representation shows interior network structure only. The adjacency matrix shown does not include feed or product connections. These could be introduced through "zero" rows and columns; then

the number of unit entries in the "zero" row would be the number of feed streams while the number of unity entries in the "zero" column would be the number of product streams.

The fifth row of the matrix (Table 4-4) has all zeroes indicating that the streams from unit 5 are product streams. Furthermore, unit 5 is not part of a recycle loop. As can be seen in Figure 4-1, the chlorinator (unit 5) is an appendage on the process. As discussed earlier in this section, its output would be the last calculated. The elements of the adjacency matrix contains only zero or one. It is referred to as a Boolean matrix by some authors[2]. Graph Theory, from whence the adjacency matrix comes, teaches that two step connections in the system may be found by forming $\mathbf{R}^2$, while n step connections between units are shown by forming $\mathbf{R}^n$. Powers of the matrix are formed through matrix multiplication: $\mathbf{R}^2 = \mathbf{R} \cdot \mathbf{R}$, $\mathbf{R}^3 = \mathbf{R}^2 \cdot \mathbf{R}$, etc. except that Boolean Algebra is used.

If you are interested in using the R matrix, you will need to know the rules for Boolean algebra. These are

$$\begin{aligned} x + y &= \max(x,y) \\ x \,.\, y &= \min(x,y) \end{aligned} \qquad [4\text{-}1]$$

For example, in Boolean addition

$$\begin{aligned} 0 + 1 &= \max(0,1) = 1 \\ 1 + 1 &= \max(1,1) = 1 \\ 2 + 1 &= \max(2,1) = 2 \end{aligned}$$

and in Boolean multiplication

$$\begin{aligned} 0 \times 1 &= \min(0,1) = 0 \\ 1 \times 2 &= \min(1,2) = 1 \end{aligned}$$

We illustrate further by applying the rules to matrix multiplication. When the elements of a row of a matrix are multiplied into the elements of a column of a matrix as follows

$$(0 \quad 1 \quad 1 \quad 2 \quad 0) \begin{pmatrix} 1 \\ 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

the Boolean matrix element formed is

$$(0 + 1 + 0 + 1 + 0) = 1$$

Taking the Boolean sum of the matrices after forming each power yields the reachability matrix

$$\mathbf{R}_n^* = \mathbf{R} + \mathbf{R}^2 + \ldots + \mathbf{R}^n \qquad [4\text{-}2]$$

An element in this matrix indicates whether a unit can be reached through the directed graph from the unit of origin in up to and including n steps. If the element is 0, the unit cannot be reached from the unit of origin.

The reachability matrix may be used to delineate recycle loops and serial regions outside of loops. The logical intersection of this matrix and its transpose, $\mathbf{R}^* \cap \mathbf{R}^{*T}$, will show these regions. The transpose, is formed by interchanging rows and columns. The logical intersection may be found by taking the Boolean matrix product. Figure 4-4 shows these operations to locate recycle loops for two simple cases. The loop representation still depends upon ascending order of numbers with information flow. If this is not the case a permutation matrix must be introduced to convert $\mathbf{R}^* \cap \mathbf{R}^{*T}$ into diagonal form. The diagonal form is given in Figure 4-4. Himmelblau and Bischoff[2] discuss this point further.

We will now demonstrate the use of the Adjacency Matrix using Figure 4-2. For convenience, Figure 4-5 summarizes the operations. Powers of the $\mathbf{R}$ on the left hand side of Figure 4-5 give the connections. Let us check. In $\mathbf{R}^4$, unit 3 should be connected to unit 4 by four steps. Referring to Figure 4-2, we see that the connection is through the sequence $3. \xrightarrow{1} 4. \xrightarrow{2} 2. \xrightarrow{3} 3. \xrightarrow{4} 4.$, that is we must cycle through unit 3 again to go from unit 3 to unit 4 in four steps. We also notice that unit 5 does not lead anywhere; so it cannot be part of a loop and must have an output stream.

Presence of recycle loops may be detected from powers of $\mathbf{R}$ or from manipulation of $\mathbf{R}^*$. The matrix of 3 step connections, $\mathbf{R}^3$, shows 4 values of unity on the diagonal. This means that any unit forming the diagonal can be reached from itself. Now a unit can only reach itself if

it forms part of a recycle loop. We can see then that units 1, 2, 3 and 4 are in recycle loops. Are they in a single loop? The $\mathbf{R}^3$ matrix tells us that they are not. If a unit can reach itself through 3 steps, the loop can only have three members. But in $\mathbf{R}^3$, there are 4 units on the diagonal. Consequently, the 4 units must be arranged in at least two three membered loops. Examination of $\mathbf{R}^2$ and $\mathbf{R}^4$ shows no diagonal elements so there are no 2 and 4 numbered loops. This means the system consists of two 3 membered recycle loops. Since we have numbered in ascending order following flow, it is evident that units 2 and 3 are common to both loops.

The Reachability Matrix through its logical intersection $\mathbf{R}^* \cap \mathbf{R}^{*T}$ does not give any more information than powers of the adjacency matrix, although the information is more graphically presented. The bottom of Figure 4-5 simply shows that units 1 to 4 form a recycle system and that the system cannot be further decomposed.

Recycle loops identified from the flow sheet or from the adjacency matrix can be represented as a table referred to as a cycle matrix[4]. This matrix is useful for ordering the calculations when iteration is used. Table 4-5 gives the matrix for Figure 4-1.

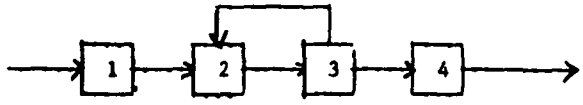
Four cycles can easily be identified in Figure 4-1. They are numbered in an arbitrary manner and form the rows of the matrix in Table 4-5. Streams form the columns. Thus, a unit element a_{ij} indicates that the stream, j, is to be found in loop or cycle i. If we call rank the number of recycle streams in each recycle loop and stream frequency the number of loops a stream is located in, then, rank and frequency are the sum of the units in the rows and columns respectively. These two quantities are shown in Table 4-5.

Stream frequency information is useful when iterative calculations must be carried out. Examination of the rows shows stream (3) is common to loops 1 and 2, while stream (9) is common to loops 3 and 4. It was pointed out earlier that to evaluate streams in a recycle loop by successive substitution values of variables in one of the streams in the

---

[4] Rudd, D.F. and Watson, C.C., "Strategy of Process Engineering" John Wiley (New York, 1968)

Case 1: Single Loop



Ultimate Reachibility Matrix $R^* = \sum_{n=1}^{3} R^n$

	1	2	3	4
1	0	1	1	1
2	0	1	1	1
3	0	1	1	1
4	0	0	0	0

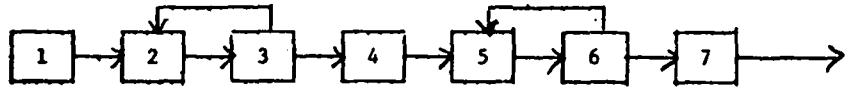
Transpose R^{*T}

	1	2	3	4
1	0	0	0	0
2	1	1	1	0
3	1	1	1	0
4	1	1	1	0

Logical Intersection $R^* \cap R^{*T}$

	1	2	3	4
1	0	0	0	0
2	0	1	1	0
3	0	1	1	0
4	0	0	0	0

Case 2: Two 1st Order Loops



Ultimate Reachability Matrix $R^* = \sum_{n=1}^{6} R^n$

	1	2	3	4	5	6	7
1	0	1	1	1	1	1	1
2	0	1	1	1	1	1	1
3	0	1	1	1	1	1	1
4	0	0	0	0	1	1	1
5	0	0	0	0	1	1	1
6	0	0	0	0	1	1	1
7	0	0	0	0	0	0	0

Transpose R^{*T}

	1	2	3	4	5	6	7
1	0	0	0	0	0	0	0
2	1	1	1	0	0	0	0
3	1	1	1	0	0	0	0
4	1	1	1	0	0	0	0
5	1	1	1	1	1	1	0
6	1	1	1	1	1	1	0
7	1	1	1	1	1	1	0

Logical Intersection $R^* \cap R^{*T}$

	1	2	3	4	5	6	7
1	0	0	0	0	0	0	0
2	0	1	1	0	0	0	0
3	0	1	1	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	1	1	0
6	0	0	0	0	1	1	0
7	0	0	0	0	0	0	0

FIGURE 4-4. LOCATION OF RECYCLE LOOPS FROM THE REACHABILITY MATRIX

Direct Interconnection (Adjacency Matrix - R)

From \ To	1	2	3	4	5
1	0	1	0	0	0
2	0	0	1	0	0
3	1	0	0	1	0
4	0	1	0	0	1
5	0	0	0	0	0

Reachability via up to 1 step(R^*)

	1	2	3	4	5
1	0	1	0	0	0
2	0	0	1	0	0
3	1	0	0	1	0
4	0	1	0	0	1
5	0	0	0	0	0

Connection via 2 steps(R^2)

From \ To	1	2	3	4	5
1	0	0	1	0	0
2	1	0	0	1	0
3	0	1	0	0	1
4	0	0	1	0	0
5	0	0	0	0	0

Reachability via up to 2 steps(R_2^*)

	1	2	3	4	5
1	0	1	1	0	0
2	1	0	1	1	0
3	1	1	0	1	0
4	0	1	0	0	1
5	0	0	0	0	0

Connections via 3 steps (R^3)

From \ To	1	2	3	4	5
1	1	0	0	1	0
2	0	1	0	0	1
3	0	0	1	0	0
4	1	0	0	1	0
5	0	0	0	0	0

Reachability via up to 3 steps(R_3^*)

	1	2	3	4	5
1	1	1	1	1	0
2	1	1	1	1	1
3	1	1	1	1	0
4	1	1	0	1	1
5	0	0	0	0	0

Connections via 4 steps (R^4)

From \ To	1	2	3	4	5
1	0	1	0	0	1
2	0	0	1	0	0
3	0	0	0	1	0
4	0	1	0	0	1
5	0	0	0	0	0

Reachability via up to 4 steps(R_4^*)

	1	2	3	4	5
1	1	1	1	1	1
2	1	1	1	1	1
3	1	1	1	1	0
4	1	1	0	1	1
5	0	0	0	0	0

Connections via 5 steps (R^5)

From \ To	1	2	3	4	5
1	0	0	1	0	0
2	1	0	0	1	0
3	0	1	0	0	1
4	0	0	1	0	0
5	0	0	0	0	0

Reachability via up to 5 steps(R_5^*)

	1	2	3	4	5
1	1	1	1	1	1
2	1	1	1	1	1
3	1	1	1	1	1
4	1	1	1	1	1
5	0	0	0	0	0

Considering more than 5 steps does not change the Reachability Matrix so if R^* = Ultimate Reachability, Matrix $R^* = R_5^* = R_6^*$, etc. Taking the transpose and forming the logical intersection:

Transpose (R^{*T})

	1	2	3	4	5
1	1	1	1	1	0
2	1	1	1	1	0
3	1	1	1	1	0
4	1	1	1	1	0
5	1	1	1	1	0

Logical Intersection ($R^* \cap R^{*T}$)

	1	2	3	4	5
1	1	1	1	1	0
2	1	1	1	1	0
3	1	1	1	1	0
4	1	1	1	1	0
5	0	0	0	0	0

FIGURE 4-5. NETWORK STRUCTURE FROM THE ADJACENCY MATRIX

TABLE 4-5. CYCLE MATRIX FOR A WASTE TREATMENT PLANT (Figure 4-1)

Cycle Number	1	2	3	4	5	6	7	8	9	10	11	12	13	Cycle Rank
1	0	1	1	0	0	0	0	1	0	0	0	0	0	3
2	0	0	1	1	0	0	1	0	0	0	0	0	0	3
3	0	0	0	0	0	0	0	0	1	0	0	0	1	2
4	0	0	0	0	0	0	0	0	1	1	0	1	0	3
Stream Frequency	0	1	2	1	0	0	1	1	2	1	0	1	1	

loop must be specified. But which stream in the loop should we specify? Clearly it would be better to specify a stream common to more than one loop. Stream frequency indicates which streams we should take and the cycle matrix tell us what loops we have made determinant by the specification. It can be seen that the stream (3) lies in both loops 1 and 2 so these become determinant if (3) is specified.

What we mean by "made determinant" needs some explanation. Suppose by some means we knew the flows and compositions leaving unit 2 - the trickling filter - in stream (3). Since we are calculating output step by step we can immediately calculate the output of unit 3, the clarifier. We then know stream (4) and we can proceed to calculate unit 4 and so on through the process. If we also specified the flows and compositions in stream (9), units 6 and 7 could be calculated directly because these units form a chain. Consequently, as a result of specifying streams (3) and (9), streams (8), (12) and (13) are established and the outputs of units 1 and 2 may be calculated.

In practice we do not know the flows and compositions in streams (3) and (9). If we guess at these, however, the iterative calculations will be faster than they would be for guessing other streams. Of course, the closer the guesses are to the actual values, the faster the iterations

will be executed.

4.4 Establishing A Calculational Sequence

Our purpose in this last section is to examine two alternative ways of establishing a calculational sequence which minimizes computating time for process simulation. Our interest is in systems containing non linear process units. To develop the argument, however, we will consider networks with linear processes first. Systems in which we follow change in composition fall into the linear class if simple lumped parameter models are employed. In some cases, a primary waste treatment plant can be modelled as a linear system.

The processes shown in Figures 4-1 and 4-2 which have been used to illustrate ideas and techniques up to now are no longer suitable. Instead, a modification of Figure 4-1 shown in Figure 4-6 will be employed.

Calculation of the output of the linear system may be accomplished by solving sets of simultaneous algebraic equations. A set arises for each variable (such as flow or composition). Since each variable occurs in each stream and there are 13 streams in Figure 4-6, each variable can have 13 values. The value in the feed stream will be known, but the remaining 12 values are unknown. Equations of the material balance type are needed to determine these unknown values. For example, unit 4 furnishes two equations for each variable. Consequently we have for the linear system 12 equations containing 12 unknowns for each variable. If we use 4 variables (say, flow, suspended solids, volatile suspended solids and BOD), we will have 4 sets each containing 12 equations. The sets can be solved by use of Cramer's rule or Gaussian elimination, but this is not the point. The point is that as the network grows, the size of determinants needed for solving the sets become large. Their manipulation quickly becomes time consuming even on a large computer.

How can the size of the set be reduced? Figure 4-6 suggests the answer. Units 1 and 6 can be stripped off. Input to unit 1 is known so that its output can be calculated. Once the recycle system containing units 2 to 5 is solved, the input to unit 6 will be known and its output can be determined. Loop 3 is independent of loops 1 and 2 so it can be solved after them as a second step. By inspection, then, we have reduced

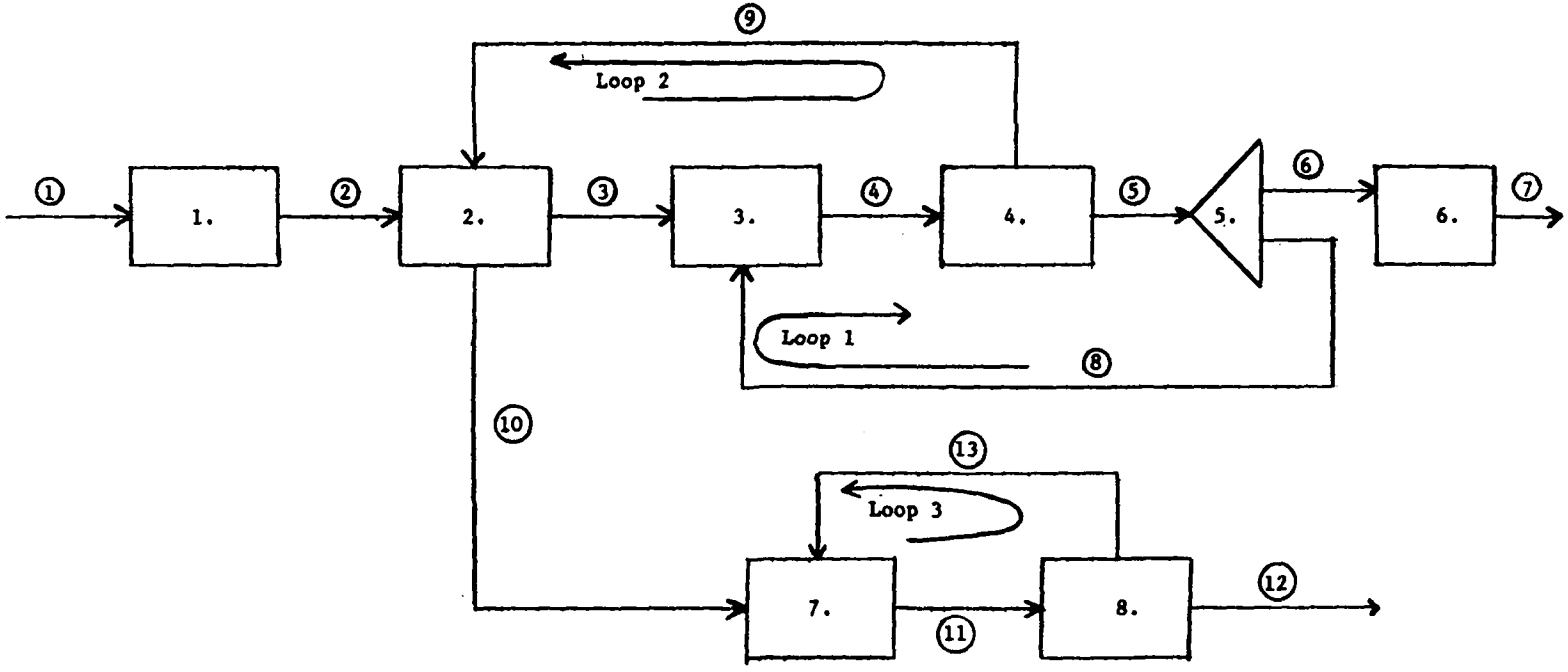


FIGURE 4-6. ILLUSTRATIVE PROCESS FLOW SHEET

a problem involving the solution of 12 simultaneous equations to one involving a set of 6 equations and a set of 3 equations. Intuitively, this is an easier job.

For networks more complex than Figure 4-6, it becomes difficult to decompose the network into structurally independent subsystems by simple inspection. The problem of decomposition has attracted a good deal of attention recently[4-8]. We will consider just the use of the adjacency matrix, discussed earlier.

A decomposition procedure, then, would proceed by first numbering units in an ascending order following the main information flow. This simplifies interpreting the R matrix. The matrix would be formed and units stripped off which are not within recycle loops. Those with zero columns would go to the beginning of a calculation list since they can be calculated directly from feed information, while those with zero rows would be placed last in the list. Next Boolean powers of the matrix would be formed to delineate recycle loops. These must be checked to find out whether the units in the loop belong to larger loops. Forming higher powers will show this, but inspection of each power also suffices. If loop members belong to a larger cycle, there will be unit entries in columns of the members below the diagonal. A loop which does not belong to a larger loop is called a "maximal cyclical net". When found, members making up the "net" can be removed from the matrix and placed in the calculation list. Figure 4-7 gives Himmelblau's algorithm for these operations[2].

---

[5] Norman, R.L., "A Matrix Method for Location of Cycles in a Directed Graph", A.I.Ch.E.J., 11, 450 (1965)

[6] Himmelblau, D.M., "Decomposition of Large Scale Systems I", Chemical Eng. Sci., 21, 425 (1966)

[7] Lee, W. and Rudd, D.F., A.I.Ch.E.J., 12, 1184 (1966)

[8] Christensen, J.H. and Rudd, D.F., A.I.Ch.E.J., 14 (1968)

[9] Sargent, R.W.H. and Westerberg, A.W., "Speed-up in Engineering Design", Trans. Inst. Chem. Engs. 42, 190 (1964)

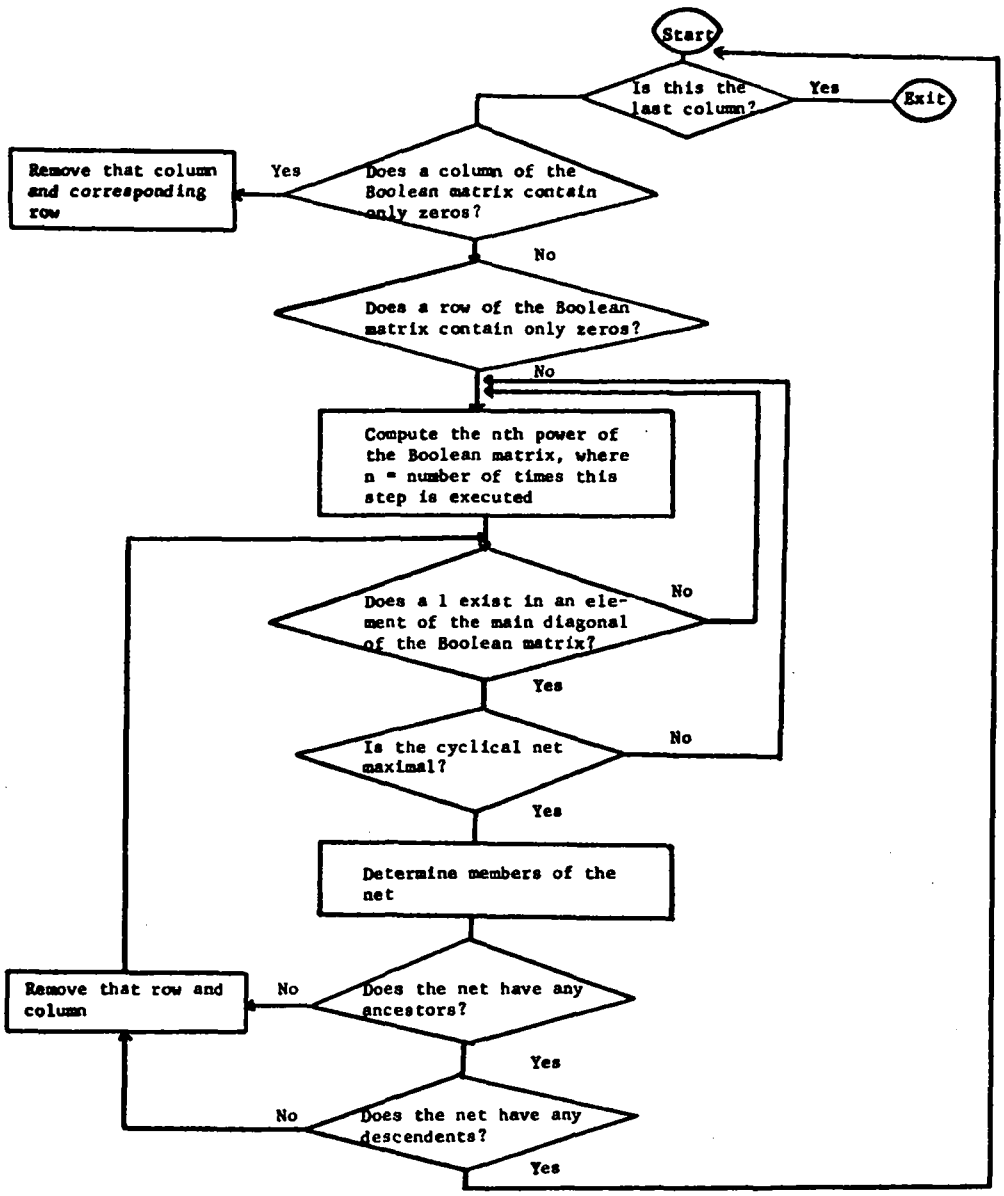


FIGURE 4-7. ALGORITHM FOR SYSTEM DECOMPOSITION*

*Figure adopted from reference (2) with the kind permission of the publisher.

Application of this algorithm to the illustrative process of Figure 4-6 is shown in Figure 4-8. The figure shows, as expected, a calculation order beginning with a direct calculation of the first unit, followed by calculations of a suitable type for the coupled recycle loops, followed once more by the same procedure for the two membered loop, and ending with direct calculation of the last unit. If successive substitution is used, streams to be specified may be obtained from the cyclic matrix as illustrated in the previous section. The procedure is also shown in Figure 4-8. Streams (4) and (11) or (13) in Figure 4-6 are the preferable streams for specification.

"Breaking" a recycle loop, as previously described, involves specifying one or more streams by assuming values for variables in the streams so that the remaining units in the loop can be calculated serially. A heuristic technique can be used in place of the Boolean and cyclic matrix procedure just discussed. The PACER and MACSIM executives and a subroutine in GEMCS employ the technique we will now describe.

By using "flags" to identify the nature of a stream in a network, the formulation of the adjacency matrix can be avoided. Starting with the process matrix (Table 4-2), a stream connection matrix (Table 4-3) is established through a search. Input streams identified in the search are "flagged" with an "1". Similarly product streams are identified and flagged with a "2". The remaining streams in the stream connection matrix are unflagged. The process matrix is then scanned row by row to find process units for which the output streams can be calculated, that is, units for which all input streams are flagged "1". When such a unit is found, the proper equipment subroutine is called to calculate the output streams of this unit. These output streams are flagged "1" since they are now known. The process unit is also flagged with a number greater than zero. In GEMCS, no calculation is performed, the streams are just flagged to indicate they can be calculated serially. Scanning the Process Matrix continues and rescanning will occur until no more equipment units can be found which may be calculated directly. If the process has one or more recycle streams the method described will be unable to solve the problem completely. The executive recognizes this situation when one or more process units are flagged zero and none of these units has all of

1) Form the adjacency matrix for suitably numbered process units or stages

From: \ To	1	2	3	4	5	6	7	8
1	0	1	0	0	0	0	0	0
2	0	0	1	0	0	0	1	0
3	0	0	0	1	0	0	0	0
4	0	1	0	0	1	0	0	0
5	0	0	1	0	0	1	0	0
6	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	1
8	0	0	0	0	0	0	1	0

Unit 1 accepts a feed stream and is not in a loop

2) Delete unit 1 from the matrix and place it at the head of calculation list.
Unit 6 discharges a product stream and is not in a loop

3) Delete unit 6 from the matrix and place it at the end of the calculation list.

4) Form the reduced adjacency matrix

From: \ To	2	3	4	5	7	8
2	0	1	0	0	1	0
3	0	0	1	0	0	0
4	1	0	0	1	0	0
5	0	1	0	0	0	0
7	0	0	0	0	0	1
8	0	0	0	0	1	0

There are no zero columns or rows so no further units may be deleted.

5) Form R^2

From: \	2	3	4	5	7	8
2	0	0	1	0	0	1
3	1	0	0	1	0	0
4	0	1	0	0	1	0
5	0	0	1	0	0	0
7	0	0	0	0	1	0
8	0	0	0	0	0	1

Units 7 and 8 form a two membered loop. Inspection of region to left of diagonal in rows 7 and 8 shows only zeroes so that 7 and 8 form a "maximal cyclical net".

FIGURE 4-8. EXAMPLE OF NETWORK DECOMPOSITION

6) Delete units 7 and 8 from the matrix and place the calculation of 7 and 8 before 6 in the list.

7) Form the reduced R^2 matrix

From \ To	2	3	4	5
2	0	0	1	0
3	1	0	0	1
4	0	1	0	0
5	0	0	1	0

8) Form R^3

From \ To	2	3	4	5
2	1	0	0	1
3	0	1	0	0
4	0	0	1	0
5	1	0	0	1

Units 2, 3,4 and 5 form two three membered loops with units 3 and 4 as common members.

9) Form R^4

From \ To	2	3	4	5
2	0	1	0	0
3	0	0	1	0
4	1	0	0	1
5	0	1	0	0

There are no non zero entries in the diagonal elements so there are no 4 membered recycle loops.
The coupled 3 membered loops are the "maximal cyclical nets".

10) Calculation list is then: - Calculate unit 1
- Calculate units 2, 3, 4 and 5
- Calculate units 7 and 8
- Calculate unit 6.

11) Form the cycle matrix using numbers of streams connecting units in recycle loops

Loop Number	Stream Number 3	4	5	8	9	11	13
1	0	1	1	1	0	0	0
2	1	1	0	0	1	0	0
3	0	0	0	0	0	1	1
Stream Frequency	1	2	1	1	1	1	1

Stream frequency and inspection of the cyclic matrix shows stream (4) is common to loops 1 and 2. Thus in successive substitution stream (4) should be specified. For loop 3, either stream (11) or (13) should be specified.

FIGURE 4-8 (continued)

its input streams flagged with "1". The operation is shown in an abbreviated computer flow diagram as Figure 4-9.

When a recycle loop is identified, a heuristic procedure shown in Figure 4-10 is used to "break" the loop. The bottom of the diagram simply shows that the executive iterates around the loop until calculations converge and continue thereafter through the process matrix. The procedure starts by assuming a zero flagged input stream known. The Process Matrix is rescanned to determine if now more units can be calculated. The executive checks to see if the stream which was assumed known is an output of one of the units which now can be calculated. If both of the above conditions are not satisfied, the executive returns to the zero flagged stream list and assumes a different stream known. If the conditions are not satisfied by assuming a single stream known combinations of two zero flagged streams are assumed known and the scanning repeated. If unsuccessful, combinations of three streams at a time are finally assumed known in an attempt to find a starting point for the iterative calculations. When the necessary conditions for an iterative solution are satisfied, a list is made of all units which now can be calculated. However, the executive removes from this list all units not contained in the loops to establish the shortest list of process units for the iterative solution.

A set of guessed values of the variables for the streams assumed known are used in performing the first iteration. Upon completion of the loop new values for these streams will have been calculated. These results are used in performing the next loop of iterations. The results of each loop are tested for convergence by comparing them with the results of the previous loop. When the absolute fractional change is less than a tolerance specified for all variables, convergence has been obtained.

Upon convergence of an iterative solution, the process matrix is again scanned to determine if any new units can be calculated. So in this way, the executive moves through the flow network. In GEMCS, no calculations are performed. After a loop is broken, the process matrix is rescanned. It is evident, thus, that the PACER, MACSIM and GEMCS

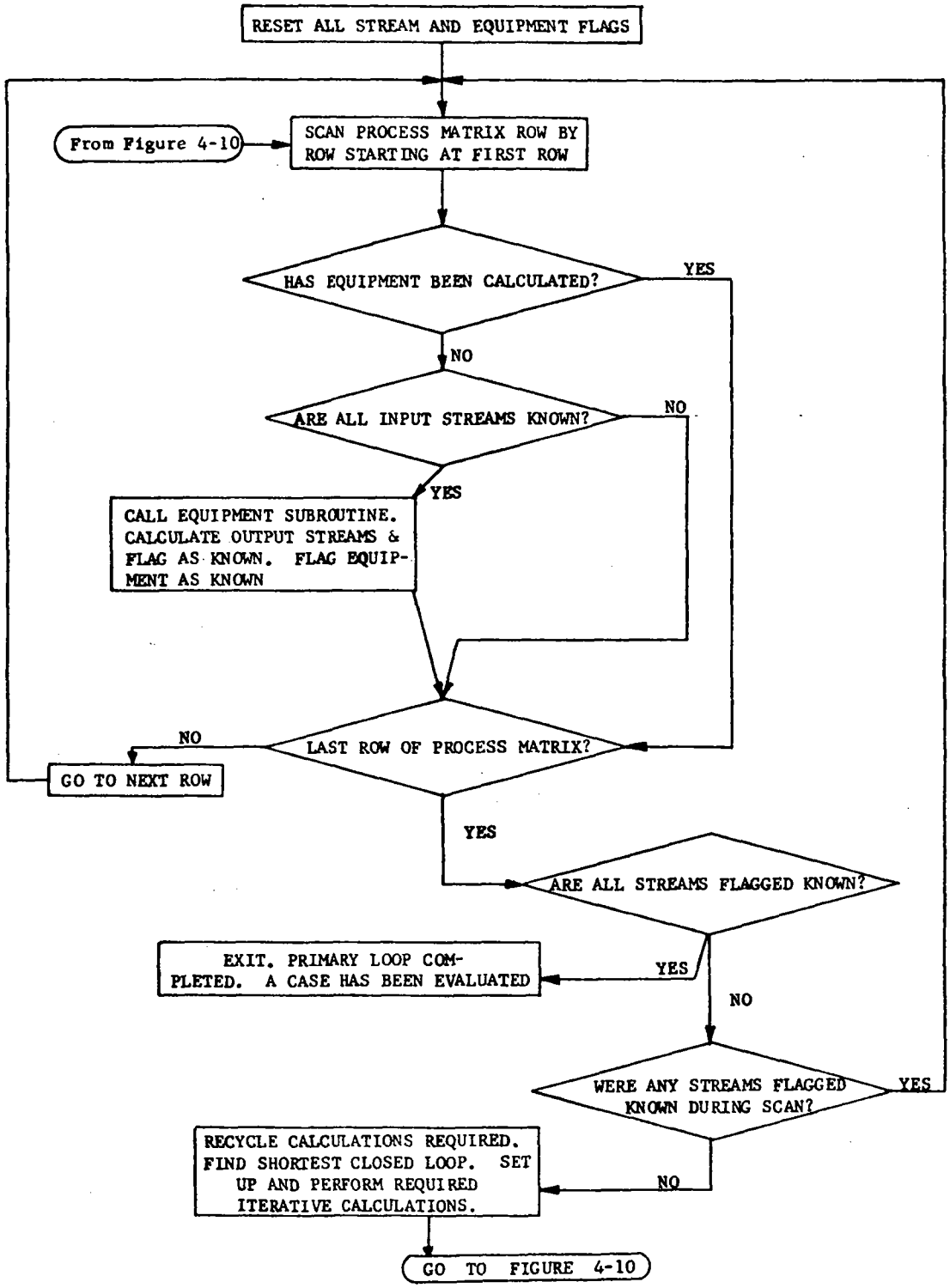


FIGURE 4-9. LOGIC FOR IDENTIFYING RECYCLE PROBLEM*

*Figure taken from reference (1) with the kind permission of the publisher.

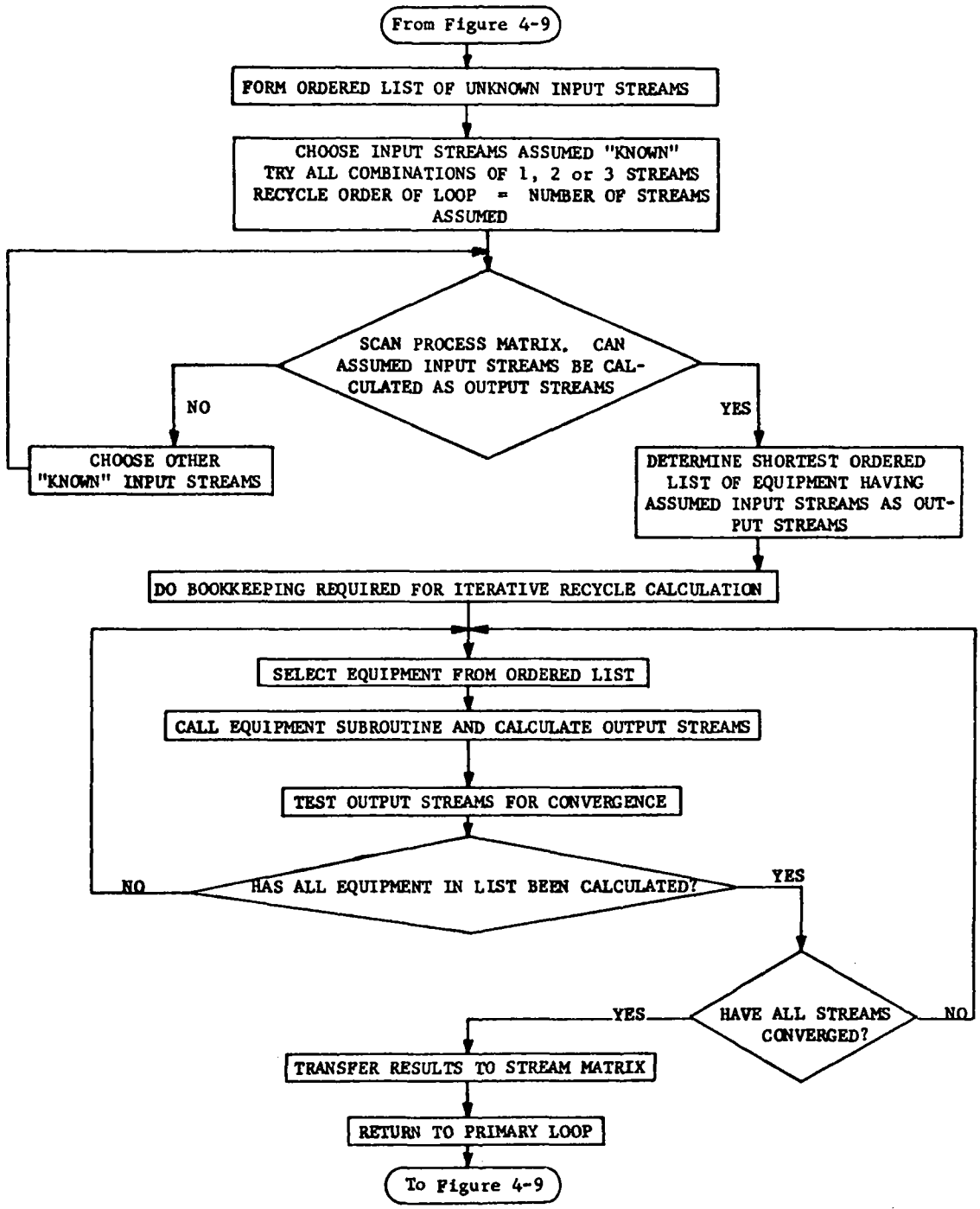


FIGURE 4-10. LOGIC FOR RECYCLE CALCULATIONS*

*Figure taken from reference (1) with the kind permission of the publisher.

executives proceed stepwise through the process network. Only the process matrix and the derived stream connections matrix are used. Although not the most sophisticated way of decomposing networks and perhaps not the most efficient, the algorithm has functioned successfully for moderately complicated networks.

SEPSIM, the executive we will use in the Workshop, does not have a network analysis capability. The user must provide the analysis.

5 STREAM VECTORS

This chapter deals with the description of streams in a process. At the beginning of the last chapter you may recall that we said that the choice of the variables to be considered is one of the central problems in the process analysis. The streams in a process are described by these variables.

Our objectives in this chapter will be to show the factors which must be considered in selecting variables, and the requirements which must be met by the variable list if an executive program is to be used. We will illustrate the discussion with vectors used in past waste treatment studies and we will close the chapter with a brief review of the correspondence of various measures of water borne wastes.

5.1 Definitions

We have used the terms "variable", "stream vector", "information content" loosely and without definition in the last three chapters. By "variable" we mean a property associated with a stream which can change from place to place in the network. BOD would be a variable since it will have one value in a stream entering a trickling filter unit and another in the stream leaving a chlorinator. Flow in the stream in gpm or temperature could be variables.

The group of variables we might choose, or all we know about a stream in a process, is the information content of the stream. For example, the information content of raw sewage might be the suspended solids, soluble BOD_5, suspended BOD_5, total dissolved solids, flow rate and perhaps also its color, odor and appearance. If we use the information modifier analogy of the last chapter, these properties of the sewage changes as it flows from unit to unit through the treatment plant. Thus, the process units operate to modify the information content of the process streams.

Stream list or vector is a more limited group. It is the set of stream properties or variables which are followed in a simulation or the set that contains the design parameters which set equipment sizes. As an example of the latter, the fractional reduction of BOD_5 is the basis

for sizing trickling filters or activated sludge units. BOD_5, consequently, would be included in a stream vector. The term vector is quite appropriate for the set of variables describing a stream. A vector in physical space has projections along the 3 coordinate directions; in "n" dimensional space, the vector will have projections along n coordinate directions. Each projection is a scalar quantity, that is, a number. The variables describing the condition of any stream are numbers. Each variable in a stream vector is like a coordinate direction. A numerical value of a variable in a stream then is like a projection along a coordinate direction.

The stream vectors are collected in SEPSIM as an array called the SN matrix. Each row of the array is a vector for a specific stream in the process. The STRMI and STRMØ matrices are smaller arrays with the same structure as the SN matrix. They are also used in SEPSIM.

5.2 Choice of Variables

Primary factors in the selection of variables are the objectives of the simulation and the nature of the unit processes in the system. If we are interested in the level of nutrients in the outfall from a municipal sewage plant, the nutrients must be variables. If one of the process units is a biological reactor, temperature may be a variable because BOD reduction depends on temperature. Only suspended solids are removed in a clarifier. Consequently, if phosphorus removal is important, then the concentration of suspended matter containing phosphorus must be a variable. The choice of variables, however, is constrained by the data available. Including a variable in the stream vector which is not or cannot be measured may be pointless. Similarly, little is gained by including a variable if models describing the change in the variable in process units are not available.

Table 5-1 compares a group of detailed vectors that have been used in both design and simulation studies. The first three were for municipal treatment plants[1,2,3]. The vectors reflect criteria now used

---

[1] Smith, R., "Preliminary Design and Simulation of Conventional Waste Treatment Systems Using the Digital Computer", Water Pollution Control Research Series WP-20-9, F.W.P.C.A./ U.S.D.I. (Washington, 1968)

for specifying water quality or those proposed for future use. BOD and TSS are used now as criteria for discharge into receiving waters. The current concern about nutrients is leading to additional criteria for nitrogen and phosphorus. Total organic carbon (SOC + DOC) may replace BOD in some quality criteria because it can be measured more easily. The division between suspended and soluble matter simply reflects the presence of clarifiers in the system. Similarly VSS is used because the biomass in an activated sludge system is frequently measured in terms of volatile suspended solids. The separation of organic carbon into biodegradable and non biodegradable recognizes that a biological reactor is not capable of converting all the organic carbon in the waste.

The municipal sewage vectors do not give a full description in as far as Coliform counts or pesticide concentrations are concerned. Selected heavy metals and color should be included. Paucity of measurements and a complete absence of models makes lengthening the vector to include these variables pointless at this time. In the WATCRAP-PACER studies[2] models could not be found or developed for all the variables in the vector. For example, we did not use models for SOC or DOC in a trickling filter. Models for DP and SOP could not be written because we are ignorant as to how phosphorus is distributed between suspended and dissolved matter in sewage. The problem was circumvented by using only BOD models and calculating SOC and DOC from BOD through rather inexact factors. Since the length of the vector increases the running time of programs and the possibility of errors in a library subroutine, the vector should be kept as short as possible. If factors are used to obtain other variables from say BOD and VSS, there is no reason to include these other variables in the vector. They can be estimated from a print-out of BOD and VSS results quickly and easily.

For measurements and models now available and criteria used now,

---

[2] Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control 69, 686 (1970)

[3] Smith, R., Eilers, R.G., Hall, E.D., "Executive Digital Computer Program for Preliminary Design of Waste Water Treatment Systems", Water Pollution Control Research Series, WP-20-14, F.W.P.C.A./U.S.D.I. (Washington, 1968)

TABLE 5-1. COMPARISON OF DETAILED STREAM VECTORS USED IN WASTE TREATMENT STUDIES

Smith in "Preliminary Design and Simulation of Conventional Waste Water Treatment Systems Using the Digital Computer" (1)	Silveston in "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System" (2)	Smith et al. in "Executive Digital Computer Program for Preliminary Design of Waste Water Treatment Systems" (3)	Hoffman et al. in "The Strategy and an Example of Simulation as Applied to a Petroleum Refinery Waste Treatment Process (4)
1. Volumetric Flow Rate (Q)*	1. Stream Number (I)	1. I	1. I
2. Suspended Organic Carbon (SOC)**	2.	2. Q	2. Stream Flag
3. Suspended Non Biodegradable Carbon (SNBC)	3. Q	3. SOC	3. Total Flow***
4. Suspended Organic Nitrogen (SON)	4. SNBC	4. SNBC	4. T
5. Suspended Organic Phosphorus (SOP)	5. DNBC	5. SON	5. Pressure, psi (P)
6. Suspended Fixed Matter (SFM)	6. SOC	6. SOP	6. Oxygen
7. Dissolved Organic Carbon (DOC)	7. DOC	7. SFM	7. Total Carbon***
8. Dissolved Non Biodegradable Carbon (DNBC)	8. SON	8. SBOD	8. Water
9. Dissolved Nitrogen (DN)	9. DN	9. VSS	9. Gaseous Carbon
10. Dissolved Phosphorus (DP)	10. SOP	10. TSS	10. DNBC
11. Dissolved Fixed Matter (DFM)	11. DP	11. DOC	11. Volatile Organic Carbon
12. Suspended BOD (SBOD)	12. SFM	12. DNBC	12. Dissolved Non Volatile Carbon
13. Dissolved BOD (DBOD)	13. DFM	13. DN	13. Immiscible Oil (as carbon)
14. Volatile Suspended Solids (VSS)	14. SBOD	14. DP	14. Organisms (as carbon)
15. Total Suspended Solids (TSS)	15. DBOD	15. DFM	15. Solid Carbonate Salts (as carbon)
16. Alkalinity (ALK)	16. TSS	16. ALK	16. Organic Sludge (no microorganisms)
	17. Temperature (T)	17. DBOD	17. Inert Solids (as carbon)
	18. VSS		18. TSS
	19. ALK		19. Phenol (in p.p.b.)
			20. pH
			21. Hydroxyl Ion Concentration
			22. Bicarbonate Concentration
			23. Carbonate Concentration

(4) Hoffman, T.W., Woods, D.R., Murphy, K.L., Norman, J.D., "The Strategy and an Example of Simulation as Applied to a Petroleum Refinery Waste Treatment Process", J.W.P.C.F., in print (1973)

* Flow in mgd

** Concentrations in milligrams/litre

*** in lbs/day

TABLE 5-2. COMPARISON OF SHORT VECTORS USED IN WASTE TREATMENT STUDIES

Silveston[2]	Singh[10]	Peeling[5]	Fan et al.[8]	Curry[9]
1. I	1. I	1. I	1. Q	1. I
2. -	2. -	2. -	2. TSS	2. -
3. Q	3. Q	3. Q	3. Substrate	3. Q
4. SBOD	4. TSS	4. TSS	4. Cell Mass	4. T
5. DBOD	5. DBOD	5. DBOD		5. P
6. TSS	6. SBOD	6. SBOD		6. pH
7. T	7. Total BOD (TBOD)	7. TBOD		7. TBOD
8. VSS	8. VSS	8. VSS		8. Total COD
9. ALK	9. pH			9. Phenol
	10. DFM			10. Mixed Liquor Suspended Solids
	11. T			11. DN
	12. SFM			12. DP
	13. -			13. Dissolved Oxygen
	14. Total Volatile Acids			

[5] Peeling, D.A., Engineering Report, Dept. of Chemical Engineering, University of Waterloo (1972)

shorter vectors are preferable. A group of such vectors are shown in Table 5-2. The structure used by Peeling[5] has been employed in all recent SEPSIM simulation studies[6][7]. The vector could have been reduced to six variables. The blank in the second element is for the flagging operation used in the MACSIM-GEMCS executive, but not used in SEPSIM. The vector was structured so that the subroutine library could be used with these other executives. Total BOD was included just for print-out convenience. SBOD and DBOD are actually calculated by the models. The ultimate vector for municipal waste treatment consisting of just 4 variables is used in Fan's ASOP-SPCHEN program[8].

By way of contrast to vectors for sewage, the last column in Table 5-1 shows the vector used by Hoffman et al.[4] for a petroleum refinery waste. The models used in Hoffman's simulation of a treatment plant utilized carbon balances. Consequently, the waste components in the vector are expressed in terms of carbon. Phenol is a particularly important component in the waste so it appears in the vector.

Table 5-2 shows the vector used by Curry[9] for a chemical waste. The vector differs substantially from those used for refinery waste and for sewage. This illustrates simply that vectors must be constructed for specific wastes as well as for the objectives of the design or simulation.

---

[6] Silveston, P.L., "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research 6, 1101-1111 (1972)

[7] Silveston, P.L., "Computer Simulation of Waste Water Treatment Plants", Proc. 1st Pacific Chem. Eng. Congress, Part III, (Kyoto, Japan, 1972)

[8] Fan, L.T., Erickson, L.E. and Chen, G.K.C., Paper, National A.I.Ch.E. Meeting, Cincinnati, Ohio (May, 1971)

[9] Curry, E.V., "Computer Simulation of a Biological Waste Treatment Facility", Eng. Report, Dept. of Chem. Eng., Univ. of Waterloo (1971)

[10] Singh, D.P., "Steady State Simulation of the Kitchener Waste Treatment Plant by Digital Computer", M.A.Sc. Thesis, Dept. of Chem. Eng., Univ. of Waterloo (1971)

All but one of the vectors in the Tables are written with a flow entry and components expressed as concentration. The other alternative is to use mass flow rates in say pounds/hour for components. This is the convention used in the Hoffman vector.

You should note in Table 5-1 the ordering of the variables. In the third column suspended matter and dissolved matter variables are grouped separately, while in the second column suspended matter are evenly numbered and dissolved matter variables bear odd numbers. In the fourth column, all the variables in terms of carbon are collected together. This ordering was intentional to simplify DO loop statements in the model subroutines.

5.3 List Restrictions

It is a good practice to use the same stream vector for all subroutines in the model library. In other words, each "library" is written for one stream vector. This practice reduces the possibility of operating on the wrong element of a vector in a subroutine which could arise if the vector changed and the user failed to recognize the change.

In the Singh vector in Table 5-2, pH and total volatile acids appear. These variables are useful only in the digester model, but they are carried throughout the design or simulation in order to keep the vector the same. Similarily, in the Curry vector, DN and DP are carried because they describe nutrient concentrations in a stream mixed with a chemical waste upstream from a trickling filter. Nutrients are not considered elsewhere in the plant.

Any vector structure can be chosen for SEPSIM provided only that the first element or entry is reserved for the stream number. Most executives have a similar requirement. In the PACER derived executives which use flagging to organize calculations (see previous chapter), the second element must be reserved for the flag.

5.4 SEPSIM Stream Vectors

In the Workshop each group will be responsible for selecting the vector which they will use for their simulation or design case. Process models each of you will write must correspond to the vector selected.

Establishing the vector is a necessary step in any application of computer-aided design or analysis. Table 5-3 sets forth guidelines for stream vectors for use with the SEPSIM Executive.

TABLE 5-3. GUIDELINES FOR SEPSIM STREAM VECTORS

SELECTION OF VARIABLES

1. Any stream property which changes from point to point in the process can be a variable.

2. Choice of variables is always a compromise between:
   a) all properties of interest in the process or in one or more output streams (in simulation),
   b) all properties used as design parameters for choosing or sizing equipment (in design)
   c) all properties which are used as water quality criteria (both simulation and design),
   d) properties which reflect the operations of the units in the process,

   on one side and on the other side:

   e) availability of data which describes the change of a property or at least sufficient information to develop suitable models,
   f) availability of data which will permit model parameters to be evaluated and the model to be tested.

3. Vector length should be as short as possible to fulfil the simulation or design requirements.

VECTOR STRUCTURE

1. 1st element in the vector is the stream number.

2. All subroutines in the model library should use the same vector.

3. Structure should permit compact and efficient statements (e.g. in DO loops) in library subroutines using the vector.

4. Library can be made compatible with the PACER group of executives by reserving 2nd element in the vector for a flag.

In the choice of variables, it is best to start with just a minimum list. Once the program is in use, the adequacy of the vector for the job required can be checked. The stream vector is not part of the executive and it can be altered, expanded, or even shrunk without difficulty by making appropriate changes in the subroutine library. Bear in mind, however, that all subroutines should be examined and possibly updated if the vector is changed.

5.5 Conversion Factors for Waste Water Measurements

If library subroutines are adopted from the Sanitary Engineering literature, it is not infrequent that the model will use one measurement for a variable, while data will be available in a different one. Rather than change the model, it is often easier to convert the data measurements to conform with those used in the model. Factors are used for this purpose. For example, the biomass in an activated sludge unit might be measured in the plant by a COD determination, but the units of biomass in a model for the unit may be mg/l. as VSS. To evaluate model parameters or test the model, it will be necessary to convert COD measurements to VSS.

Three main types of measurements are used for organic matter in wastes: biochemical oxygen demand (BOD), chemical oxygen demand (COD), and total organic carbon (TOC). BOD, as you know, is measured by mixing a waste sample with clean water whose dissolved oxygen level is known, inoculating the mixture with an acclimatized seed bacteria and incubating the air tight system for either 5 or 20 days. The BOD is determined from the change in the oxygen level of the water. A thorough description of the method is given in "Standard Methods"[11]. The test and its interpretation are also discussed by Eckenfelder and Ford[12].

COD is measured by digesting the waste sample with an acid and oxidizing agent for about two hours. The consumption of oxidizing agent

---

[11] "Standard Methods for the Examination of Water and Waste Water", 12th Edition, Am. Public Health Service, Inc. (New York, 1965)

[12] Eckenfelder, W.W., Jr. and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970)

gives the COD of the sample. Total organic carbon can be obtained via a special instrument for this purpose. A waste sample is catalytically oxidized at high temperature in an air stream and the amount of CO_2 formed is measured by an infra red spectrophometer. Details of both tests are given in the references above.

Not all of the biodegradable organic matter of the waste will be consumed even after 20 days incubation. The actual biodegradable organic matter is termed the theoretical BOD, while the maximum BOD which can be measured in the standard test is called the ultimate BOD (BOD_u). BOD_u can be assumed to be 0.9 times the theoretical BOD[12]. A twenty day incubation period will often give a good estimate of BOD_u. The five day incubation period BOD (BOD_5) is related by a factor to the ultimate BOD, but the factor depends on the rate constant for oxidation in the incubation bottle; that is, it depends upon the waste. Figure 5-1 taken from Seminar Notes[13] illustrates the waste dependence and shows that BOD_u will measure ammonia nitrogen as well as organic carbon. For raw sewage $0.8 < BOD_5/BOD_u < 0.9$, although Eckenfelder and Ford[12] suggest 0.77 for the ratio. The ratio ranges from 0.5 to 0.6 for secondary effluent.

The factor relating COD to BOD_5 (COD/BOD_5) will be a function of the waste and the treatment it has undergone. Figure 5-2 taken from Eckenfelder and Ford[12] shows the variation in the factor. The figure suggests a factor of 1.5 for raw sewage. Smith[1] proposes the same factor. Other sources suggest the factor is 1.9[13] and as high as 3.0[12] for sewage. Eckenfelder and Ford tabulate data which show $3.2 < COD/BOD_5 < 4.2$ for primary effluent (clarifier discharge) and $5.0 < COD/BOD_5 < 7.0$ for secondary effluent. This latter range agrees with Figure 5-2.

TOC is based on carbon rather than oxygen so the COD/TOC factor will be greater than one. Smith[1] suggests the factor is 3.2. Eckenfelder and Ford show data with a range of 3.3 to 4.6 for raw sewage, 3.2 to 5.8 for primary effluent and 2.0 to 2.6 for secondary effluent. For the mixed liquor suspended solids Smith suggests COD/TOC = 2.7. The

---

[13]"Biological Waste Treatment", Notes for a Technical Seminar, University of Waterloo, Waterloo, Ontario (1967)

theoretical ratio based on molecular weights of carbon and oxygen is 2.66.

BOD_5/TOC range from 1.3 to 1.9 for sewage according to data given by Eckenfelder and Ford. In the same section they quote a study by Wuhrman setting the factor ≈ 1.87. Smith suggests the same value. Seminar notes[13] employ 2.23. For primary effluent, $1.0 < BOD_5/TOC < 1.3$, while for secondary effluent the range extends from 0.3 to 0.7.

Volatile suspended solids are another measure of organic suspended matter. Smith gives two values for COD/VSS. The value for sewage is 1.5 while for mixed liquor suspended solids the ratio is 1.42. Smith estimates VSS/TOC from the previous values as 2.1 and 1.9 for sewage and the biomass respectively.

According to limited data given in Design Guides[14], volatile suspended solids account for 85% of the total suspended solids (VSS/TSS = 0.85). The value used by Smith in his study[1] is 75%. Design Guide[14] also indicates 60% of the suspended solids are non biodegradable.

The BOD of sewage, according to Smith, is 30% dissolved and 70% suspended. Smith assumed in his work[1] that 1/3 of the nitrogen and phosphorus occurs in sewage as suspended matter.

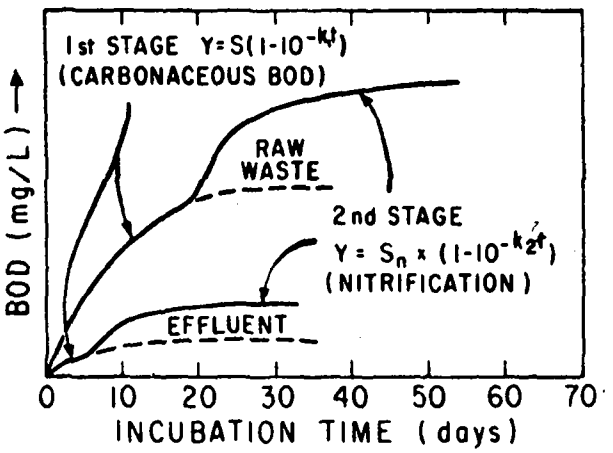


FIGURE 5-1 VARIATION OF MEASURED BOD WITH INCUBATION TIME AND WASTE*

---

[14] "Design Guides for Biological Waste Water Treatment Processes", Water Pollution Control Research Series, 11010 ESQ, E.P.A. (Washington, D.C., 1971)

* Taken from reference (14).

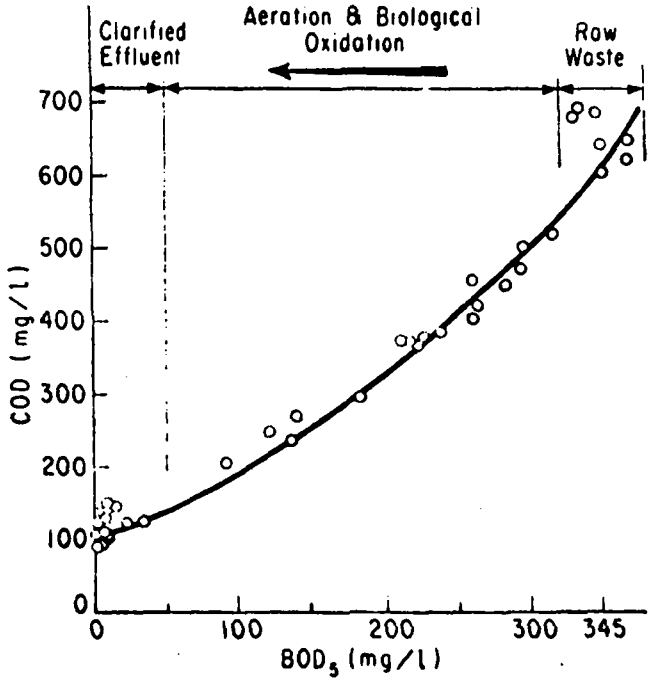


FIGURE 5-2. BOD-COD RELATIONSHIP**

Conversion of units will also be necessary for preparing data and in writing models. Table 5-4 gives some of the more useful conversion factors for such purposes.

**Taken from reference (12) with the kind permission of the publisher.

TABLE 5-4. USEFUL CONVERSION FACTORS

Measurement in Units of	X	Multiply by — to Convert to	=	Measurement in Units of
gallons (U.S.)		0.833		gallons (Imp.)
gallons (U.S.)		0.134		cu. ft.
gallons (Imp.)		0.16		cu. ft.
acres		43,560		sq. ft.
gallon per day (U.S.) (gpd)		0.00557		cu. ft./hour
lbs.		453		grams
mg/l.		1		ppm
mg/l.		6.24×10^{-5}		lbs/cu. ft.
gallons (U.S.)		0.00379		cu. meters
ft.-lbs/sec		0.00182		horse power
cm/sec		30.48		ft/sec.

Density of Water = 62.4 lbs/cu. ft.

$g = 32.2 \text{ ft/sec}^2 = 980.7 \text{ cm/sec}^2$

6 SEPSIM

In Chapters 3 and 4 we have examined how an executive program handles either simulation or design. Our purpose in this chapter is to look into the details of how an executive functions. We will consider SEPSIM, the executive to be used in the Workshop. It is a "bare bones" executive developed for pedagogic purposes and for relatively simple process systems, such as those used in waste treatment. Despite its simplicity, SEPSIM is typical of larger and more complex executives. It is thus admirably suited for the purpose of this chapter. We will examine the organization of an executive, how models in the subroutine library are related to specific units in a proposed or existing flow sheet, and the procedure for converging iterative calculations. We will also look at how information is fed to the program and how certain built-in or user initiated execution controls operate.

However, unless you are interested in the design of simulation or design executive programs, you need not study this chapter. It serves as an appendix to earlier chapters.

6.1 Background

SEPSIM - Short Executive Program for SIMulation - was developed in 1969 partially at the University of the Witwatersrand in Johannesburg, South Africa, and partially at the National Research Institute of Mathematical Science of the South African Council on Scientific and Industrial Research by Professor Silveston and Mr. D. P. Laurie. It was intended originally for use in courses on process simulation, as well as for use by the South African National Institute for Water Research who sponsored its development.

Immediate ancestors of SEPSIM are the PACER executive and an untitled design program developed at the Cincinnati Water Research Laboratory of the U.S. Environmental Protection Agency by Robert Smith. Both executives have been briefly discussed in earlier chapters. Smith's Executive was at least partially inspired by the same research thesis[1]

[1] H. Mosler, M.S. Thesis in Chemical Engineering, Purdue University, Lafayette, Indiana (1963).

which was the source of much of the PACER Executive.

The problem with the Smith Executive is that it is a design program grafted on to a simulation structure. One or more of the outlet variables for a process unit are specified and a model in the subroutine library is used to calculate equipment size and cost. It is this specification of variables in outlet streams which make the Executive unsuitable for simulation. The PACER Executive, on the other hand, is a simulation program, but it contains a large and cumbersome decomposition module and in its early version it contained controls and data input provisions which are unnecessary for simple process systems. What we have done in SEPSIM is to adapt PACER's useful information storage and transfer routines. These have been combined with algorithms for handling recycle loops and for identifying library models with process units taken from Smith's Executive and modified for our use.

Our objectives in the SEPSIM development were to provide an executive which would offer most of the advantages of powerful executives such as PACER but one which could be used on a small computer without resorting to overlays. Furthermore, we wanted to have an executive which would handle all calculations, including the tedious iterative ones, but leave the pedagogically instructive task of network analysis to the student.

6.2 Organization

SEPSIM consists of a mainline program and, in the version we consider in this chapter, 3 operational subroutines: NØMEN, SELECT and RPRINT. The read in of data, manipulation of arrays, organization of calculations and convergence testing are handled by the main program. It also calls the other subroutines as they are required.

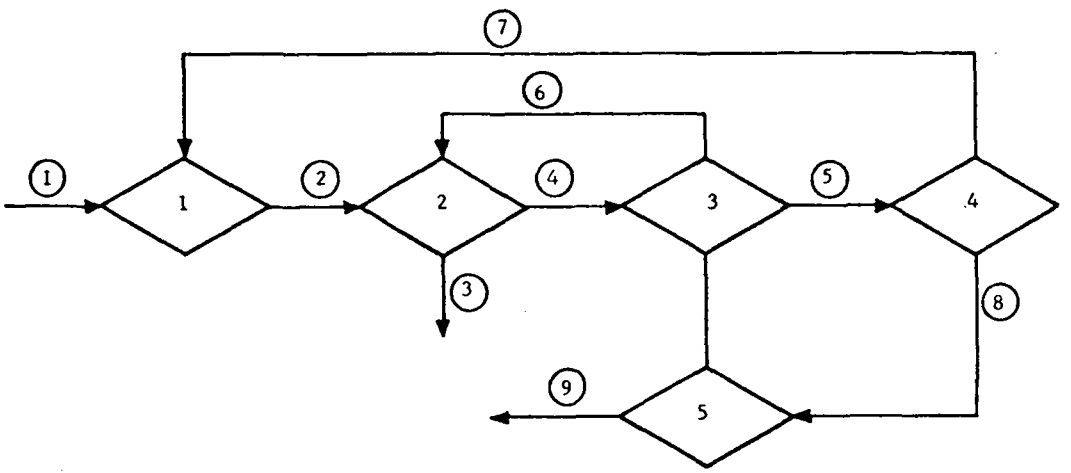
The NØMEN subroutine was included to permit a variety of names to be used for models in the SEPSIM subroutine library. SELECT acts solely as a calling program to bring in the proper model subroutine when it is required for calculations. The subroutine RPRINT handles all the output printing for successful SEPSIM runs.

Compilers normally require that a subroutine must exist for all

subroutines specified in SEPSIM. SELECT contains provision for calling up to 50 subroutine. Thus, SEPSIM must include up to 50 dummy subroutines. These are very brief programs which simply provide for return to the calling subroutine. The dummy subroutines are replaced by the actual subroutines to be used in a run by a number of methods.

6.3 Organization of Calculations

Calculations performed by SEPSIM are controlled by the process matrix. This matrix is always part of the input data prepared by the user. In principle, therefore, it is the user who decides on the calculation sequence to be used. Figure 6-1 shows a simple recycle system which we will consider in this section. The SEPSIM process matrix for this system appears immediately below it. We will use this matrix to discuss how the SEPSIM mainline program operates.



SEPSIM PROCESS MATRIX

K	Equipment No.	Mode Name	III	Associated Streams
1	1	MIXER3	-	1 7 - - - 2 - - - -
2	2	MIXER3	-	2 6 - - - 3 4 - - -
2	3	MIXER3	-	4 - - - - 5 6 - - -
1	4	MIXER3	1	5 - - - - 7 8 - - -
-	5	MIXER3	2	8 - - - - 9 - - - -

FIGURE 6-1. SIMPLE RECYCLE EXAMPLE FOR SEPSIM

The index K in the first column of the process matrix numbers recycle loops and shows their extent if units in the array are arranged to follow forward flow in the process. From Figure 6-1 we see that units 2 and 3 (joined by streams (4) and (6)) form a loop. K = 2 marks the start and end of this loop. An outer loop marked by K = 1 embraces units 1 to 4 (joining streams are (2), (4), (5) and (7)). Units 2 and 3 are contained in this outer loop because they appear in the array between units which are designated by K = 1. A second index, III is employed to indicate those units not contained in any loop (III = 2) or which terminate an outermost loop (III = 1). Unit 4 in the Figure 6-1 ends the loops so III in the fourth column of the matrix is set equal to 1, while unit 5 is outside of any loop so III = 2 for it.

The status of the calculations during execution are followed by a set of internal indicators. These are given and explained in Table 6-1.

TABLE 6-1. INTERNAL CONTROL INDICATORS IN SEPSIM

Indicator	Explanation
INDC	Number of last calculational loop SEPSIM has started to calculate. If no loop has been started INDC = 0. Note that loops are numbered in SEPSIM by K.
KØUT	Position in loop. KØUT = 0; no loop is being calculated. KØUT = 1; a loop is active. KØUT = 2; end of a loop has been reached.
IN	Nesting level of a loop. SEPSIM allows IN = 10.
IFLUN(IN)	If currently active loop of nesting level IN is to be repeated IFLUN(IN) = 1. If not, IFLUN(IN) = 0.
IFLUNK	If the outer loop in which the currently active loop is nested is itself to be repeated IFLUNK = 1. If not, IFLUNK = 0.
LOOP(IN)	Identifies loop of nesting level IN.

The process units are numbered sequentially and ordered in the process matrix following the main flow of information in the network.

SEPSIM begins its calculation by reading the first row of the process matrix. If the first element in the row contains a zero, this unit will not be in a recycle loop. The Executive will call the appropriate subroutine, transfer stream values needed to execute the calculations in the subroutine and transfer the resulting stream values to the SN matrix, filling empty rows of this matrix. However, this is not the case in Figure 6-1. When a recycle loop is encountered ($K \neq 0$), INDC is set equal K, the appropriate subroutine is called and it is executed. The stream values obtained are tested for convergence with the vector EPS against values in the SN matrix for the output streams. Since they normally will not converge for the first iteration, IFLUN(IN) which becomes IFLUN(1) is set to 1. The flow diagram of SEPSIM, Figure 6-2, shows the sequence. Since we are in the first pass in the iterative procedure, the tests shown in the figure send us back to (B) and another row of the process matrix will be read in. Suppose that we have a new loop starting at the unit now considered (as in Figure 6-1). The next row will contain a value of $K \neq$ INDC. This indicates a nesting of recycle loops and we let LOOP(IN) = INDC. We next reset INDC to the K of the new loop and IN is augmented. IN will have the value 2 for the second and third row of the process matrix shown in Figure 6-1. Thus, IN indicates the nesting order of loops. Next a subroutine will be called and executed. Normally, testing of the output stream value will not show convergence so IFLUN(2) will be set to 1 and another row of the matrix will be called.

When the last row of the now active inner loop is reached, K = INDC and KOUT is incremented to 2. This permits us to return to the first terminal of the nested loop. This terminal will be marked by INDC = K and is found by scanning the K column starting with row one of the process matrix. We now iterate the inner loop until convergence is achieved. This is indicated by IFLUN(2) = 0. However, IFLUNK = IFLUN(1) is not zero so we set INDC to its previous value and proceed with calculating any further process units in the outer or primary loop.

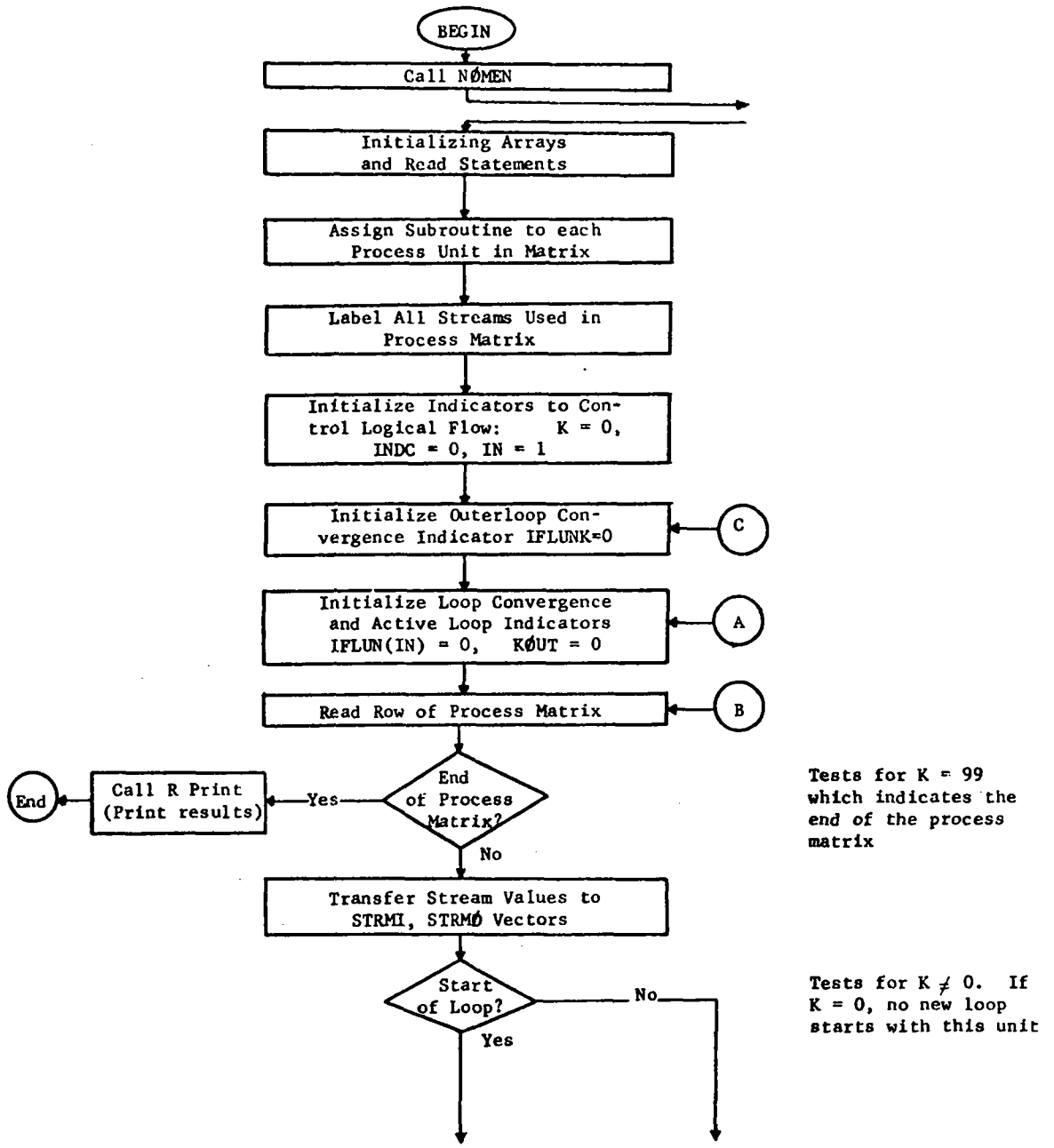


FIGURE 6-2. LOGICAL FLOW DIAGRAM FOR SEPSIM

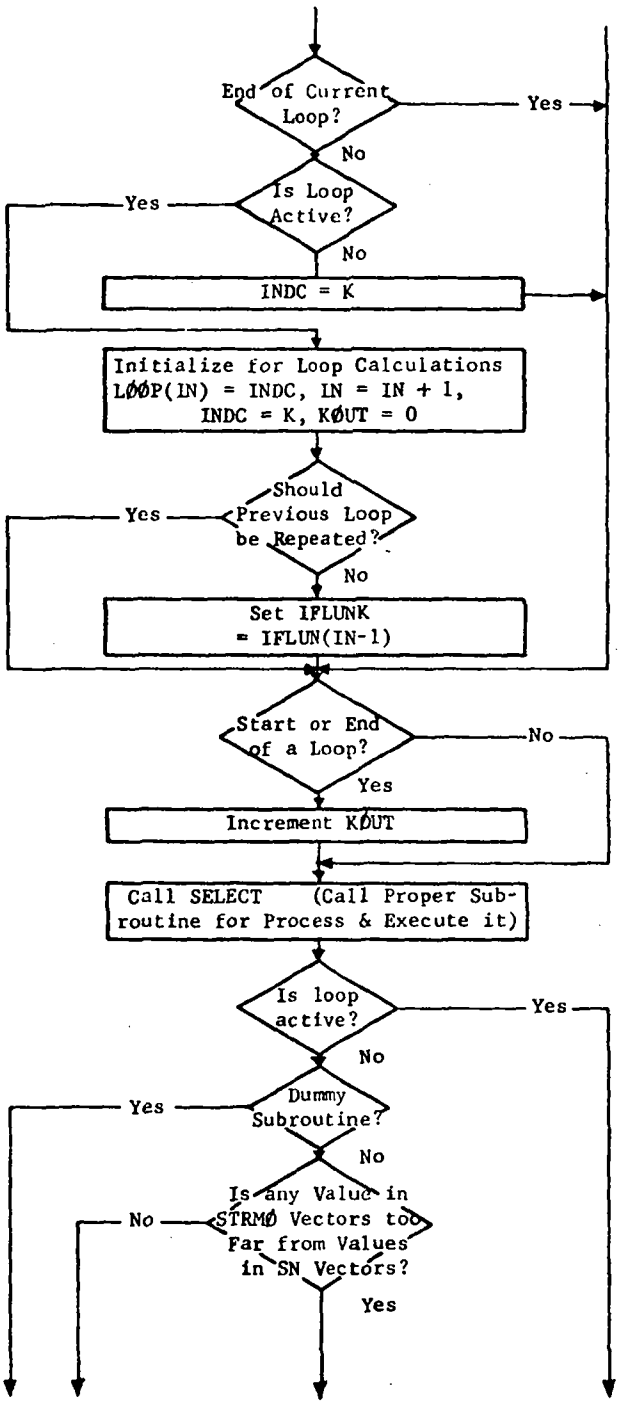


FIGURE 6-2 (cont'd)

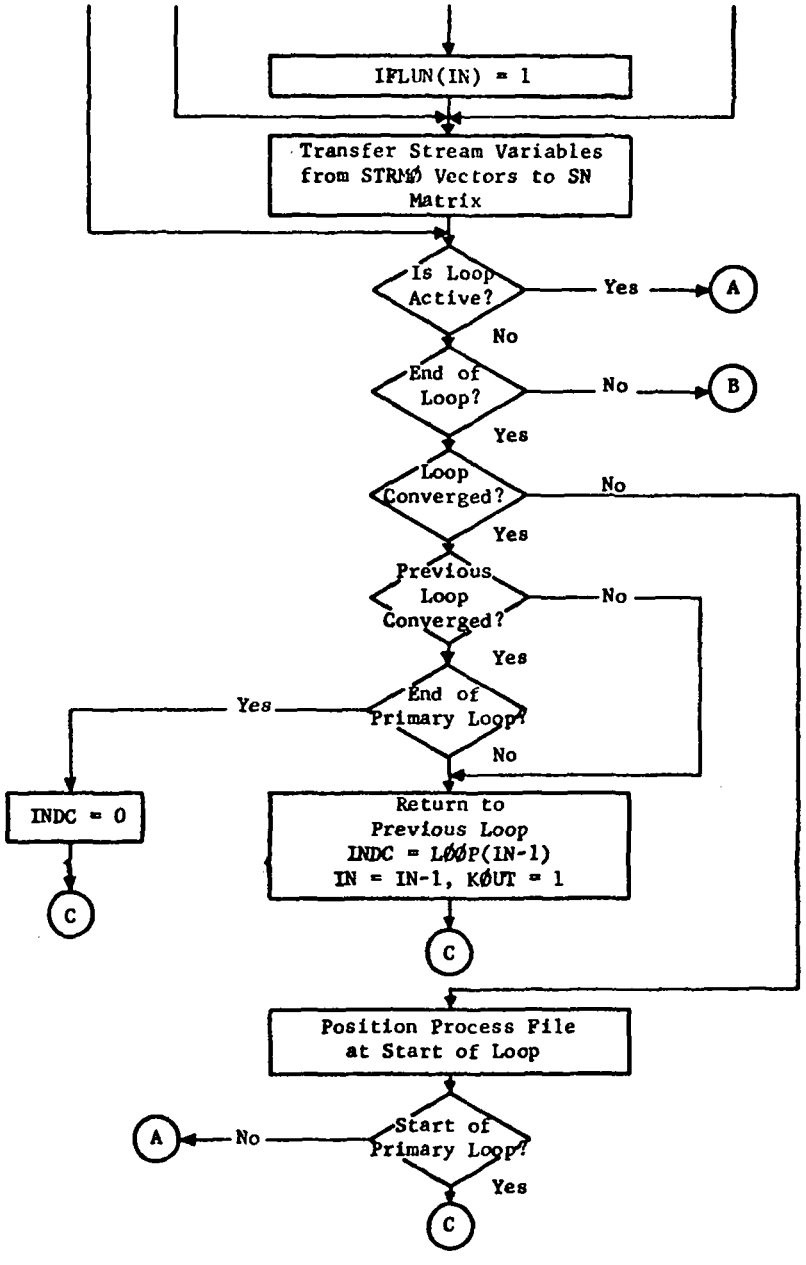


FIGURE 6-2 (cont'd)

The end of this loop is found when K = INDC and we return to the beginning of the outer loop. We now iterate on the primary loop, but in each cycle through this loop we must converge the inner loops.

Convergence of the outer loop is indicated by IFLUN(1) = 0. When the last unit in this loop indicated by III = 1 is reached we set INDC = 0. We now return at (C) in Figure 6-2, initialize all indicators and proceed with the calculations by reading in another row of the matrix.

SEPSIM cannot handle flow sheets where there are interlocking recycle loops or where two or more loops terminate or originate at the same process unit. These network situations can be handled by introducing fictitious process units or streams to convert the network to nested loops. We will discuss this in a latter section.

The flow diagram you will notice contains a number of "IF" and directed "GO TO" statements. These statements lead to a compact, efficient program, but they make the program seem much more complicated than it really is. Notes on the right hand margin describe how the "IF" and directed "GO TO" statements function.

We have sketched out in the preceding paragraphs the function of the Executive in broad terms. It will probably help you to understand the function if we show how the network shown in Figure 6-1 is handled in SEPSIM. The network consists of a recycle loop containing 4 process units, totally enclosing a two member loop. In the terminology introduced in Chapter 4, this is a second order nested recycle system. A single chained unit is appended after the outer recycle loop. The process matrix encodes the structure for SEPSIM. The index K numbers the loops and shows the end of the network. The III column shows the end of the recycle loop portion and indicates chained units.

SEPSIM begins by reading the input data as suggested in Figure 6-2. The values in the first row of the SN matrix will be specified. All other rows will contain zero or guessed values. After initializing all the indicators, we read in the first row of the Process Matrix and transfer rows 1 and 7 from the SN matrix to the STRMI matrix used by the subroutine. A value of K = 1 is encountered indicating that we enter

a primary recycle loop. The program sets INDC = 1, KØUT = 1 and calls subroutine MIXER3 to calculate values for stream (2). These are stored in a STRMØ row and are tested for convergence. Convergence, of course, is not obtained since the stream vector in the SN matrix which we compare to the STRMØ values contains zeroes or guessed values. The Executive therefore sets INFLUN(1) = 1. We return to (B) in Figure 6-2 and read in row 2 of the matrix. We now encounter K = 2 so for this row K ≠ INDC. This indicates to the program that an internal or nested loop has been encountered. SEPSIM sets its loop indicators LØØP(1) = 1, and IN = 2. It also changes INDC to 2 and resets KØUT = 0. The latter is subsequently changed to 1. IFLUNK is set to IFLUN(1). Since IFLUN(1) = 1, the program now requires that the outer loop calculations be repeated after we exit from the inner loop calculations.

After these operations MIXER3 is called and executed giving values to streams (3) and (4). A convergence test is run which normally will fail in the first pass so IFLUN(2) = 1. We continue to the end of the diagram (Figure 6-2) and return to (B). The next line read contains K = 2. Since K = INDC this indicates the end of a loop. This causes KØUT = 2 and we proceed to call and execute MIXER3 once more. Values for streams (5) and (6) are obtained. Convergence test will be negative usually so IFLUN(2) = 1 as for unit 2. Again this takes us to the bottom of Figure 6-2. This time we reposition our process file at the second row of the process matrix and begin a first iteration of the inner loop. INDC, IN continue to be equal to 2 and we proceed as indicated in the above lines.

Let us assume that after three or four iterations of loop 2 we obtain convergence so IFLUN(2) = 0. The nested loop no longer needs iterations so INDC, IN and KØUT are reset to one and we return to (C). SEPSIM now reads line 4 where it encounters K = 1 so again K = INDC indicating the end of a loop. KØUT is reset to 2 and we call and execute the subroutine MIXER3 to calculate values for streams (7) and (8). Convergence will not be obtained so IFLUN(1) = 1 as before. Since IFLUN(1) ≠ 0, the process file is now positioned to the beginning of the primary loop, that is, unit 1. We return at (C), initialize some indica-

tors and we are back where we started. However, at this point we have evaluated streams (2) to (8). We now read in the first row again and begin to iterate our outer loop. Bear in mind, though, that each time we calculate through the outer loop, we must iterate many times through the inner loop until the inner loop converges.

After say 5 or 10 iterations of the outer loop involving perhaps a hundred iterations about the inner loop, let us say we achieve convergence of both loops. This will be indicated by IFLUN(2) = 0 followed by IFLUN(1) = 0 after we complete the outer loop. When this occurs we are in line 4 with unit 4. SEPSIM identifies the end of a primary loop because III = 1. Since it has converged we set INDC = 0 and return at (C) (The flow diagram simplifies the logic at this point). From (C), we initialize our indicators and read in the next line which is line 5. We find K = 0, III = 2, so this unit is not inside a loop. We call and execute the subroutine MIXER3 for this unit and calculate values for stream (9). This completes the simulation and SEPSIM calls the RPRINT subroutine which prints out the simulation results.

There is one final operation of the executive which needs a brief discussion. This is the way in which the appropriate subroutine is called for each process unit. The process matrix contains the model name as shown in the third column in Figure 6-1. Just after the matrix is read in by SEPSIM, the last three alpha numberic characters in the model name are compared with the vector NAME established by the NØMEN subroutine. Each element in NAME is indexed with an integer J. When the last characters of the model name in the process matrix correspond to an element in NAME, SEPSIM replaces the subroutine name in the process matrix by J. When a new line of the process matrix is called in during calculations, NDX, the index in the subroutine SELECT is set equal to J in column 3 of the matrix. The proper subroutine for calculation is brought in by a call to the subroutine SELECT(NDX) (see Figure 6-2).

6.4 NØMEN and SELECT Subroutines

The purpose of these subroutines in SEPSIM is to permit different sets of names to be used for models in the subroutine library without rewriting the executive. A change of names requires only changes

in SELECT and NØMEN.

NØMEN has a simple function. It takes the list of model names, splits out the last three characters in the name and stores these in a vector NAME(J). This vector is used by the mainline program to set up the model calling sequence as we discussed at the end of the previous section. A second vector NAME2(J) is also formed from the remainder of the model name. This vector is used only when the computer results are printed out.

Although a NØMEN version was used in the Workshop, it has now been replaced by a BLØCK DATA statement attached to SELECT in what we call the "Standard Version" of SEPSIM. The statement performs the same function as NØMEN but uses a different technique. You can refer to Appendix A - "User's Manual for SEPSIM" - to see how this is done. To use another set of names, a new BLØCK DATA statement must be prepared.

SELECT consists of a series of CALL statements for the models forming the SEPSIM subroutine library. These are selected through a GO TO statement controlled through the index NDX. For example, if NDX is 4, the subroutine named ACSLD1 will be called. ACSLD1 usually designates a model for an activated sludge aerator. As discussed, NDX is set equal to J after a line of the process matrix is read in during the calculation sequence. It is established then by the process matrix befor SELECT is called. After a subroutine has been called and executed, control returns to the mainline program from SELECT.

Names of models can be changed quite simply by replacing the CALL statement with statements bearing the new names.

The presence of CALL statements containing subroutine names in SELECT means for most compilers that the subroutines named must be included when the program is compiled into machine language. This is rather awkward and the normal practice is to put in one line dummy subroutines for those which will not be used in a SEPSIM application. A typical dummy would be:

```
      SUBRØUTINE UNAME1
C     THIS IS A DUMMY SUBRØUTINE AND MUST BE REPLACED
C     BY A LIBRARY MØDEL WHEN UNAME1 IS USED
      RETURN
      END.
```

6.5 RPRINT Subroutine

The subroutine RPRINT has the single function of printing out the results of a simulation or a design run. Splitting this task out from the mainline program permits a user to change the print-out without substantially altering SEPSIM. The user, if he wishes, can choose the information, the print-out format and labeling that he feels is appropriate to his job. However, it is not necessary for a user to write his own printing subroutine. The RPRINT currently part of SEPSIM prints out the compositions and flows in all streams. It also gives the parameters associated with all the units in the process and it prints the process matrix for the system as well. All entries can be labeled, mostly by abbreviations. If the user wishes, the print-out can include a list of definitions which interpret the abbreviations. Table 6-2 shows the information printed and its order in the RPRINT subroutine.

The labeling of the SN vector entries (Table 6-2) is achieved by reading in the abbreviation for each of the variables as part of the data for each SEPSIM run. The table explaining the abbreviations is obtained in the same way. The abbreviations used to label model parameters or design results, however, are part of the model in the subroutine library. Although RPRINT permits bypassing most of the labeling, this is a poor practice. Labeling is essential if the print-out is to be passed on someone who is unfamiliar with SEPSIM or if print-out is retained for record purposes.

As Table 6-2 shows, RPRINT is called by SEPSIM after the last row in the process matrix has been executed and all recycle calculations have converged. The subroutine, therefore, only functions for successful runs. When a run is terminated through faulty data, a message is printed out through the mainline program.

TABLE 6-2. RPRINT STRUCTURE

TITLE AND RUN NUMBER

INPUT PROCESS MATRIX

Loop No. Eqp't. No. Loop Indicator Input Streams Output Streams

VARIABLE DEFINITIONS

List prepared by user and submitted as data for each SEPSIM run. The list can have no entries or can have any number of entries.

OUTPUT EQUIPMENT PARAMETERS MATRIX

Process No.

For each unit a list containing a 4 character abbreviation for the parameter and the value can be printed. If the user wishes to dispense with abbreviations, only the parameter values will be printed.

ADDITIONAL EQUIPMENT PARAMETER MATRIX

Just values of the parameters are printed for each process unit.

RESULTS STREAM VARIABLES MATRIX

Stream No.

An abbreviation for each variable and its value are printed out for each stream in the process matrix.

6.6 Use of SEPSIM

You do not need to understand how the Executive operates to carry out simulation or design with SEPSIM. If models are available, all you need to know is how to form the process matrix and how the input data must be structured. We will consider formulating the process matrix now. The next section treats input data. Further details are contained in Appendix A.

To illustrate formulation of the process matrix, we will use Figure 4-6. This was the flow sheet used as an example for network decomposition. Notice that the flow sheet contains chain units, a single primary loop and two coupled recycle loops. Coupled loops, unfortunately, cannot be handled by SEPSIM's simple logic. Only nested loops can be dealt with.

The first task in preparing a system for a SEPSIM study is to inspect the process flow sheet. The type of recycle loops must be identified. Chain units outside of loops should be noted as well. Where coupled loops occur, the flow sheet must be converted to an equivalent nested structure. Fortunately, conversion is usually simple. Introducing into the flow sheet "dummy" units which do not change flow or composition and "dummy" streams which carry no flow is all that is required. Techniques for obtaining equivalent networks which can be used with SEPSIM are discussed in the "User's Manual", Appendix A.

Suppose in Figure 4-6 we introduce a fictitious splitter in stream (6) between units 5 and 6. This unit will be joined to a fictitious mixing junction by line (15) which accepts stream (9) from unit 4. Figure 6-3 shows the introduction of these units and streams. It is equivalent to the system shown in Figure 4-6 because these fictitious units change no flows or compositions. To achieve this means that we must model the fictitious splitter, unit 9, so that all of stream (6) goes into stream (14). Stream (15) contains no flow so stream (16) = stream (9). What we have accomplished is to convert the coupled loops embracing units 2 to 5 into a nested loop containing units 3, 4, 5 and a primary loop made up of units 2 to 5, 9 and 10.

The process matrix for Figure 6-3 appears in Table 6-3. Notice that our ordering of the process units prescribes a calculation order: unit 1, nested recycle loops embracing units 2 to 10, primary recycle loop embracing units 7 and 8, and finally unit 6. Since the branches containing units 7 and 8 and unit 6 are chained, the order is not important. Unit 6 could be inserted before 7 and 8. Setting III = 2, K = 0 for units 1 and 6 indicates that they are not part of any loop and may be calculated directly. K = 1 delineates a primary loop stretching from unit 2 to unit 10. The III = 1 for unit 10 indicates the end of this loop. K = 2 now delineates a nested loop, while we can see that K = 3 gives the extent of a separate primary loop. We have used a set of permissable, but non specific SEPSIM subroutine names for the model names in Table 6-3 with the exception of MIXER3 which is the junction model name. The first group of associated streams are input streams to

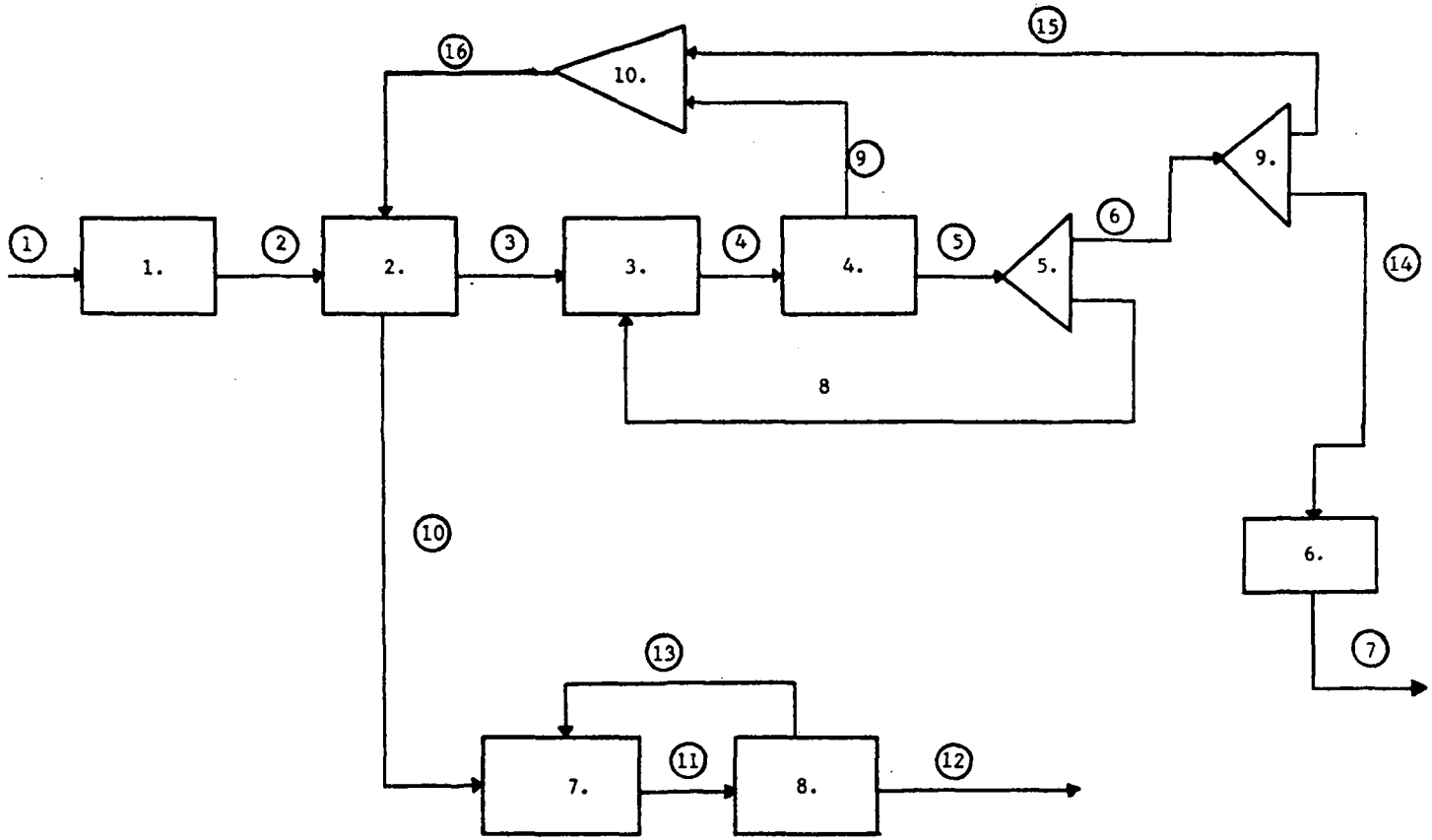


FIGURE 6-3. "FICTITIOUS" FLOW SHEET FOR SEPSIM USE OF THE PROCESS OF FIGURE 4-6

the unit, while the second group are output ones. There is no way of telling from the matrix that stream 15 is fictitious or that units 9 and 10 are dummy units.

TABLE 6-3 SEPSIM PROCESS MATRIX FOR ILLUSTRATIVE EXAMPLE (FIGURE 6-3)

K	Equipment No.	Model Name	III	Associated Streams
-	1	UNAMEO*	2	1 - - - - 2 - - - -
1	2	UNAME1	0	2 15 - - - 3 10 - - -
2	3	UNAME2	0	3 8 - - - 4 - - - -
-	4	UNAME3	0	4 - - - - 5 9 - - -
2	5	MIXER3**	0	5 - - - - 6 8 - - -
-	9	MIXER3	0	6 - - - - 14 15 - - -
1	10	MIXER3	1	9 15 - - - 16 - - - -
3	7	UNAME4	0	10 13 - - - 11 - - - -
3	8	UNAME5	1	11 - - - - 12 13 - - -
-	6	UNAME6	2	14 - - - - 7 - - - -
99				

* UNAMEO, etc. are SEPSIM subroutine names for arbitrary process units

** MIXER3 is the SEPSIM subroutine name for splitting and mixing junctions

6.7 Input Data For SEPSIM

In common with most executive programs, SEPSIM is designed to use general models for process units. These models are adapted to specific units in a simulation or a design through the model parameters. Parameters for models are placed in an array called the EN matrix in SEPSIM. Each unit in the process with the exception of "DUMMY" units is represented by a row in the matrix. The first element in the row contains the number of the process unit as given in the process matrix. The maximum "length" of the row, that is, the number of elements is usually 20 so up to a maximum of 19 parameters may be used in a model.

The user must supply as input to the EN matrix the parameters necessary for the model to function. These are normally constants or exponents in mathematical functions. In a simulation, they would also be sizes of equipment, while for design the parameters could be design criteria. The EN matrix can also be used to store results calculated by the model. For example, in a simulation, the performance of the unit could be calculated by a library routine and put into an element of the EN row for the unit. The sizes of equipment and/or costs calculated by a design subroutine would be stored in the matrix.

A second array, the AEN matrix is also available in SEPSIM for the somewhat unusual case where a model requires a large number of parameters. A row in this matrix usually will have 40 elements, the first of which is reserved for the unit number. Data tables in which the output is tabulated against input are acceptable models for SEPSIM. An example of such a table would be settling data obtained in a quiescent column, in which suspended solids concentrations are tabulated against time at different depths (see Figure 8-16). The AEN matrix thus permits this type of model to be used. In the "Standard Version", more than one row can be used for the EN vector in place of using the AEN vector.

The third array in SEPSIM contains the flows and/or compositions which characterize all the streams in the process flow sheet. As in the case of the other arrays referred to above, we use the PACER names. Thus, we call the array containing stream information the SN matrix. In this matrix, each row corresponds to a stream in the flow sheet. The first element in the row contains the number of the stream which appears in the process matrix. Fictitious streams used to rearrange the flow sheet into nested recycle loops must be included. Most current versions of SEPSIM permit the "length" of the SN row to be 25 elements. Consequently, up to 24 properties may be used to characterize each stream. Properties such as density, or heat capacity can be used along with flow or composition.

Information which must be fed as input data into the SN matrix are the properties of all the feed streams entering the process. Other rows can be left blank in the input data, although it is often a good practice to enter guessed values. Convergence of the recycle calculation can be significantly speeded up in this way.

Data provided for a run must be exactly organized. "User's Manual for SEPSIM" discusses input data formulation thoroughly, so we will just suggest in this section the structure used by reproducing as Table 6-4 a table from the Manual which shows the organization of the input data deck for a run using the "WATFIV Version" of SEPSIM. The maximum number of cards indicated in groups 4 and 5 in the table depend on the dimensions of the EN and SN matrices. Data organization differs slightly in the "Standard Version" of SEPSIM.

TABLE 6-4. DATA FORMAT FOR SEPSIM (WATFIV VERSION)

1. One card - title in columns 1 - 72

2. One card - 15 - 4 character names of stream vector parameters. Punched with no spaces between names in format 15 A 4.

3. One card - dimension and control parameters in format 8 I 3 and in the same order as in Table 7.

4. Card group - row of SN matrix in format 8 F 10.3 or 8 E 10.3. Rows are required for all streams with known initial values. A row may consist of up to 4 cards. A row with zero components is used to indicate end of the stream input.

5. Card group - row of EN matrix in the same format as above. Rows are required for all process units and a row may consist of 3 cards. The input is ended as above.

6. Card group - row of AEN matrix. Format, repetition, end as above.

7. Card group - EPS vector in 8 F 10.3 or 8 E 10.3 format. No end cards required.

8. Card group - process matrix. Read in as K, NE, subroutine name, III, numbers of 5 input streams, numbers of 5 output streams. Format 2I4, 2X, 2A3, 11I4 - the subroutine name needs at least 4 alphanumeric characters and must be right-adjusted.

9. End of file card - 99 in format I4.

10. One card - number of definitions to be printed. Must be an integer.

11. Card group - definitions of abbreviations and names punched one per card in columns 1-60.

6.8 User Chosen Control Parameters In SEPSIM

There are three groups of control parameters which must be specified by the user to execute a SEPSIM run. The first group delineates the actual storage space used and controls the reading in of data and the printing out of computed results. Members of this group are:

NELMAX - Length of the longest equipment vector. (<20)

NEMAX - Highest equipment number used. (<20)

NSLMAX - Length of stream vector. (<25)

NSMAX - Highest stream number used. (<75)

NOAEN - Length of AEN vector. (<40)

The parentheses show the maximum length of the vectors permitted by the current SEPSIM versions.

In the strictest sense the control parameters are not chosen by the user. They are determined by the system under examination, the information vector used, and the models employed. For example, NELMAX is determined by the model which uses the largest number of parameters. Suppose UNAME1, the model for unit number 2 in Table 6-3, requires 5 parameters such as constants, equipment dimensions, etc., and calculates as the result of a run two additional numbers, such as a percent removal and an operating temperature. UNAME3, however, makes use of or calculates just a total of 5 parameters and the other UNAME and MIXER3 models involve just 3 parameters. The UNAME1 model therefore utilizes the "longest" EN row and it determines NELMAX. NELMAX would be seven plus one or eight because the unit number is part of the vector. If we tried to run a case with NELMAX = 6, the last two elements of the EN row for unit 2 would not be read in to the computer, nor would there be any print-out from these positions even though the UNAME1 subroutine could calculate and store numbers in those positions. With the proper value of 8 for NELMAX, the EN row for unit 5 which uses a 3 parameter MIXER3 model would contain numbers in the first 4 elements, but the remaining 4 would be blank.

The NEMAX parameter controls the number of rows of the EN matrix. Since each unit uses a row in the matrix, if units are numbered continuously from one on, the highest number gives the number of rows and will be NEMAX.

NSLMAX specifies the number of columns in the SN matrix, while NSMAX sets the number of rows. Like NEMAX, it is assumed that the streams are numbered continuously. If this practice is followed, the highest stream number is the number of rows in the SN matrix and will be NSMAX.

The parameters NELMAX and NSLMAX indicate how many computer cards are needed for each row in both the EN and SN matrices. You will see in Table 6-4 that data are entered into these matrices through an 8E10.3 or 8F10.3 format. This means each entry can take up to 10 digits

and each card contains 8 entries. If NELMAX is set at 8, then a row of the EN matrix will fit on one card.

The second group of control parameters has just one member, KSETS. It is used to control print-out from the models in the subroutine library as a tool for "debugging" SEPSIM runs which fail in execution. KSETS has just two values: zero or unity. If a value of unity is assigned, messages encoded in a model subroutine will be printed when the subroutine is executed. A zero assignment suppresses printing.

The third control parameter group in SEPSIM also has just one member, the EPS vector. Accuracy of the calculations on one hand and execution time on the other are controlled by this vector. On each pass through an iterative calculation of output streams from a unit, SEPSIM calculates the fractional change of each variable in the stream vector from its previous value. The absolute value of this fractional change is compared with values in the EPS vector for each variable. If all fractional changes are less than corresponding values in the vector, convergence has occurred.

Usually "coarse" values such as 0.05 are used in early runs while the simulation or design is under study. This means convergence can be obtained after just a few iterative passes and execution time is kept short. Once "debugging" and sensitivity studies are over and higher accuracy is needed, values in the EPS vector may be reduced to 0.005 or 0.001. It is not necessary to use the same value in all elements of the EPS vector, but this is frequently done.

6.9 Subroutine Library and Subroutine Names

A subroutine library, as we have used the term in Chapters 2 and 3, refers to a collection of mathematical models for the units in a process. These models are compatible with a particular executive program. Thus, the SEPSIM subroutine library is a collection of models which can be used with SEPSIM. A small library of about 6 models is currently available at the University of Waterloo[2]. A much larger library specifically for waste treatment processes was developed for the PACER execu-

[2] Silveston, P.L., "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research, 6, 1101 (1972).

tive[3]. Only part of this package has been rewritten for SEPSIM. A waste treatment subroutine library written for the GEMCS executive is described by Hoffman et al. in a paper to appear soon[4]. An extensive library is also able for the E.P.A. preliminary design executive[5]. As we mentioned earlier the library, normally, is not part of an executive. Model subroutines are added to the executives as required for either design or simulation.

Because of the structure of the NØMEN and SELECT subroutines, names of the model subroutine in the SEPSIM library must conform with the list of names contained in these subroutines. The list is given in Table 6-5. Although it is possible to substitute different names, this involves modifying subroutines and we will not do this in the Workshop. The names in the table are appropriate for a wide variety of waste treatment processes, while the UNAME title can be used to cover other types of models. This restriction, therefore, should not be a problem.

---

[3] Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control 69, 686 (1970).

[4] Hoffman, T.W., Woods, D.R., Murphy, K.L. and Norman, J.D., "The Strategy and an Example of Simulation as Applied to a Petroleum Refinery Waste Treatment Process", J.W.P.C.F., accepted for publication.

[5] Smith, R., Eilers, R.G., Hall, E.D., "Executive Digital Computer Program for Preliminary Design of Waste Water Treatment Systems", Water Pollution Control Series WP-20-14, F.W.P.C.A., U.S.D.I. (Washington, D.C.), 1968)

TABLE 6-5. CURRENT SEPSIM SUBROUTINE NAMES

Subroutine Name	Suggested Use	Subroutine Name	Suggested Use
MIXER 3	Junction or Splitter	STRIP	Ammonia Stripper
PRISTL	Primary Clarifier	XCHAN	Ion Exchanger
TRFLTR	Trickling Filter	XCIN	Incinerator
ACSLD1	Activated Sludge Reactor	XTRANS	Reverse Osmosts
ACSLD2	Sludge Holding Vessel	DSTIL1	Distillation
DIGSTR	Digester	FLASH	Flash Distillation
CHLOR	Chlorinator	XTRAC2	Extraction
SECSET	Secondary Clarifier	CRYST	Crystallization
BFLTER	Sand Filter	BLOW2	Compression
VACFL	Vacuum Filter	COOL4	Heat Exchange
MECFIL	Mechanical Filter	REACT1	Reactor
DRYER	Dryer	UNAME0	Arbitrary
THICK	Thickener	UNAME1	Arbitrary
WASHR	Elutriator	UNAME2	Arbitrary
XFLOT	Flotation Tank	UNAME3	Arbitrary
BIOXP	Oxidation Pond	UNAME4	Arbitrary
COAG	Coagulation Contactor	UNAME5	Arbitrary
XFLOC	Flocculation Contactor	UNAME6	Arbitrary
PHCONT	CO_2 Absorber	UNAME7	Arbitrary
ADSORP	Adsorption Column	UNAME8	Arbitrary
DIALS	Dialysis or Electro-dialysis Unit	UNAME9	Arbitrary

7 DEVELOPING A MODEL LIBRARY

The success of a plant simulation or of a design rests upon the adequacy of the models used. If an executive program is employed, the executive may make the task easy or perhaps difficult for the user. It can be thrifty in its demand on the central processor and the storage capacity of the computer or it can be wasteful. Nonetheless, an executive will deliver a simulation or a design. If the models are not correct, however, the design or simulation will be useless. The preparation of satisfactory models lies at the heart of simulation and computer-aided design.

The object of this chapter is to introduce you to the "art" of model development. We will consider what modelling is, classes of models and how they are formulated. Special requirements imposed on modelling by the SEPSIM executive will be dealt with and we will end the chapter by proposing a modelling procedure.

We have intentionally avoided mathematical formulations wherever possible. If you find the treatment too elementary, there are a number of excellent textbooks dealing specifically with the construction of models for process units and systems[1,2,3].

7.1 What Is Modelling?

Models extend from miniature replicas of a process unit to groups of mathematical statements. Here we are concerned only with mathematical models. For these models, modelling is the operation of converting physical observations, concepts, or verbal statements into sets of mathematical statements. Sometimes this is elementary because the verbal statements are in mathematical form. Consider, for example, the type of description which arises in transportation problems. Daily cost of opera-

---

(1) Himmelblau, D.M. and Bischoff, K.B., "Process Analysis and Simulation", John Wiley (New York, 1968)

(2) Himmelblau, D.M., "Process Analysis by Statistical Methods", John Wiley (New York, 1970)

(3) Smith, C.L., Pike, R.W. and Murrill, P.W., "Formulation and Optimization of Mathematical Models", International Textbook Co. (Scranton, Pennsylvania, 1970)

ting a delivery truck consists of fuel at 50¢/gallon with a usage of 20 miles per gallon, wages and benefits for a driver of $24/day, and a distributed maintenance cost of $3/day and 1¢/mile. The daily cost may be written without hesitation as

$$C = 0.50\ (X/20) + 24 + 3 + .01X = .035X + 27 \qquad (7\text{-}1)$$

with X as miles travelled per day. The equation is a simple mathematical model describing the daily cost of a delivery truck.

Models can be more than just equality statements, such as eqn. (7-1), although most of the models we will use in the workshop have this form. Inequality statements do arise, usually in the form of a restraint on one of the variables. Restraints are frequently expressed in a form which is tantamount to a mathematical statement. For the elementary case of the delivery truck cost, the restraint might be that the maximum daily mileage for the truck is 200 miles. This may be written as

$$X \leq 200 \qquad (7\text{-}2)$$

If our model is in the form of a differential equation, boundary or initial conditions will be part of the model. These conditions are often algebraic equality statement. Occasionally, they too can be readily deduced from verbal statements.

There are cases, on the other hand, when the concepts or verbal statements cannot be converted easily or without introducing additional information. For example, a chlorinator in a sewage plant may be described as a section of pipe in which chlorine gas is mixed with liquid secondary effluent leaving a header. After mixing, the stream flows into a tank, emerging midway between walls of the tank and two thirds of the distance from the tank bottom. The liquid in the tank circulates slowly before overflowing into the outfall. A 4" o.d. cast iron pipe is used and the gas enters through a nozzle located midway in the pipe. Only a faint chlorine odor is evident above the tank. Now a model for the chlorinator cannot be written even though the description is fairly detailed. One needs to introduce the reactions of chlorine in water, knowledge of its disinfection action, flow rates, concentrations and temperature changes,

and the like before the model can be formulated (see Chapter 12).

There are few theoretical concepts involved in most modelling except mathematical ones which are necessary when models contain differential or integral equations. The modelling activity depends on stating concepts unambiguously, understanding of physical laws, broad background in physics and chemistry and, in fairness, some physical intuition. Experience is important.

7.2 Model Classification

Models can be grouped according to various but overlapping characteristics set forth in Table 7-1.

TABLE 7-1. MODES OF CLASSIFICATION

1. Treatment of Time
   - Transient
   - Steady-State

2. Character of Physical Knowledge
   - Deterministic
   - Probabilistic
   - Statistical
   - Mixed

3. Level of Internal Detail
   - Microscopic (but excluding Molecular level)
   - Simplified (Averaged) Microscopic
   - Macroscopic

4. Discreteness of Variables
   - Lumped Parameter
   - Distributed Parameter

5. Structure of Relationships
   - Linear
   - Non-linear

6. Mathematical Description
   - (See Figure 7-1)

The first classification in the table is a simple one. Models which allow time to be an independent variable are transient, whereas those which do not are classed as steady state. As time goes to infinity, transient models should give the same behaviour as steady state ones, unless the inputs or boundary conditions vary with time. Transient models are often referred to as dynamic or unsteady state models.

Design and simulation models used for waste treatment have been exclusively steady state until just recently. Transient models are being developed for waste treatment process as interest in starting up biological reactors, process control and system stability continues to grow.

Perhaps the most consequential choice of model class is between deterministic, probabilistic and statistical models. The equation for pressure drop when a fluid flows through a pipe is an example of a deterministic model. Models which are formulated on the bases of heat, mass and momentum balances or through physical relationships are usually deterministic. Probabilistic or statistical models in contrast are characterized by uncertainty. The variables or parameters of the model or its boundary conditions are not precisely known. The model may contain parameters which include a random contribution or which may be described by a frequency distribution. In statistical models, parameters uncertainty is expressed by a probability. For example, the value of γ is $(a \pm b)$ with 95 percent probability, meaning that in the long run the value of γ will be greater than $(a + b)$ or less than $(a - b)$ just 5 percent of the time. Probabilistic models are becoming more popular. Although they are more difficult to develop and to use, they have the advantage that they provide a measure of the confidence we may place on the behaviour shown by the model. Probabilistic models make use of balance and physical relations. Statistical models, on the other hand, do not make use of these relations. Statistical models are often polynomials but they may assume any algebraic form. They may be looked on as compact representation of data which in turn represent the behaviour of the component modelled. Some form of regression analysis will always be the source of statistical models.

In practice we often use mixed models. The structure of the model is deterministic, but because of simplifications or an incomplete

fundamental description, the parameters of the model must be fitted by statistical methods employing experimental data.

By level of internal detail, we mean whether we take into account in formulating a model spatial variation of a variable within a piece of equipment, say a tank, or whether we simplify the picture by taking into account only some of the variation or ultimately simplify it by neglecting all variation and assigning an average value to the variable in the equipment. The first mentioned approach yields a microscopic model. As an example, consider an activated carbon adsorption column such as is now under study as a tertiary treatment technique. A microscopic model would employ expressions for what happens at a point in the column. It would allow for flow around particles in the column, mass transfer of organic matter to the surface of individual carbon particles, and for the rate of adsorption inside the particle. For most process units we do not have sufficient information to construct a microscopic model. They are not encountered in waste treatment.

If we must deal with continuously changing variables, microscopic models are frequently simplified by averaging some of the spatial variations. This provides a class of useful models which are referred to in Table 7-1 as simplified microscopic models. We will encounter this class in Chapter 9 when we model a conventional activated sludge unit in which the substrate and the biomass concentrations change continuously down the tank. Both microscopic and simplified models are distributed parameter models. This is a classification which simply says one of the variables is changing along at least one of the coordinate directions.

The bulk of the models used in describing waste treatment process units are macroscopic. Consequently, this is the model we will encounter most frequently in subsequent chapters. A variable is either assumed to have no spatial variation in a macroscopic model or we assume the behaviour is adequately represented by using a spatial average for the variable. A completely stirred tank exemplifies a unit in which concentration or indeed any property is uniform throughout.

Just as a "distributed parameter model" refers to a mathematical description in which variables vary spatially, its converse, a "lumped

parameter model", refers to a description where there is no spatial variation. Macroscopic models, therefore, are all "lumped parameter models".

We are interested in distinguishing between linear and nonlinear models simply because linear models are much easier to manipulate.

Many models are nonlinear. The widely used Monod equation (see Chapter 9) which relates the rate of cell growth (R_X) to the concentrations of cells (X) and of substrate (S),

$$R_X = \frac{\mu S X}{k_m + S} \tag{7-3}$$

is a good example of a nonlinear model. A plot of R_X vs. S is parabolic. Furthermore X may vary as well as S.

The last classification in Table 7-1 is a mathematical one employing the class of equations which arise in forming the model[1]. Mathematical classes are shown in Figure 7-1 and the related classifications according to Table 7-1 are shown in parentheses in the figure.

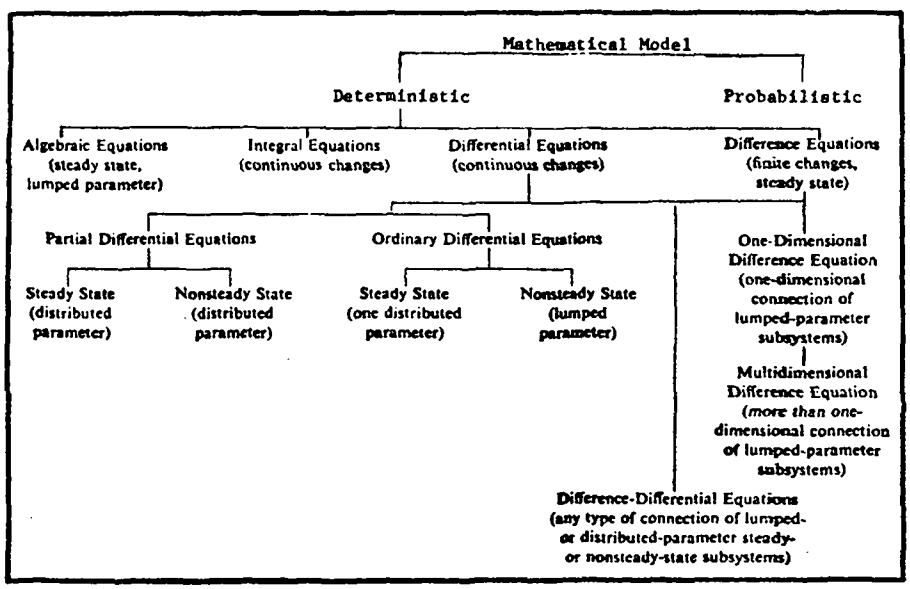


FIGURE 7-1. CLASSIFICATION BASED ON MATHEMATICAL STRUCTURE*

*Figure adapted from Reference (2) with the kind permission of the publisher.

The choice of a model class for a unit will depend upon the information available. If conditions in the unit change with time, the model must fall in the transient class. If we know that continuous variations occur along one coordinate, the model must be of the distributed parameter type. Once the information needed for modelling is assembled, the first task in formulating a model is to select the class. There is little point in choosing a class which will require more information than is readily available.

The complexity of a model and the ease with which it can be used depends upon a model's class. This is an important consideration. It is difficult to illustrate with waste treatment models because they are mostly in the macroscopic/lumped parameter class. We will consider a case from chemical reactor design instead. Consider a reaction of the type $A \rightarrow B$ with a heat of reaction ΔH_r occuring in a fluid following through a tube (tubular reactor). Both temperature (T) and the concentration (c) of A vary spatially in the tube. The velocity v_z varies radially. In the figure that follows, $\bar{D}$ is a dispersion coefficient, $\bar{k}$ is a conductivity, r and z represent the radial and axial coordinates. U and P, S are associated with heat transfer.

The left top hand drawing in Figure 7-2 represents the physical phenomena which would be included in a microscopic model of the reactor (velocity, concentration and temperature profiles, axial and radial dispersion of heat and the chemical species). The microscopic model itself is shown to the right. It consists of two second order partial differential equations coupled through the rate of reaction R which itself is nonlinear $[R = f(c)e^{-E/RT}]$. There are eight boundary conditions. No exact analytical solution exists so the model must be expressed in this way. The output concentration of A can be obtained only by integrating the two simultaneous partial differential equations; a formidable task!

The middle drawing represents a simplification whereby the radial variations are neglected. The model, to the right, is now reduced to two second order ordinary differential equations still coupled by a nonlinear rate term. Only four boundary conditions are required. Output and input can be related only by integration; but integration is consi-

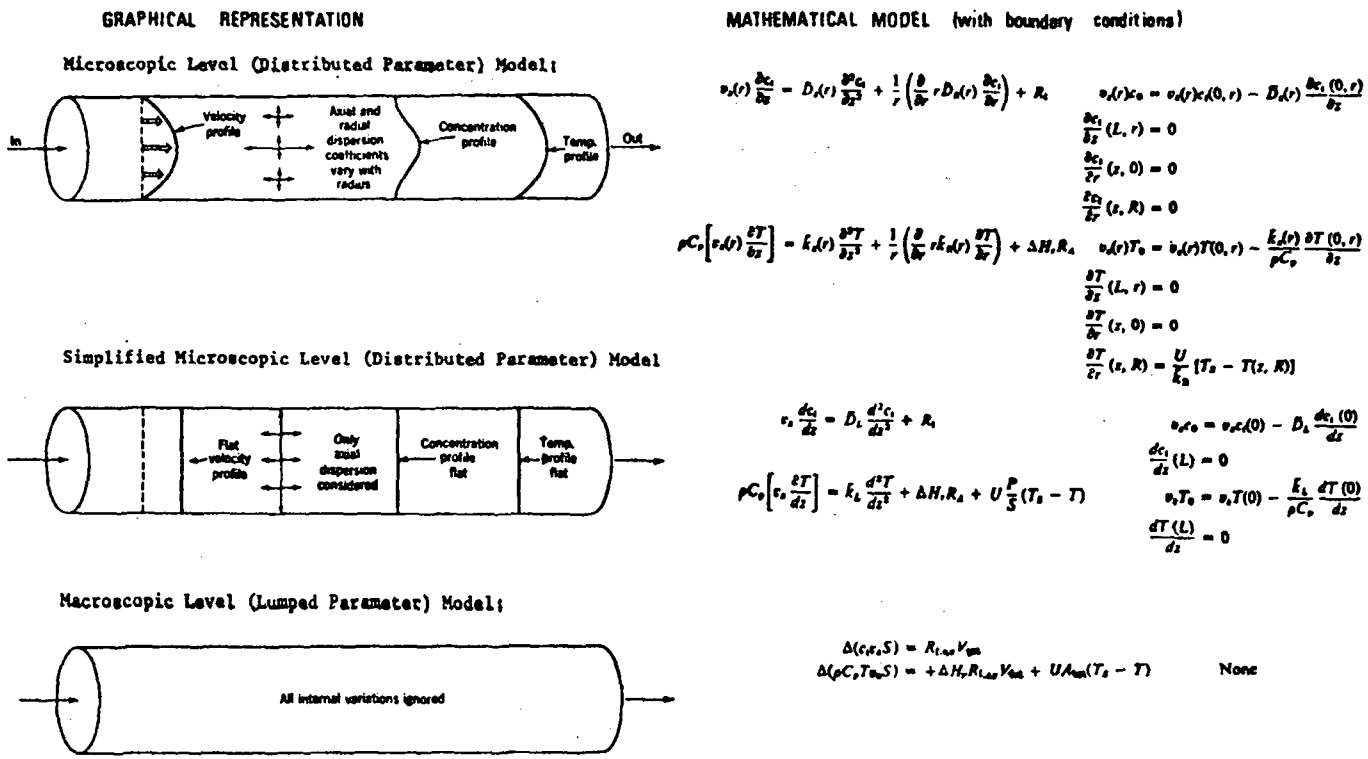


FIGURE 7-2. LEVEL OF DETAIL FOR TUBULAR REACTOR MODEL*

*Adapted from Reference (1) with the kind permission of the publisher.

derably easier to perform.

The bottom left-hand drawing now represents the ultimate simplification - all internal variations are ignored. We have now a lumped parameter system. The model consists of two simultaneous algebraic equations. In some special cases these can be solved to give analytical relations relating the output (of species A, say) to the input. The model is of course very much easier to manipulate than the two just discussed.

In many waste treatment applications the lumped parameter model will be adequate. It is questionable, given the uncertainties associated with the kinetics, cell yields, cell lysis in the activated sludge process, whether a distributed parameter model which requires integration is worth the effort when a lumped parameter model could be adequate. Generalizing, you should choose in modeling the class which results in the simplest model which meets the purposes of the design or simulation undertaking.

We now turn our attention to formulating models. We will consider each of the classes in Table 7-1 important for waste treatment units.

7.3 Mixing Model

A model will be developed for a sludge elutriator to illustrate the formulation of perhaps the simplest type of deterministic, lumped parameter model.

Elutriation is used to reduce the alkalinity of a digested sludge in order to reduce the chemicals required for the subsequent sludge dewatering. It is a simple process; water (often treatment plant effluent) is mixed with the sludge to dilute the liquid phase. The sludge is then allowed to settle and the liquid phase is decanted. The alkalinity of the sludge or rather the liquid remaining in the sludge is thereby reduced. Figure 7-3 illustrates the continuous process.

We note that alkalinity A_{Alk} in mg/l. is neither created nor destroyed in the process. Thus alkalinity entering must leave, so:

$$(A_{Alk})_o \; Q_o + (A_{Alk})_w \; Q_w = (A_{Alk})_e \; Q_e + (A_{Alk})_u \; Q_u \qquad (7\text{-}4)$$

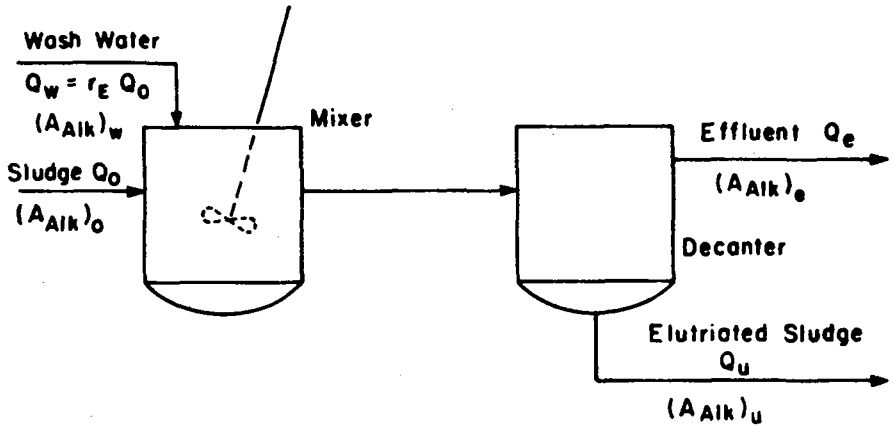


FIGURE 7-3. SCHEMATIC DIAGRAM OF A SLUDGE ELUTRIATOR

Replacing Q_w and noting that if the sludge and water are thoroughly mixed the alkalinity concentration remaining in the sludge must be the same as in the decanted supernatant. So $(A_{Alk})_e = (A_{Alk})_u$ and

$$Q_o \left((A_{Alk})_o + r_E (A_{Alk})_w \right) = (A_{Alk})_e \ (Q_e + Q_u) \qquad (7\text{-}5)$$

where r_E is the ratio of wash water (mgd) to sludge volume (mgd). A water balance

$$Q_o + Q_w = Q_o (1 + r_E) = Q_e + Q_u \qquad (7\text{-}6)$$

was also used to obtain eqn. (7-5). Normally a fraction of the sludge solids (f_E) will be lost to the wash water. By definition,

$$f_E \equiv 1 - \frac{Q_u M_u}{Q_o M_o} \qquad (7\text{-}7)$$

Also the sludge after settling may have a different consistency.

$$y_E \equiv \frac{M_u}{M_o} \qquad (7\text{-}8)$$

defines a factor relating sludge concentration before and after elutria-

tion.

With the definitions of eqns. (7-7) and (7-8), we can find Q_u - the sludge flow after elutriation:

$$Q_u = \frac{1 - f_E}{y_E} \tag{7-9}$$

What we wish to model is the reduction of sludge alkalinity. Consequently we want the alkalinity in the washed sludge as a function of the initial alkalinity and r_E. Equation (7-5) can be solved, using $(A_{Alk})_e = (A_{Alk})_u$, to give

$$(A_{Alk})_u = \frac{(A_{Alk})_o + r_E (A_{Alk})_w}{1 + r_E} \tag{7-10}$$

If we are interested in the suspended solids, M_e, in the wash liquor, it can be found from a sludge solids balance and is

$$M_e = \frac{y_E f_E M_o}{y_E (1 + r_E) + f_E - 1} \tag{7-11}$$

The flow of sludge is given by eqn. (7-9), while the supernatant flow is

$$Q_e = Q_o \left(1 + r_E - \frac{(1 - f_E)}{y_E}\right) \tag{7-12}$$

The set of equations (7-9) to (7-12) provide a complete model for the continuous operation of an elutriator. Figure 7-4 is a FORTRAN version of the model.

Simple models of this class (lumped parameter) can be written for all process units in a sewage plant. They provide a first level of approximation. They are usually easy to manipulate because output is frequently a simple algebraic function of the input.

```
C       IN THIS DEMONSTRATION ALKO = ALKALINITY OF DIGESTED
C       SLUDGE, ALKW = ALKALINITY OF WASH WATER, ALKU =
C       ALKAL. OF ELUTRIATED SLUDGE, RE =
C       VOLUME RATIO OF WASH WATER TO SLUDGE, QO
C       = SLUDGE FLOW RATE, QU = ELUTRIATED SLUDGE
C       FLOW RATE, XMO = SLUDGE CONC'N, XME = SOLIDS CONC'N
C       IN OVERFLOW, YE = THICKENING RATIO, FE = FRACTION OF
C       SLUDGE SOLIDS LOST IN WASHING
C
        READ 1, RE, YE, FE,
      1 FORMAT (3F 5.3)
        READ 2, ALKO, ALKW, QO, XMC
      2 FORMAT (4F W.3)
C
C       CALCULATE ALKALINITY OF ELUTRIATED SLUDGE
        ALKU = (ALKO + RE * ALKW) / (1.0+RE)
C
C       CALCULATE ELUTRIATED SLUDGE
C       FLOW RATE
        QU = QO * (1.0-FE)/YE
C
C       CALCULATE EFFLUENT WASH WATER RATE
        QE = QO * (1.0+RE) - QU
C
C       CALCULATE SOLIDS IN WASH
        XME = (YE * FE *XMC) / (YE*(1.0+RE)+FE-1.0)
C
        PRINT 3, QU, QE, ALKU, XME
      3 FORMAT (4F 20.3)
        END
```

FIGURE 7-4. FORTRAN ELUTRIATOR MODEL

7.4 Macroscopic-Lumped Parameter Models

In this class of model, we are interested only in overall behaviour, not with internal detail.

A blower is an example of a process unit well represented by this model. Figure 7-5 is a schematic drawing of a blower installation. The blower is driven by a motor which supplies energy through a variable speed transmission. The blower has an adiabatic efficiency, η, and an overall efficiency including the motor, η_T. The blower jacket is not cooled.

Gas flow and pressure delivered by a blower depend upon shaft angular velocity (rpm), power delivered by motor W, inlet pressure and temperature. These are then the independent variables describing blower

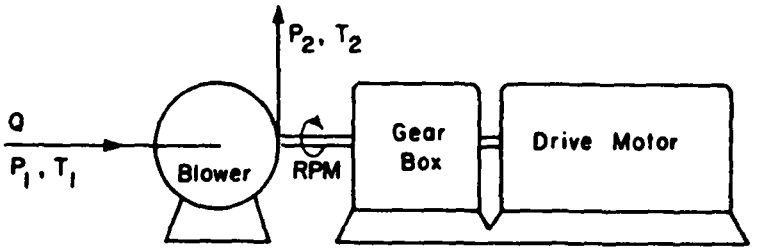


FIGURE 7-5. AIR BLOWER AND DRIVE SYSTEM

operation. Notice that we cannot formulate a model directly from the description in the previous paragraph or the diagram. We must introduce some elementary thermodynamics. Shaft work per unit time in a flow process is

$$W = \int_{p_1}^{p_2} Q \, dp \tag{7-13}$$

where Q = volumetric flow, and p_1 and p_2 are upstream and downstream pressure respectively. Blowers operate over a small pressure change so we can take Q to be independent of p. Integration of the above equation gives the power required to achieve a pressure p_2 for an air flow at the inlet of Q cfm and a pressure of p_1 in psia:

$$W = \frac{4.36 \times 10^{-3} (p_2 - p_1) Q}{\eta_T} \tag{7-14}$$

W is horsepower allowing for the mechanical efficiency η_T.

The effect of shaft speed on performance may be found from the aerodynamics of rotary machinery. If $(p_2)_o$, Q_o represent the pressure developed at a standard flow rate for the design shaft speed ω_o, then theory says that

$$Q/Q_o = \frac{\omega}{\omega_o} \tag{7-15}$$

and

$$p_2/(p_2)_o = \left(\frac{\omega}{\omega_o}\right)^2 \tag{7-16}$$

If the motor used has a fixed power delivery, the effect of changing rpm is

$$p_2 = \left(p_1 + \frac{229\ \eta_\tau W}{Q_o}\right)\ \left(\frac{\omega}{\omega_o}\right)^2 \tag{7-17}$$

and

$$Q = \left(\frac{229\ \eta_\tau W}{(p_2)_o - p_1}\right)\left(\frac{\omega}{\omega_o}\right) \tag{7-18}$$

The temperature rise of the air may be calculated by assuming the gas is compressible in the blower and adding heat generated by the irreversibilities in the blower casing. Thus,

$$T_2 = T_1 \left(\frac{p_2}{p_1}\right)^{\frac{k-1}{k}} + \frac{(1 - \eta)\ W}{\rho \bar{c}_p\ Q} \tag{7-19}$$

where ρ and $\bar{c}_p$ are the inlet gas density and specific heat.

What we have with these equations are a set of explicit equations which give the output of the device as a function of the inputs and the design parameters. This is typical for lumped parameter models and explains, of course, why they are widely used for simulation and design.

Figure 7-6 is a computer program for the blower model.

```
C       FOR THIS EXAMPLE W=WORK OF BLOWER
C       IN HP, Q=GAS FLOW IN CFM, P=PRES
C       SURE IN PSIA, ETA=ADIABATIC EFF.,
C       ETAT= OVERALL EFF. WMEGA= SHAFT
C       RPM. A VARIABLE ENDING IN C MEANS
C       THE VARIABLE REPRESENTS THE DESIGN
C       CONDITION. A VARIABLE ENDING IN I
C       IS AN INLET CONDITION
C
        READ 1,P2O,PI,QO,TI,XK,ETA,ETAT,
         WMEGAO,RHOI,CPI
C
C       CALCULATE HORSEPOWER OF BLOWER
        W=4.36E-03*( P2O-PI )*QO/ETAT
C
```

```
C       CALCULATE TEMP. OF AIR AFTER BLOW
C       ER
        T2=TI*(P2O/PI)**((XK-1.0)/XK) + ((
        1.0-ETA)*W)/(RHOI*CPI*QO)
C
C       CALCULATE EFFECT OF CHANGING SHAFT
C       SPEED
        READ 2, WMEGA
        P2=(PI+(229.0*ETAT*W/QO))*(WMEGA/
        WMEGAO)**2.
        Q=(229.*ETAT*W/(P2/-PI))*(WMEGA/
        WMEGAO)
C
        PRINT3, W,T2,P2,Q
      1 FORMAT (10F10.3)
      2 FORMAT(1F10.3)
      3 FORMAT(4F15.3)
        END
```

FIGURE 7-6. FIGURE BLOWER MODEL

7.5 Distributed Parameter-Simplified Macroscopic Model

Two separate steps normally encountered in model formulation were illustrated by the two previous examples. In the first example we formulated the model by writing material balances, while in the second just physical laws (eqns. (7-13), (7-15) and (7-16)) were used. In many cases, both steps must be used. This is always the case for distributed parameter models. Employing balances and physical laws for distributed parameter models imposes a special requirement. Since the variables are not spatially constant, physical laws must be written for a point in space and balances must be made over differential zones or volumes.

Let us briefly review model formulation. Two choices are open for balances. The first is to choose an appropriate control zone (2 dimensional cases) or volume (3 dimensional cases) and write balances of the form

$$\left\{\begin{matrix}\text{Net}\\ \text{accumulation}\\ \text{in system}\\ \text{volume}\end{matrix}\right\} = \left\{\begin{matrix}\text{Net}\\ \text{transport}\\ \text{in through}\\ \text{system surface}\end{matrix}\right\} - \left\{\begin{matrix}\text{Net transport}\\ \text{out through}\\ \text{system}\\ \text{surface}\end{matrix}\right\} + \left\{\begin{matrix}\text{Net}\\ \text{generation}\\ \text{in system}\\ \text{volume}\end{matrix}\right\} - \left\{\begin{matrix}\text{Net}\\ \text{consumption}\\ \text{in system}\\ \text{volume}\end{matrix}\right\} \tag{7-20}$$

If we have a one or two dimensional system (this happens when the variables vary in one or two coordinate directions), a boundary is used instead of a surface and a zone is used instead of a volume in the above equation. Physical laws are introduced either into the balance and replace any of the terms on the right hand side or they are included as separate relations. Balances may be on molecular species (ammonia) or identifiable components (BOD_5), mass (suspended solids), force (momentum), or energy. Each balance in a distributed parameter model yields an ordinary or partial differential equation.

The second choice is to use detailed general balances available in the literature* and simplify these until they accord to the physical conditions of the unit being modelled and meet the modeling objectives. This alternate route is probably less satisfactory for the mathematically unsophisticated models normally used for waste treatment.

With either procedure, the next step is to devise the boundary conditions for the set of differential equations obtained from balancing. Boundary conditions for many process units may be deduced directly from descriptions of the unit and reflect statements that a variable must have a fixed value at a boundary, or the rate of transport is fixed or that planes of symmetry exist. Boundary conditions are difficult to formulate only when the phenomena are complex or when they are difficult to state verbally. Ordinarily, we will need $\sum_{j=1}^{\ell} O_j$ boundary conditions for each differential equation where O_j is the order of the derivative for the j^{th} independent variable of that equation and ℓ is the number of variables. If we have a hyperbolic partial differential equation in two variables, 2 + 2 or 4 boundary conditions will be needed.

With these preliminary comments, let us now formulate a model for a trickling filter (see Chapter 10).

---

*Tables of balance equations may be found, for example, in reference (1) or in Bird, Stewart, Lightfoot, "Transport Phenomena", Wiley (New York, 1960); Bennett & Myers, "Momentum, Heat and Mass Transfer", McGraw-Hill (New York, 1962); Rosenhow and Choi, "Heat, Mass and Momentum Transport", Prentice Hall (New York, 1963).

Figure 7-7 shows a vertical section taken out of a trickling filter. Composition in a plane perpendicular to this section does not change, so that instead of a three dimensional body we need only consider what happens in the vertical direction, that is along the z axis. The system reduces in this way from a three to a one dimensional one.

We will write a balance on the biodegradable organic matter and we will assume that BOD_5 (mg/l.) measures the concentration of this matter. Our symbol for BOD will be S^*, while X will stand for the weight of active slime per unit filter volume at the point considered. We will assume, however, that X does not vary. BOD removal in mg/volume/time of filter will be, say,

$$R_S = kS^*X \tag{7-21}$$

where k is a rate constant.

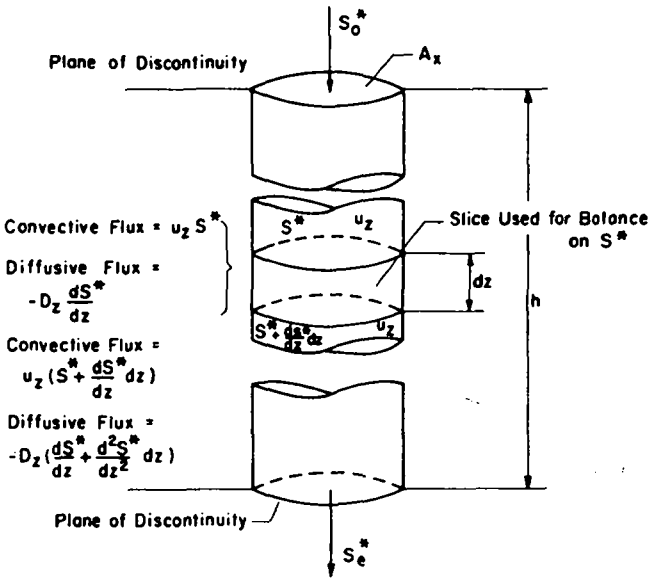


FIGURE 7-7. CONTROL VOLUME AND BOUNDARIES FOR FORMULATING A TRICKLING FILTER MODEL

Consider now the intersection of a plane of thickness dz with the vertical section. A slice is formed with a cross sectional area A_x and a thickness dz. Writing a mass balance on S^* around this slice following eqn. (7-20) for a short time period dt:

$$\frac{\partial(S^* A_x dz)}{\partial t} dt = u_z S^* A_x dt - D_z A_x \frac{\partial S^x}{\partial z} dt -$$

$$(u_z S^* + \frac{\partial(u_z S^*)}{\partial z}) A_x dt - (D_z \frac{\partial S^*}{\partial z} + \frac{\partial}{\partial z}(D_z \frac{\partial S^*}{\partial z}) dz)$$

$$A_x dt - R_S A_x dz dt \qquad (7\text{-}22)$$

Two flux contributions appear in this equation, a diffusive flux (with D_z) and a convective flux (with u_z). If we assume that the velocity, u_z, with which the waste trickles through the slime bed does not change, that the dispersion in the axial direction is invariant, and that the cross section of the vertical section is constant; eqn. (7-22) becomes

$$\frac{\partial S^*}{\partial t} = -u_z \frac{\partial S^*}{\partial z} + D_z \frac{\partial^2 S^*}{\partial z^2} - kS^* X \qquad (7\text{-}23)$$

We consider only steady-state systems in this Workshop so the $\frac{\partial S^*}{\partial t}$ term vanishes and

$$D_z \frac{d^2 S^*}{dz^2} - u_z \frac{dS^*}{dz} - (kX)S^* = 0 \qquad (7\text{-}24)$$

The boundary conditions for this system need careful consideration. There is a plane of discontinuity where the waste stream dribbles onto the top of the filter bed. Below the plane, the waste trickles through bed, mixing occurs and BOD is removed by bacterial action, while above the plane the waste simply drops downward. We must consider the two fluxes below the plane, but only the flow of waste (convective flux) above.

A similar situation occurs at the bottom of the bed where drops and rivulets leave the bed and drop onto the tile collectors. We will distinguish between above the plane and below it by a + and - subscript.

At the top of the filter, a mass balance for S on the infinitesimally thin boundary plane gives

$$(u_z)_+ (S_o^*)_+ = (u_z)_- (S_o^*)_- - D_z \left(\frac{dS^*}{dz}\right)_{o_-} \tag{7-25}$$

This is the boundary condition at $z = 0$.
If $D_z \approx 0$, this reduces to an "initial" condition,

$$S^* = S_o^* \tag{7-26}$$

a form which is quite frequently used.

At the bottom of the bed, a mass balance over the same infinitesimally thin plane gives

$$(u_z)_+ (S_e^*)_+ - D_z \left(\frac{dS}{dz}\right)_{e_+} = u_{z_-} (S_e^*)_- \tag{7-27}$$

Since $\left(\frac{dS}{dz}\right)$ must be negative if it is not zero, eqn. (7-27) means that $S_{e_+}^* < S_{e_-}^*$ or that a jump in concentration must occur. A jump is physically impossible so the current wisdom is to make

$$\left(\frac{dS}{dz}\right)_e = 0 \tag{7-28}$$

and use this as the boundary condition.

The system of equations (7-24), (7-25) and (7-28) is linear as long as X does not vary with z. Integration is possible and gives

$$S_e^*/S_o^* = \frac{4\beta \exp\left[\frac{1}{2} u_z h/D_z\right]}{(1+\beta)^2 \exp\left[\frac{\beta}{2} u_z h/D_z\right] - (1-\beta)^2 \exp\left[\frac{\beta}{2} u_z h/D_z\right]} \tag{7-29}$$

where

$$\beta = (1 + (4 \text{ k X } h/u_z)\ (D_z/u_z h))^{\frac{1}{2}} \qquad (7\text{-}30)$$

If the rate expression involved $(S^*)^n$ where n is neither 1 nor 0 or if X is a function of S^* an analytical solution does not exist. A numerical solution must be employed. Numerically integrating from $z = 0$ to n can give poor results. The integration of this boundary value problem is improved if integration is carried out from $z = h$ to $z = 0$. This is easily arranged by replacing z by $x = h - z$. A change of variables via the chain rule gives

$$D_z \frac{d^2S^*}{dx^2} + u_z \frac{dS^*}{dx} - kXS^* = 0 \qquad (7\text{-}31)$$

The boundary conditions become

$$(u_z)_- (S_o^*)_- = (u_z)_+ (S_o^*)_+ + D_z \left(\frac{dS^*}{dx}\right)_{o_+} \qquad (7\text{-}32)$$

and

$$\frac{dS^*}{dx} = 0 \qquad (7\text{-}33)$$

A variety of methods are available for numerical integration. The 4th order Runge Kutta method is popular. Use of the method requires the reduction of the 2nd order differential equation to first order. Let $S^* = Y_1$ to conform with the variable used in a library subroutine RUK4 (X,Y,H,N, VECTOR). Thus eqn. (7-31) becomes

$$D_z \frac{d^2Y_1}{dx^2} + u_z \frac{dY_1}{dx} - kXY_1 = 0 \qquad (7\text{-}34)$$

If we let

$$\frac{dY_1}{dx} = Y_2 \qquad (7\text{-}35)$$

eqn. (7-34) becomes

$$D_z \frac{dY_2}{dx} + u_z Y_2 - kXY_1 = 0$$

or

$$\frac{dY_2}{dx} = \frac{kXY_1 - u_z Y_2}{D_z} \qquad (7\text{-}36)$$

Thus, we have replaced a 2nd order differential equation (7-34) by two first order ones (eqns. (7-35) and (7-36)). The boundary conditions at $x = 0$ are $Y_1 = S_e^*$, $Y_2 = 0$. Since S_e^* is what we want to find, numerical integration requires a trial and error procedure. We begin by assuming a value of S_e^*. Equations (7-35) and (7-36) are integrated by the RUK4 subroutine to $x = h$. We can now evaluate the right-hand side of eqn. (7-32) which can be rewritten:

$$(S_o^*)_o = Y_1(h) + \frac{D_z}{u_z} Y_2(h) \qquad (7\text{-}37)$$

The zero subscript on S_o^* indicates it is our first guess at S_o^*. The true value of S_o^* is known, so we can augment or decrease S_e^* in the trial procedure and re-integrate until eqn. (7-37) gives the true value of S_o^*.

Figure 7-8 shows a computer listing of a trickling filter model incorporating the RUK4 subroutine.

7.6 Probabilistic Models

Probabilistic models, like deterministic ones, may be either microscopic or macroscopic. The class includes stochastic models which provide results in terms of distributions if the input is given as a distribution. Our example considers the simplest type of probabilistic model that of a residence time distribution.

Before formulating the model, we briefly review the theory.

```
C     IN THIS DEMONSTRATION, SO,SE ARE THE
C     INFLUENT AND EFFLUENT BOD OF
C     THE WASTE STREAM. UZ,DZ ARE SUPERFICIAL
C     VELOCITY OF THE WASTE AND THE
C     DISPERSION COEFF. IN THE FILTER. K AND X ARE A RATE
C     COEFF. AND BIOMASS DENSITY, BOTH CONSTANT.
C
C     INITIALLY SO IS KNOWN, SE IS ASSUMED. SE IS INCREMENTED
C     UNTIL CONVERGENCE WITH SO OBTAINED. IN THE PROGRAM
      Y=S, HT=FILTER HEIGHT, N=NO. OF
C     DEP. VARIABLES. VECTOR CONTAINS THE TWO EQUATIONS IN
C     THE MODEL.
C     ***************************************************************
C     REAL*8 Y(25),W(25),HT,H
      EXTERNAL VECTOR
      N=2
C
C     READ IN INITIAL VALUES OF VELOCITY, DIFFUSIVITY,
C     INITIAL ESTIMATE OF SE(LESS ONE INCREMENT)
C     ACTUAL INFLUENT CONC., SO, KAND X,
      READ10, UZ,DZ,SO,SE,K,X,
    2 SE=SE + 1.0
C
C      INITIALIZE X,Y(1),Y(2) AT BOTTOM BOUNDARY VALUE
C
      X=0.
      Y(1)=SE
      Y(2)=0.
C
C     CALC. NUMBER OF INCREMENTS FOR INTEGRATION
C     BY DIVIDING FILTER LENGTH BY INCREMENT LENGTH
C
      NI=HT/H
      DO 1 I=1,NI
      CALL RUK4(X,Y,W,H,N,VECTOR)
    1 CONTINUE
C
C     CALC. ERROR IN INFLUENT CONC. USING
C     TOP BOUNDARY VALUE
C
      DIFF=UZ*SO-UZ*Y(1)+DZ*Y(2)
C
C     IF ERROR IS WITHIN TOLERANCE, OUTPUT
C     Y(1) IF NOT INCREMENT SE & RECYCLE.
C
      IF (DIFF.LT.0) DIFF=DIFF*(-1.0)
      IF (DIFF.GT.1.0) GO TO 2
      PRINT 20Y(1)
   10 FORMAT(6F10.3)
   20 FORMAT(10H EXIT BOD=,F5.2)
      STOP
      END
C
C
      SUBROUTINE VECTOR (X,Y,EQU,N)
      REAL *8X,Y(25),EQU(25),X
      EQU(1)= |(2)
      EQU(2)=(KXY(1)-UZY(2))/DZ
      RETURN
      END
```

FIGURE 7-8. FORTRAN MODEL FOR A TRICKLING FILTER USING A LIBRARY SUBROUTINE FOR INTEGRATION

We are dealing with counts of entities, for example, microorganisms of a certain size or age. The fraction at a specific age or size can be represented by a frequency distribution function,

$$\text{Fraction between } \gamma \text{ and } \gamma + \gamma\Delta = f(\gamma)\Delta\gamma \qquad (7\text{-}38)$$

If we take a microscopic view, we can write a balance on the fraction at a spatial point allowing for the flow (with velocity u_x) into and out of the differential volume around the point, change at some known rate in the property γ which effects $f(\gamma)$, and the sudden appearance, B, or disappearance, D, of quantities measured by γ (such as the destruction of microorganisms). This balance may be written for a one dimensional microscopic system[1,4,5]:

$$\frac{\partial f(\gamma)}{\partial t} + \frac{\partial}{\partial x}(u_x f(\gamma)) + \frac{\partial}{\partial \gamma}\left(\frac{\partial}{\partial t} f(\gamma)\right) + D - B = 0 \qquad (7\text{-}39)$$

For the macroscopic case, the balance becomes

$$\frac{\partial f(\gamma)}{\partial t} + \frac{\partial}{\partial \gamma}\left(\frac{\partial \gamma}{\partial t} f(\gamma)\right) + D - B = \frac{1}{V}\left(Q_o f(\gamma)_o - Q_e f(\gamma)_e\right) \qquad (7\text{-}40)$$

where V is the volume under consideration.

The distribution function $f(\gamma)$ can be replaced by a moment of the distribution[4]. This is usually undertaken because the moments of the distribution are often directly related to important properties such as the biological activity of a microorganism colony. See Himmelblau and Bischoff[1] for a compact summary of the technique which they refer to as the population balance technique.

For our example, we will model the steady state performance of

---

[4] H. M. Hulburt and S. Katz, Chem. Eng. Sci., 19, 555 (1964)

[5] A. D. Randolph, Can. J. of Chem. Eng. 42, 280 (1964)

a rotating disc contactor (see Chapter 10). We assume that the movement of the discs stirs the waste and that the slime layer on all discs is uniform and constant. The rate of removal of biodegradable organic matter by the slime can be represented just as in the previous example by $R_S = kXS^*$ where S^* is again BOD_5, X is the active slime mass/volume of the contactor, and k is a rate constant. If the contactor is filled initially with waste of BOD level S_o^* and no further waste is added or effluent removed, the reduction of BOD in the contactor will be given by

$$\frac{dS^*}{dt} + kXS^* = 0 \tag{7-41}$$

If X does not change with time, the solution of this equation is

$$S^*/S_o^* = e^{-kXt} \tag{7-42}$$

where t is the time the waste is subject to the action of the slime.

Neither eqns. (7-39) nor (7-40) are useful with residence time distributions. However, if Y represents the time a minute amount of the waste stream remains in the disc contactor, the function $f(Y)$ describes the distribution of residence times in the contactor for the fluid leaving the vessel at any instant. The function is known as a residence time distribution. It is usually represented by $E(t)$. The t in the function has the meaning of Y above. It is a <u>residence time</u>. It is a distributed variable and has a most probable value. Viewing t as a "random" variable, $E(t)$ may be thought of as a probability density function. Thus, $E(t)$ is the probability that a minute, identifiable volume of waste emerging from the contactor resided in that vessel for a time between t and $t + \Delta t$.

The reduction in BOD of the waste is also a function of "residence" time according to eqn. (7-42). Since both the BOD reduction equation and $E(t)$ hold for linear systems, superposition applies. Consequently, if BOD reduction occurs while the waste flows through the disc contactor, the expected value theorem can be used to predict the effluent level S_e^* if the contactor operates continuously. For this

application, the theorem can be written as

$$S_e^* = \int_o^\infty S^* E(t)\, dt \qquad (7\text{-}43)$$

where S^* is given by eqn. (7-42).

Residence time distributions are usually measured by tracer techniques (see Himmelblau and Bischoff[1], for example). Expressions are available for some idealized systems, however. If the disc contactor can be represented by two equally sized, completely stirred tanks in series,

$$E(t) = 4\bar{t} \exp(-2t/\bar{t}) \qquad (7\text{-}44)$$

where $\bar{t}$ = mean residence time = $\int_o^\infty t\, E(t)\, dt$.

Equation (7-43) becomes

$$S_e^* = 4S_o^* \int_o^\infty \bar{t}\, e^{-(2t/\bar{t} + kXt)} dt \qquad (7\text{-}45)$$

Integration gives

$$S_e^* = \frac{S_o^*}{(\frac{kX\bar{t}}{2} + 1)^2} \qquad (7\text{-}46)$$

Our probabilistic model, eqn. (7-43), may be formulated without any reference to the expected value theorem by considering the flow through the contactor to consist of microscopic "batches" of fluid. In each minute "batch", bio oxidation following eqn. (7-42) occurs. Consequently, when each "batch" emerges from the contactor it will have a concentration $S^*(t)$ where t is the time the "batch" spent in the contactor. To obtain the mean concentration in the outlet we sum over all batches. Now, if $E(t)\Delta t$ is the fraction of batches which spend a time t in the contactor, clearly,

$$S_e^* = \sum_{t=0}^{\infty} S^*(t)\, E(t)\, \Delta t \qquad (7\text{-}47)$$

A linear reaction rate expression has been used so far. Equations (7-43) or (7-46), however, can be used with other kinetics, for instance the Monod equation. In such cases, the model becomes an approximation whose accuracy depends on how intimately the fluid in the contactor is mixed. If the mixing is slow so the fluid is not well mixed, eqns. (7-43) or (7-47) can give quite good approximations of S_e^*.

Figure 7-9 is a computer program of a model based on eqn. (7-47). We assume that laboratory measurements have established S^* vs. t under the conditions at which the prototype unit will operate. Tracer measurements on the prototype have been taken. They have been calculated as $E(\theta)$ vs. θ where θ is a dimensionless residence time t/τ. τ is the detention time in the tracer study. Residence time data is often handled this way because $E(\theta)$ is much less dependent on flow rate than is $E(t)$. The relation between the two expressions is

$$E(\theta) = \tau\, E(t) \qquad (7\text{-}48)$$

```
C     IN THIS EXAMPLE, SO IS INLET BOD
C     OF WASTE, S(TP) ARE BOD LEVELS
C     MEASURED IN A BATCH UNIT AT TIMES
C     TP,TAU IS DETENTION TIME, ET IS
C     EXIT AGE DIST., ETHETA IS DIMENSIO
C     NLESS DIST. AND THETA IS DIMENSION
C     LESS TIME. THE SPACING OF S AND THE-
C     TA ARE DIFFERENT SO INTERPOLATION
C     IS USED.
C
      READ 1, T(J),S(J)
      READ 1 (I),ETHETA(J)
      READ2 DELT,TAU,N,NE
C
C     INIALIZE FOR INTEGRATION
      SE = 0.0
      DO 20 I = 1,N
C     CALCULATE DIMENSIONLESS TIME
      THETA=TAU*ETHETA(I)
C     LOOK UP PROPER BOD VALUE
      DO 10 J== 1,NE
      IF (TP(J).GE.T(I)) GO TO 15
```

```
   10 CONTINUE
   15 DIFF1 = TP(J) - TP(J-1)
      DIFF2 = TP(J) -T(I)
      DIFF3 = S(J)-S(J-1)
      S= S(J)- DIFF1*DIFF2/DIFF3
C     AUGMENT SUM
   20 SE=SE + DELT*THETA*S
      PRINT3, SE
    1 FORMAT(2F10.3)
    2 FORMAT(2F10.3,2I3)
    3 FORMAT(1F10.3)
      END
```

FIGURE 7-9. FORTRAN VERSION OF A PROBABILISTIC MODEL FOR A BIOLOGICAL OXIDATION UNIT

7.7 Statistical Models

For our final example, we return to a very simple and frequently used model class. Statistical models are employed where the physical phenomena are so complex that other classes of models become too difficult or too costly to formulate. This class of model may be suitable also where there is an ill-defined random behaviour which may obscure or partially obscure any deterministic pattern.

Statistical models are formulated by fitting a data set representing the behaviour of the process unit by an algebraic expression containing one or more coefficients. Typical expressions are linear:

$$y = ax + b \tag{7-49}$$

One dimensional polynomial:

$$y = a_1 + a_2x + a_3x^2 + ... + a_nx^n \tag{7-50}$$

or where there are more than one independent variables, multidimensional polynomial:

$$y = A + a_2x + ... + a_nx^n + b_2w ..+ b_mw^m + c_2z + ... + c_\ell z^\ell$$

$$+ d_2xw + ... + d_px^nw^m + e_2xz + ..+ e_qx^nz^\ell + f_2wz +$$

$$..+f_r w^m z^\ell \qquad (7\text{-}51)$$

Frequently the data will be transformed so that one of the three expressions apply.

Problems encountered while using statistical models are the selection of the variables which should be included in the model and the evaluation of exponents and coefficients. Highly sophisticated techniques are available to solve these problems if required. Linear least squares routines may be used to obtain the coefficients for eqn. (7-49). By redefining terms to a power as new variables, that is, $v = x^2$, this simple technique can also be used for eqn. (7-50). Stepwise multiple regression methods, however, must be used for eqn. (7-51). A wide variety of techniques exist; space and time limitations do not permit even a cursory treatment. Himmelblau's "Process Analysis by Statistical Methods"[2] provides an excellent discussion of procedures in a way which facilitates their adoption by users.

A sedimentation basin for clarifying sewage is considered in this example. The A.S.C.E. Manual on Sewage Treatment Plant Design[6] tabulates performance data for 58 full scale rectangular and circular clarifiers. The percent removal of suspended solids is plotted versus the overflow rate as gallons (U.S.)/day/ft^2 of basin surface in the Manual and is reproduced as Figure 7-10. A median curve in the figure shows that removal vs. overflow rate is not linear. Thus a multidimensional polynomial must be used to fit the data. Testing shows that the percent removal, f_R, seems to be an exponential function of the overflow rate, Q/A. We let $y = \log(f_R)$, $x = Q/A$ and take w as a shape variable which assumes the values 1 if the tank is circular, but 0 if the tank is rectangular. The data shown in Figure 7-10 can now be fitted by a simplified form of eqn. (7-51):

$$y = A + a_2 x + b_2 w \qquad (7\text{-}52)$$

---

[6] Manual of Engineering Practice - No. 36, "Sewage Treatment Plant Design", A.S.C.E. (New York, 1959)

Smith[7] has carried out the fit and found that $A = -0.086$ and $a_2 = 3.6 \times 10^{-4}$. The b_2 term was found to be very small; tank shape is not important therefore. The fitting procedure yields,

$$f_R = 0.82\, e^{-Q/2780A} \qquad (7\text{-}53)$$

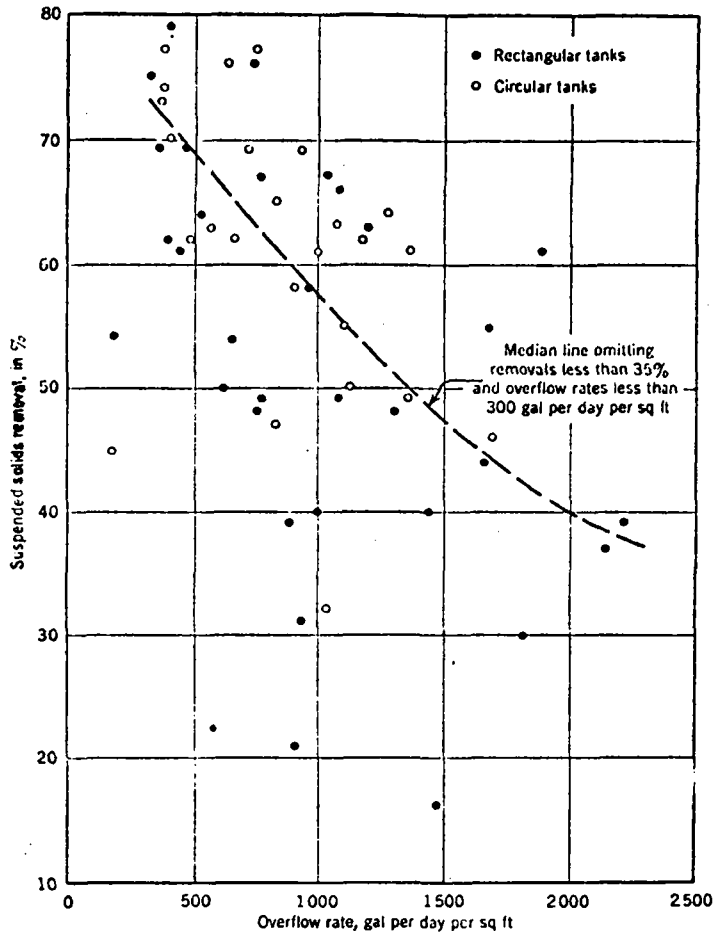


FIGURE 7-10. REPRESENTATION OF SUSPENDED SOLIDS REMOVAL DATA FROM FULL SCALE PLANTS

---

[7] Smith, R. "Preliminary Design and Simulation of Conventional Waste Water Renovation Systems Using the Digital Computer", Water Pollution Control Research Series, WP-20-9, F.W.P.C.A. - U.S.D.I. (Washington, 1968)

7.8 Requirements For A Model Library

We have reviewed to this point model classification and how models in various classes can be formulated. The examples have not been left as mathematical statements; they have been converted into FORTRAN statements so that the models, in principle, could be run on a computer. There are further requirements, however, before the models could be used as part of a model library. We will examine these in a general way first and in the next section go on to see how models must be written for the SEPSIM library.

In Chapter 3 we found that a modularity organized simulation or computer-aided design program is often advantageous. Modularity means, we repeat, that the various operations taking place in simulation or design are contained in separate subroutines. Modularity makes an executive program necessary. In turn the existence of an executive imposes restrictions on models of the library.

Executives invariably have these features:

i) Stream information is stored in a matrix accessible to the subroutines.

ii) Testing for convergence in iterative calculations is done in the executive or a special testing subroutine, but not in a model subroutine.

iii) Printing is done by the executive or a special subroutine except during debugging.

iv) Control of the calculations including termination if necessary should reside with the executive program.

v) Parameters for the models are stored in a matrix accessible to the subroutines.

The last feature is important in modelling because it permits generality. For example, a single model can be used to represent two sizes of the same type of equipment or the same piece of equipment handling streams of different compositions.

For models, the consequence of these features are:

i) Information needed for calculations in a model subroutine must be taken from an array whose structure is constant and

whose name is imposed by the executive (in SEPSIM, the array name is STRMI).

ii) Results of calculations of flows and compositions must be transferred to an array similar to that in i) (this array is STRMØ in SEPSIM).

iii) Parameters for a model must be drawn from a list named as specified by the executive. Parameters calculated must be transferred to the same list (the list is called EN in SEPSIM).

iv) Overflows caused by division by zero which will stop a computer run must be prevented.

v) Model subroutines should contain PRINT statements which will assist debugging.

vi) Model subroutine should be written as generally as possible making maximum use of the separate parameter input.

vii) Model subroutines should be adequately documented through comment cards so they can be readily adopted to other equipment of a similar type.

7.9 Requirements For The SEPSIM Model Library

Items i) to iii) must be followed in SEPSIM model libraries; the remaining items are good practice. Stream information in SEPSIM is stored in an array called SN. The columns in the array reflect the structure of the information list for streams chosen beforehand as discussed in Chapter 5. Each row corresponds to a stream in the process matrix. Through a COMMON statement SN is made accessible to all the model subroutines if it is necessary to draw or replace information directly in the array. However, the Executive as part of its subroutine calling procedure transfers all rows of the SN array associated with the unit being calculated to two smaller arrays called the STRMI and STRMØ arrays. The purpose of this is to place the stream information into the proper lists used by the unit calculation. It makes the model independent of the process flow sheet. A model subroutine must be written to use the STRMI array.

Stream information calculated by the subroutine is returned to

the SN array through the STRMØ array to keep the model independent of the flow sheet and to facilitate testing for convergence as discussed in the previous chapter. Both transfer procedures are illustrated in Figure 7-11.

	K	NR	NAME	III	INPUT STREAMS	OUTPUT STREAMS
Sample Row of Process Matrix:	0	6	WASHR	0	11 12 0 0 0	13 14 0 0 0

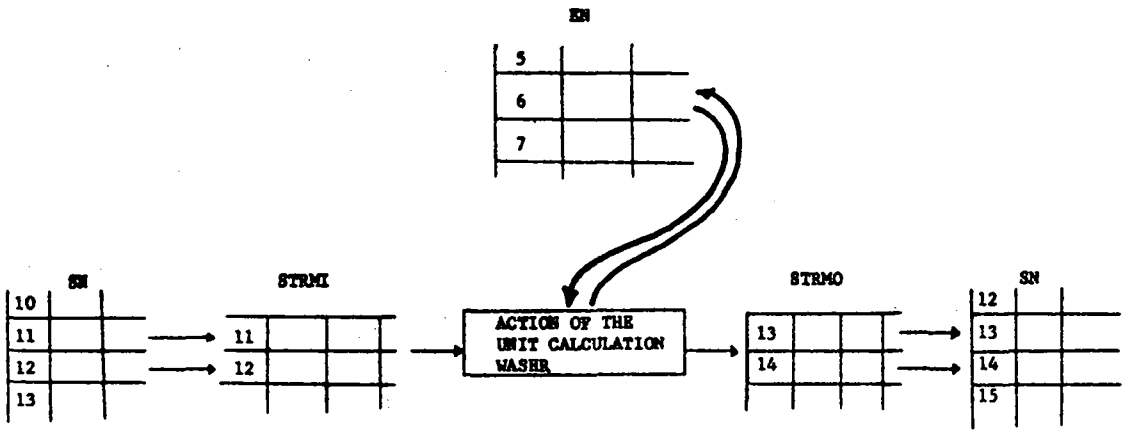


FIGURE 7-11. TRANSFER OF STREAM INFORMATION AND MODEL PARAMETERS

SEPSIM labrary programs must use the variable designation STRMI (I,J) for all members of the stream vector for each inlet stream and the designation STRMØ (I,J) for the same member for each outlet stream.

In the elutriator model (Figure 7-4), the Fortran for the change in alkalinity was

$$ALKU = (ALK\emptyset + RE * ALKW)/(1.0 + RE) \qquad (7\text{-}54)$$

Designating the sludge as the first stream entering or leaving the elutriator (I = 1) and the wash water as the second stream (I = 2) and assuming that alkalinity is stored in the fifth column of the SN matrix, the equivalent SEPSIM statement would be

$$STRM\emptyset\ (1,5) = (STRMI(1,5) + RE * STRMI(2,5))/(1.0 + RE) \qquad (7\text{-}55)$$

If flow rate is stored in the 3rd column of the SN array, the statement fixing the sludge flow rate

$$QU = Q\emptyset * (1.0 - FE)/YE \tag{7-56}$$

becomes

$$STRM\emptyset(1,3) = STRMI(1,3) * (1.0 - FE)/YE \tag{7-57}$$

Figure 7-12 shows a SEPSIM version of the elutriator model using the STRMI, STRMØ variable names.

Parameters used in the subroutines are stored in SEPSIM in an array called the equipment parameters array and designated EN in the program. Since each unit has just one row of this array associated with it, numbers stored in the array can be transferred directly to the subroutine. Direct transfer is illustrated schematically in Figure 7-11.

Using an EN element to designate the parameter RE used in Figure 7-4, eqn. (7-54) becomes

$$ALKU = (ALK\emptyset + EN(NE,3) * ALKW)/(1.0 + EN(NE,3)) \tag{7-58}$$

The EN term means RE has been stored in the third column of the row in the EN array reserved for the elutriator through the number NE. The alkalinity change can be written entirely in terms of EN, STRMØ, STRMI as

$$STRM\emptyset(1,5) = (STRMI(1,5) + EN(NE,3) * STRMI(2,5))/(1.0 + EN(NE,3)) \tag{7-59}$$

If YE is stored in the fourth column and FE in the fifth, eqn. (7-56) becomes

$$QU = Q\emptyset * (1.0 - EN(NE,5))/EN(NE,4) \tag{7-60}$$

Equation (7-57) appears as

$$STRM\emptyset(1,3) = STRMI(1,3) * (1.0 - EN(NE,5))/EN(NE,4) \tag{7-61}$$

```
      SUBROUTINE WASHR
C     THIS SUBROUTINE MODELS AN ELUTRIA-
C     TOR FOR DIGESTED SLUDGES. SLUDGE IS
C     MIXED WITH WATER, SETTLED AND WATER DECANTED.
C     IN THE MODEL RE IS THE VOLUME RATIO
C     OF WASHWATER TO SLUDGE, YE IS THE
C     RATIO OF SLUDGE % PERCENT SOLIDS
C     BEFORE AND AFTER WASHING AND FE IS
C     THE FRACTION OF SOLIDS LOST TO THE
C     WASH
C
C     THE FIRST INPUT AND OUTPUT STREAMS
C     ARE SLUDGES
C
C     A SPECIAL STREAM VECTOR IS USED
C     ***************************************************************
C     1. STREAM NO.
C     2.
C     3. FLOW (MGD)
C     4. SUSP. SOLIDS (MG/L)
C     5. DISSOLVED BOD
C     6. ALKALINITY
C     ***************************************************************
C
C     THE EN VECTOR
C     ***************************************************************
C     1. EQUIPM'T NO. 6. VOLUME   CU FT
C     2. COST CLASS
C     3. RE
C     4. YE
C     5. FE
C     ***************************************************************
C
C     COMMON AND DIMENSION STATEMENTS MISSING
C
C     DEBUG PRINTOUT
      IF (KSETS) 50,50,60
   60 PRINT 70, NE
   70 FORMAT(10X18H CALL. REACHED WASHR,
     NE=,I4/)
   50 CONTINUE
C
C     CALC.FLOWS
      STRMO(1,3)=STRMI(1,3)*(1.-EN(NE,5)/EN(NE,4))
      STRMO(2,3)=STRMI(1,3)*(1.+EN(NE,3))-STRMO(1,3)
C
C     CALC.SLUDGE SOLIDS
      STRMO(1,4)=STRMI(1,4)*EN(NE,4)
C
C     CALC.SOLIDS IN OVERFLOW
      STRMO(2,4)=EN(NE,4)*EN(NE,5)*STRMI(1,4)/
     1(EN(NE,4)*(1.+EN(NE,3))+EN(NE,5)-1.)
C
C     CALC.ALKALINITY
      STRMO(1,6)=(STRMI(1,6)+EN(NE,3)*STRMI(2,6))
     1/(1.+EN(NE,3))
      STRMO(2,6)=STRMO(1,6)
C
C     DISS.BOD WILL CHANGE PROP. TO ALKALINITY
C     CAL.BOD OF SLUDGE AND WASH
      STRMO(1,5)=STRMI(1,5)*STRMO(1,6)/STRMI(1,6)
      STRMO(2,5)=STRMO(1,5)
C
C     DESIGN SECTION REMOVED FOR BREVITY
C
      RETURN
      END
```

FIGURE 7-12. SEPSIM MODEL LIBRARY SUBROUTINE USING STRMI AND STRMØ VARIABLES AND EN PARAMETERS

Figure 7-12 shows what a model looks like using the SEPSIM convention for information transfer with the Executive directly in the equation statements forming the model. The SEPSIM model shown in the figure is illustrative only. COMMON and DIMENSION statements have been left out and a brief stream vector unlike any we have examined in Chapter 5 is employed to condense the subroutine.

Using the transfer names for parameters and variables in the model makes it very difficult to understand the statements as you can see by looking at Figure 7-12. Interpretation would be utterly hopeless without the commentary provided at the top of Figure 7-12. In vii) of the model requirements we spoke about the necessity of documentation to assist in using a subroutine for more than one unit or for more than in a single design or simulation study. Documentation is necessary also just to understand what the model does. Anyone who has programmed knows that even after just a few weeks of neglect a program will become unintelligible unless documentation is complete. It is important therefore to document all model subroutines to the fullest possible extent.

STRMI, STRMØ, EN are necessary in SEPSIM subroutines for information transfer, but if they are used in model statements they make the programs difficult to understand. Model subroutines for SEPSIM might be better written using conventional symbols for variables and parameters. Translation statements could appear at the beginning and end to relate the variables and parameters used in the statements to the STRMI, STRMØ and EN terms. Figure 7-13 illustrates the structure this leads to.

In Figure 7-14, we have rewritten the elutriator model, Figure 7-4, for the SEPSIM library using the structure shown in Figure 7-13. Compare Figure 7-14 with Figure 7-12. The former is considerably easier to follow. Thus, we recommend that library models should be written using conventional symbols for variables and model parameters. If this is done, it is necessary that SEPSIM model library subroutines must be written with statements taking or adding information to STRMI and STRMØ arrays and the EN list.

Model subroutines should be written so as to anticipate problems. The SEPSIM subroutine WASHR (Figure 7-14) contains a

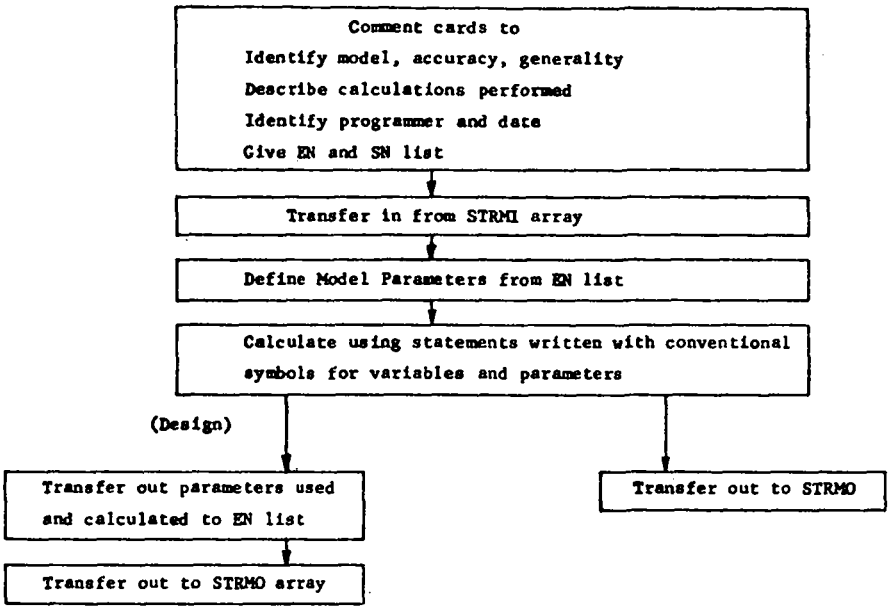


FIGURE 7-13. STRUCTURE OF A SEPSIM LIBRARY PROGRAM USING CONVENTIONAL SYMBOLS IN MODELS*

Debug Printout to indicate if the subroutine was used. This permits the user to follow the progress of a simulation or a design if the program fails to operate. It is a useful "debugging" aid.

```
      SUBRCUTINE WASHR
C     THIS SUBROUTINE MODELS AN ELUTRIA-
C     TOR FOR DIGESTED SLUDGES. SLUDGE IS
C     MIXED WITH WATER, SETTLED AND WATER DECANTED.
C     IN THE MODEL RE IS THE VCLUME RATIO
C     OF WASHWATER TO SLUDGE, YE IS THE
C     RATIC OF SLUDGE % PERCENT SCLIDS
C     BEFORE AND AFTER WASHING AND FE IS
C     THE FRACTION OF SOLIDS LOST TO THE
C     WASH
C
C     THE FIRST INPUT AND OUTPUT STREAMS
C     ARE SLUDGES
C
```

*Figure adapted from Reference (8) with the kind permission of the publisher.

(8) Crowe, C.M., Hamielec, A.E., Hoffman, T.W., Johnson, A.I., Shannon, P.T. and Woods, D.R., "Chemical Plant Simulation", Prentice-Hall (Englewood Cliffs, New Jersey, 1971)

```
C      A SPECIAL STREAM VECTOR IS USED
C      ************************************************
C      1. STREAM NO.
C      2.
C      3. FLOW (MGD)
C      4. SUSP. SOLIDS (MG/L)
C      5. DISSOLVED BOD
C      6. ALKALINITY
C      ************************************************
C
C      THE EN VECTOR
C      ************************************************
C      1. EQUIPM'T NO. 6. VOLUME   CU FT
C      2. COST CLASS
C      3. RE
C      4. YE
C      5. FE
C      ************************************************
C
C      COMMON AND DIMENSION STATEMENTS MISSING
C
C      DEBUG PRINTOUT
       IF (KSETS) 50,50,60
   60  PRINT 70, NE
   70  FORMAT(10X18H CALL. REACHED WASHR,
       NE=,I4/)
   50  CONTINUE
C
C      TRANSFER STREAM INFO.
       QO=STRMI(1,3)
       XMO=STRMI(1,4)
       DBODC=STRMI(1,5)
       ALKC=STRMI(1,6)
       ALKW=STRMI(1,6)
C
C      TRANSFER PARAMETERS
       RE=EN(NE,3)
       YE=EN(NE,4)
       FE=EN(NE,5)
C
C      CALC.FLOWS
       QU = QO * (1.0-FE)/YE
       QE = QO * (1.0+RE) - QU
C
C      CALC.SLUDGE SOLIDS
       XMU=YE*XMO
C
C      CALC.SOLIDS IN OVERFLOW
      XME = (YE * FE *XMO) / (YE*(1.0+RE)+FE-1.0)
C
C      CALC.ALKALINITY
     ALKU = (ALKO + RE * ALKW) / (1.0+RE)
       ALKE=ALKU
```

```
C
C       DISS.BOD WILL CHANGE PROP. TO ALKALINITY
C       CAL.BOD OF SLUDGE AND WASH
        DBODU=DBODO*ALKU/ALKC
        DBODE=DBODU
C
C       TRANSFER STREAM INFO
        STRMC(1,3)=QU
        STRMC(2,3)=QE
        STRMC(1,4)=XMU
        STRMC(2,4)=XME
        STRMC(1,5)=DBODU
        STRMC(2,5)=DBODE
        STRMC(1,6)=ALKU
        STRMC(2,6)=ALKE
C
C       DESIGN SECTION REMOVED FOR BREVITY
C
        RETURN
        END
```

FIGURE 7-14. SEPSIM MODEL LIBRARY SUBROUTINE FOR AN ELUTRIATOR USING CONVENTIONAL SYMBOLS FOR VARIABLES AND PARAMETERS

Item iv) of the list of requirements for library subroutines cautions that division by zero should not occur. This problem arises because in the iterative procedures used by SEPSIM to solve a recycle problem stream variables in a STRMI vector may have zero values. If one of the variables appears as a divisor an "overflow" will occur during computation. This would terminate the computer run. Inspection of Figure 7-14 shows that division by a variable does not occur. Consequently no "protection" statements appear in the subroutine. In the Blower model, Figure 7-6 the statement giving the effect of RPM on delivered pressure does contain a stream variable, the flow rate. Since this variable might take a zero value, a SEPSIM subroutine should provide protection. This is easily accomplished by testing the variable and assigning a suitable value if zero is detected. Figure 7-15 shows the statements which would appear in a subroutine assuming Q (flow rate) is the variable causing concern.

```
C       PREVENT DIVISION BY ZERO
C       Q SPEC IS GUESSED VALUE OF Q AND IS SPECIFIED IN EN LIST
        IF (Q) 80,80,90
   80   Q = Q SPEC
        PRINT 200, Q
  200   FORMAT (10X 34H DIVISION BY ZERO ATTEMPTED
        Q SET =, F10.3)
   90   CONTINUE
```

FIGURE 7-15. OVERFLOW PROTECTION SEQUENCE

Other sources of trouble to look at are substraction of roughly equal number which in an iterative loop could create negative numbers. Negative numbers and zeros will terminate a run if they are used as arguments in logarithmic or square root terms. To avoid trouble later on, models should be examined for execution problems; protection statements and those to assist debugging should be added as necessary.

Item vi) of the requirements list is important, but the other extreme of all too general models should be avoided. Such models can be excessively long and time consuming in execution. Judgment is necessary. Models for a subroutine library should be constructed to be as general as possible commensurate with reasonable length and intended use.

7.10 Procedure For Modelling

Developing or choosing a model is a challenging engineering activity. Although no two modelling jobs will be exactly the same , the four phases shown in Figure 7-16 always occur. Each phase has been subdivided into specific activities. In some jobs one or more of these activities may be very important while others may be handled virtually without thought. Some of the mathematical activities (8., 11., 12. in

Figure 7-16) will be unnecessary for lumped parameter models because of their simplicity.

The procedure outlined in Figure 7-16 assumes a model is to be developed from first principles. However, selecting a model from those given in the literature will be the situation encountered most frequently. The procedure for this situation is not substantially different from that shown in the figure. The definition phase hardly changes. The planning phase, however, becomes a search for different models; their assumptions, strengths and deficiencies. Activities 9. to 12. of the "action" phase are no longer relevent. They are replaced by comparison of possible models to find which most closely meets the selection criteria and determination of what modifications to the chosen model are necessary if indeed any are.

Selection of a model or its development must reflect modelling objectives, the unit being model and the character and reliability of the data that the model is to be used with. Even with these considerations firmly in hand, there is still a good deal of scope for choice. Sophisticated models which are normally more accurate and more general than simpler ones are more costly to develop. They use more computing time; they are more prone to errors, and since they are difficult to understand, they are more likely to be misused. This conflict between accuracy and generality on one side and simplicity and ease of use on the other calls for judgment.

In their pioneering treatment of process simulation[8], Crowe et al. of McMaster University give this question their attention more than once. They conclude that models should be developed sequentially in simulation studies. At first, simple, easily formulated models should be used. These models would be employed in preliminary studies whose purpose is to investigate calculation sequence, computing problems, and convergence requirements, but primarily to determine which process units dominate the behaviour of the simulation. In subsequent work, the early models will be replaced by more sophisticated ones for the key process units. Minor equipment will not require comprehensive models even in the later stages of development. There is little point in using such a model for,

FIGURE 7-16. MODELLING PROCEDURE

Definition Phase

1. Establish need for a model.
2. Frame objectives for modelling (what properties must the model have?)
3. Delineate scope of model (what part of the physical unit is to be modelled?)
4. Frame criteria for judging a successful model.
5. Establish characteristics of unit to be modelled.

Planning Phase

6. Select class of model.
7. Determine additional information needed for modelling.
8. Review of mathematical tools for solution.

Action Phase

9. Decompose unit into sub elements when possible.
10. Formulate mathematical relationships through balance techniques or from application of physical laws.
11. Formulate boundary conditions as in 10.
12. Solve model equations when possible or choose integration or root finding procedure.
13. Evaluate parameters of model from experimental data.
14. Prepare FØRTRAN version.
15. Convert to SEPSIM.

Review Phase

16. Compare model with experimental data
17. Evaluate model accuracy, versatility and execution time.

say, an elutriator if imprecision in its modelling has a negligible effect on the simulation of the whole system.

There is no reason to select or develop just a single model for a type of unit. In most cases it will be convenient to have separate models for design and for simulation. Even just for simulation, models for the same unit can have different applications. In our WATCRAP studies[9] at Waterloo and in South Africa, we had at one time four alternate clarifier models, 3 digester models and 5 aerator models. Once the first model has been developed, the succeeding ones are much easier.

This discussion of the modelling procedure can be closed perhaps best by bringing together in one place the suggestions we have made in different sections of this chapter.

TABLE 7-2. SOME GUIDELINES FOR SEPSIM MODELS OF PROCESS UNITS

1.	Choose the simplest permissible model class for your model appropriate to your objective and the information available.
2.	Document all model subroutines to the fullest possible extent.
3.	Write model subroutines using when possible conventional symbols for model variables and parameters.
4.	SEPSIM model library subroutines must be written with statements taking or adding information to STRMI and STRMØ arrays and the EN list.
5.	Models should be examined for execution problems and protection statements plus statements to assist debugging should be added as necessary.
6.	Models for a subroutine library should be constructed to be as general as possible commensurate with reasonable length and intended use.

[9] Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control 69, No. 6, 686 (1970)

7.11 Preface To Subsequent Chapters

One of the purposes of the Workshop, stated in Chapter 1, was to offer you experience in formulating computer models for either simulation or design. As should be evident from this chapter, models cannot be synthesized out of a vacuum. A good deal of information about how waste treatment units operate, theory of the physical and biological phenomena occuring, and modelling technique should be known before a computer model is attempted. All this information is available in journal articles, symposium proceedings, textbooks or monographs. You may be familiar with some of it from your training and experience. However, to draw the information from the literature, even for those who are versed in waste treatment, is a time consuming task. It is a task far beyond the time available in the Workshop. Thus, in subsequent chapters, we have broached the collecting and organizing job to eliminate as much as possible this step for the models you will prepare in the Workshop.

No apology is needed for the following chapters. They are not intended to be complete discussions of different process units. The information is intended only to suffice for the Workshop. In what follows, many of the statements we make as "truths" are really just generalizations. We do not pretend that the models presented are all that are available, but we hope that they are representative.

The structure of the next six chapters will be about the same. We begin by defining the objective of the process unit. We then consider how it operates as a system and examine the theory of the various phenomena which are thought to occur. Those experienced generally in waste treatment will be able to skip through it hurriedly as it rarely exceeds what is taught in an undergraduate Sanitary Engineering course. Modelling is handled next. We look at models for all important changes which occur in the unit and at mixing phenomena when appropriate. At the end of a chapter we consider models from a design standpoint.

8 CLARIFIER MODELS

Clarifiers are probably the lowest cost units on a $/lb. BOD removed basis in waste treatment systems. They are, nonetheless, the "work horses" of these systems. Two banks of clarifiers are normally part of a treatment plant: primary clarifiers which operate on raw sewage; secondary or final clarifiers which handle the effluent from biological treatment units. The former removes about 60 to 70% of the suspended matter in the sewage and 20 to 30% of the BOD and nutrients present. The final clarifiers determine the level of suspended solids in the treatment plant outfall.

We will consider both primary and final clarifiers in this chapter. We will also examine thickening, a unit less frequently found in municipal sewage plants. Thickening has been added here because it is similar to sedimentation and furthermore because it occurs in clarifiers and determines the solids concentration in the underflows from these units.

Our objectives in this chapter are to furnish you with the models and information you will need to write model library subroutines for settlers. To provide the background for the proper use of these models, we will review the function and operation of clarifiers. We will then examine briefly the theory that has been developed. After this introduction, we will discuss models available in the literature. The sequence of model presentation and discussion will be primary clarifiers, thickeners and final clarifiers. A discussion of design considerations will conclude the chapter.

8.1 Function

Both primary and final clarifiers have the dual functions of 1) removing suspended matter from the stream to produce an effluent low in suspended solids and 2) producing an underflow of a relatively high solids content. The latter is important because the sludge passes on to subsequent treatment units whose size depends on the flow volumes they must accept. A dense sludge, therefore, will reduce the cost of these "downstream" units. Thickening has the single function of volume reduction of sludges. It is justified as a separate unit on the grounds of lower cost

for digesters, vacuum filters, drying beds, etc. generated by denser sludges.

BOD and nutrients in a waste stream are contained in suspended matter so that "clarifying" has the secondary, but still important benefit of BOD and nutrient reduction.

8.2 Clarifier Operation

Clarification of a solids laden stream occurs through the physical process of sedimentation. Often, sedimentation is preceded by the physio-chemical process of flocculation.

Sedimentation occurs through the action of gravity on solid particles whose density is greater than the density of the liquid which contains them. Separation of the solid takes place if the differential velocity established by gravity is larger than the random motion in the liquid (due to turbulence or Brownian phenomena). The velocity depends on particle size, the density difference and the liquid properties. Flocculation occurs through "collisions" of the dispersed solid particles and "adhesion" which yields larger sized particles. These particles settle faster. Flocculation is a kinetic phenomena and thus the degree to which it occurs depends on time.

Clarification requires equipment, therefore, which has minimal mixing to reduce the level of turbulence and sufficient detention time to permit flocculation and let suspended matter to settle out of the liquid. A shallow effective depth keeps the detention time reasonable. Provision must be made for withdrawing clarified waste and a sludge separately.

Shallow basins, either rectangular or circular are used for clarification. A wide variety of designs are possible. Figure 8-1 shows a circular basin with center feed, one of the most widely used designs. It is compared with other designs in Figure 8-2.

The depth of basin lies usually between 7 and 12 ft. Circular tanks often are 100 ft. in diameter, but their size may vary between 35 and 200 ft. Rectangular tanks, when used, normally have lengths of about 100 ft. The width of the tank is governed by the sludge collection and re-

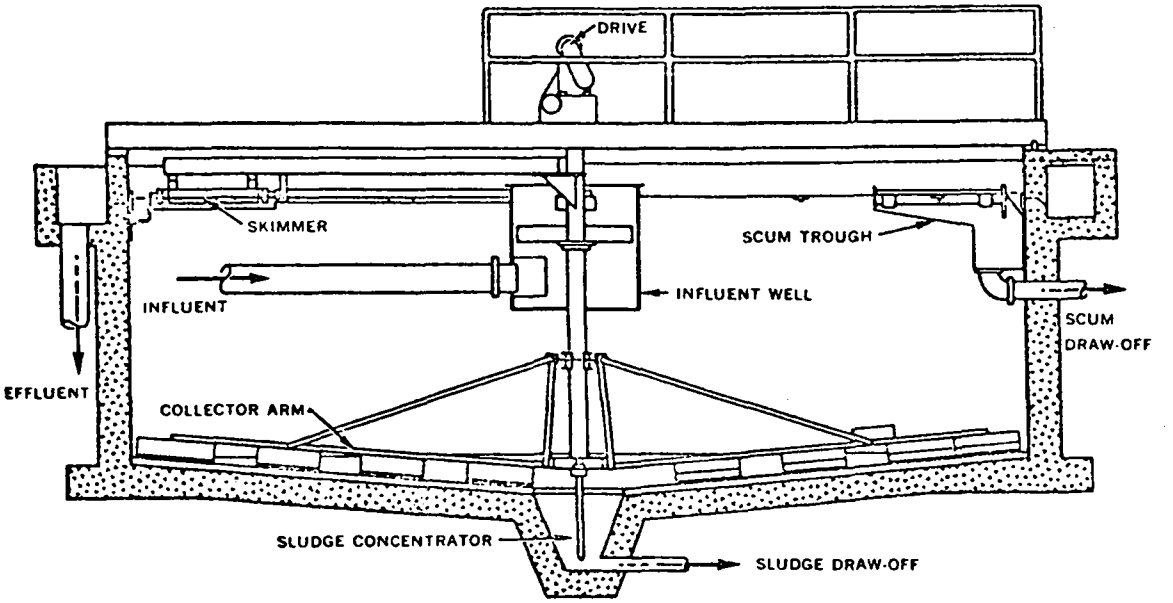


FIGURE 8-1. CIRCULAR CLARIFIER WITH CENTER FEED, SLUDGE RAKES WITH A CENTRAL DRAW OFF*

moval equipment to be used. Common length-to-width ratios employed are from about 3:1 to 5:1. Bottom slopes range from 1% in rectangular tanks to about 7 or 8% in circular tanks.

Inlet flow distributers and the design of the outlet weir are quite important. The inlet devices prevent short circuiting across a portion of the basin by providing uniform radial or linear distribution of flow and by dissipating the kinetic head of the influent jet. This also reduces mixing and turbulence in the basin. A number of proprietary devices are marketed for these purposes.

Clarified overflow is collected over weirs by launders on the periphery or on a side of the basin. The weirs are designed for maximum overflow velocities so as to prevent carry over of suspended matter into the launders.

In rectangular clarifiers scraper flights extending the width

---

*Figure taken from reference (1) with the kind permission of the publisher.

(1)Weber, W.J., Jr., "Physicochemical Processes for Water Quality Control", Wiley-Interscience (New York, 1972)

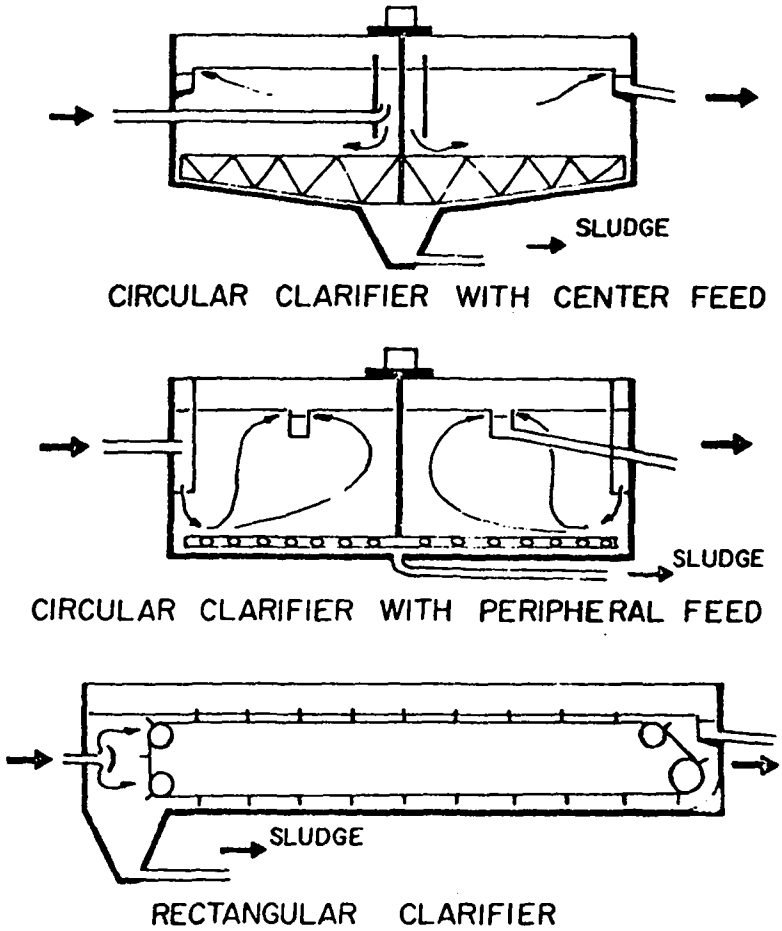


FIGURE 8-2. VARIOUS CLARIFIER DESIGNS*

of the tank move the settled sludge toward the inlet end of the tank at a speed of about one foot per minute, although in some designs the scrapers move towards the other end to conform with the direction of density currents.

Circular tanks are generally designed for center sludge withdrawal. The flow of sludge to the center well is forced by the collection

*Figure taken from reference (2).

(2)"Design Guides for Biological Waste Water Treatment Processes" Water Pollution Control Research Series, No. 11010 ESQ, U.S. Environ. Protect. Agency (Washington, D.C., 1971)

mechanism rather than the slope of the tank bottom. The clarifier mechanisms commonly employed are plows, rotary hoes, and vacuum draw-off. Peripheral speeds range from 2 to 12 ft/min. depending on sludge density. A median speed is about 10 ft/min.

In Europe and other parts of the Commonwealth, sludge blanket or vertical flow clarifiers are used for waste treatment. The influent in this type of clarifier is distributed below the sludge zone. Suspended matter in the influent is carried upwards through the blanket which acts as a "filter". The vessel is designed so that in the upper portions of the clarifier the upflow velocity is sufficiently low so that fine suspended matter not entrapped by the blanket settles out.

Sludge blanket clarifiers are relatively deep circular vessels with steeply sloping conical bottoms. The influent is introduced centrally well within the conical portion of the vessel. Overflow is collected peripherally over weirs. The sludge settles out past the inlet distributer into the neck of the cone. Its density is such that it can be removed by a siphon.

When the sludge blanket in a conventional secondary clarifier is located fairly high in the basin, it is likely that these conventional clarifiers operate at least partially as sludge blanket units.

8.3 Theory of Clarification and Thickening

If we were dealing in waste treatment with very dilute suspensions made up of near spherical particles, the theory of clarification could be described quantitatively and succinctly through Stokes' Law. This law holds for fine particles which settle slowly enough so that flow is laminar and non separating (no wake) around a particle. The law

$$v_t = \frac{g}{18} \frac{(\rho_* - \rho)}{\mu} d_p^2 \qquad (8\text{-}1)$$

where v_t is the terminal settling velocity in the medium at a specified temperature, d_p is the equivalent spherical particle diameter. ρ, μ, g are the density (* = solid), viscosity and the gravitational acceleration. For larger particles where wakes occur, Newton's Law is used,

$$v_t = \frac{4g}{3} \frac{\rho_* - \rho}{\rho C_D} d_p \qquad (8\text{-}2)$$

in which C_D is a drag coefficient whose value depends on the particle Reynold's number $(\rho v_t d_p/\mu)$.

Unfortunately, suspended matter in wastes is far from ideal. Particles are irregularly shaped and may flocculate. Flocculated solids have a porous structure. Furthermore clarification is carried out at high enough solids concentrations that particles influence each other's terminal settling velocities appreciably. The behaviour of different classes of suspended matter in a clarifier can differ drastically. Figure 8-3 is a conventional classification schema for suspensions. Where a particular suspension fits depends upon concentration and ionic media (coagulation). Class 1 is usually referred to as discrete settling (often fairly well described by eqn. (8-1) and (8-2)) while class 2 is often called flocculent settling or flocculation controlled settling.

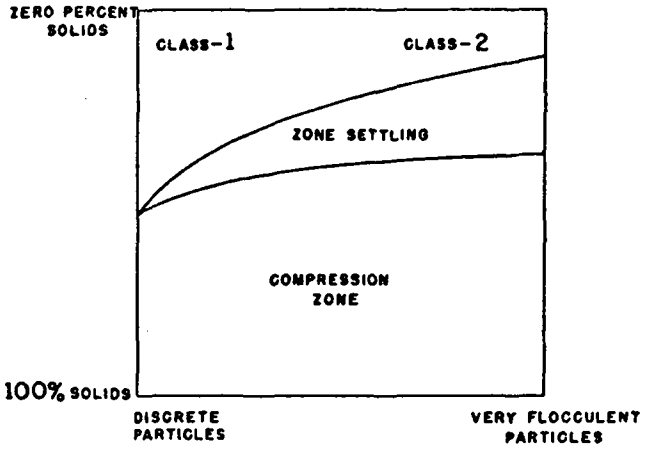


FIGURE 8-3. CLASSIFICATION OF SUSPENSIONS*

Eckenfelder and O'Connor give the classifications succinctly: "These are discrete settling, flocculent settling, zone settling and compression.

*Figure taken from reference (1) with the kind permission of the publisher.

In the first type a particle maintains its individuality and does not change in size, shape or density. Flocculent settling is characterized by agglomeration of the particles which is associated with a changing settling rate. In zone settling the particles settle as a mass and exhibit a distinct interface between the supernatant and the settling solids. During compression, solids are mechanically pressing on layers beneath resulting in a slow displacement of liquid."[3]

Suspensions following class 1, are described by Stokes' or Newton's Laws in principle. Particle shape influences the drag coefficient (C_D) appreciably as well as the particle size at which Stokes' Law gives way to Newton's. Flat particles show higher coefficients, although stringy, flexible particles may exhibit lower values because they can rotate and "bore" their way downward. Nonetheless, terminal settling velocities for class 1 suspensions may be estimated from particle dimensions through eqns. (8-1) and (8-2) and settling rate measurements, conversely, may be used to measure particle size.

Particles settling in a vessel displace liquid which is forced upwards countercurrent to the particles. Furthermore as the number of particles in a unit volume increases, the velocity fields surrounding individual particles interfere. Both effects reduce the absolute settling velocity. The phenomena is called hindered settling. Many relations have been proposed; of these the equation proposed by Richardson and Zaki (see reference (4)) seems most useful. The relation is,

$$v_t = v_t^o \, \varepsilon^n \qquad (8\text{-}3)$$

where v_t^o is the terminal settling velocity at high dilution and ε is the liquid volume fraction,

$$\varepsilon = (1 - M/\rho_*) \qquad (8\text{-}4)$$

---

[3] Eckenfelder, W.W., Jr., and O'Connor, D.J., "Biological Waste Treatment", Pergamon Press (London, 1961)

[4] Silveston, P.L., "Design of Settling Basins with Allowance for Residence Time Distributions", Can. J. Chem. Eng., 47, 521 (1969)

M is the concentration (mg/l.) of suspended matter and ρ_* is the particle density in the same units. The exponent $n = 4.65$ for regularly shaped particles.

Camp[5] suggests that the effect of hindered settling becomes significant only if the volumetric ratio of solids to liquids in the suspension exceeds 0.5%. It is negligible when the ratio is less than 0.1%. For sewage, the upper limit works out to about 1000 mg/l. suspended solids. Hindered settling, therefore is not important in the top portion of primary clarifiers.

Flocculating suspensions (class 2) exhibit increasing particle size during sedimentation. Suspended matter of this class will agglomerate on contact to form larger and therefore faster settling solids (see eqn. (8-1) for the v_t versus d_p relation). The process occurs through diffusion and low intensity mixing in the clarifier, which cannot be eliminated, as well as through an "overtaking" phenomena discussed by Camp[5]. In the former, particles are brought into proximity by "random walk," while in the latter, larger or denser particles overtake smaller slower settling particles putting them near enough to coalesce.

Flocs formed in waste treatment, particularly those found in the activated sludge process have densities of the order of 1.005 and appear as a loose gelatinous matrix. Under discrete settling conditions, their equivalent spherical diameters will be less than 1 mm. However, in concentration ranges found in the influent to final clarifiers, the floc-floc spacing is such that a dynamic interaction becomes possible. Particles, regardless of size, settle with neighboring particles. Indeed, the suspended matter settles as a zone with a distinct interface and with just a small axial density gradiant (unlike discrete settling). Figure 8-3 suggests that with flocculating solids zone settling can occur at low concentrations.

In a batch or column settler, as the zone settles it reaches a depth where the solids concentration begin to increase. Downward movement

---

[5] Camp, T.R., "Sedimentation and the Design of Settling Tanks", Trans. Am. Soc. of Civil Eng., III, 895 (1946)

of the sludge-clarified liquid interface eventually becomes very slow. Figure 8-4 taken from Camp[5], illustrates the time behaviour of the top of the blanket, that is, the sludge-liquid interface.

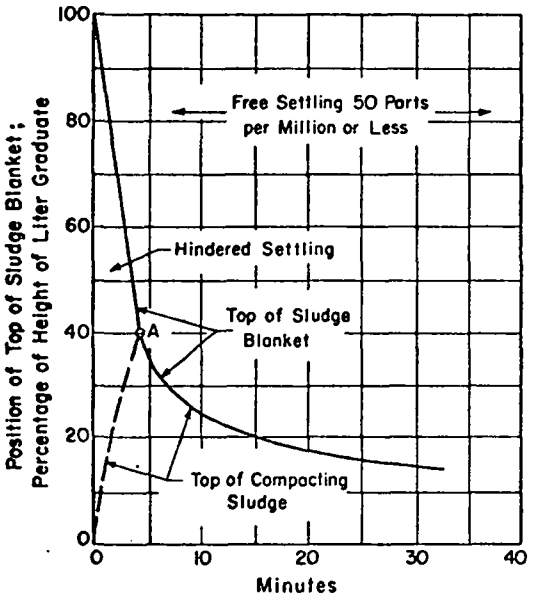


FIGURE 8-4. SETTLING AND COMPACTING OF TYPICAL ACTIVATED SLUDGE MIXED LIQUOR WITH AN INITIAL SUSPENDED SOLIDS CONTENT OF ABOUT 2,000 PPM

The region around "A" in the figure is termed the transition zone, while below "A" the sludge is said to be compressed. Figure 8-5[6] is a schematic presentation of the settling and thickening states occurring in Figure 8-4.

The upward flow of liquid through the suspended solids matrix is thought to govern the movement of the interface. This movement is the rate of zone settling. When the transition condition is reached, the movement of the interface becomes the rate of compaction. This viewpoint suggests that zone settling and compaction under the transition zone conditions should be described by equations for the flow of liquids through randomly packed beds of solids.

The phenomena, however, are more complex under compression

---

*Figure taken from reference (5) with the kind permission of the publisher.

(6)Eckenfelder, W.W., Jr. and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970)

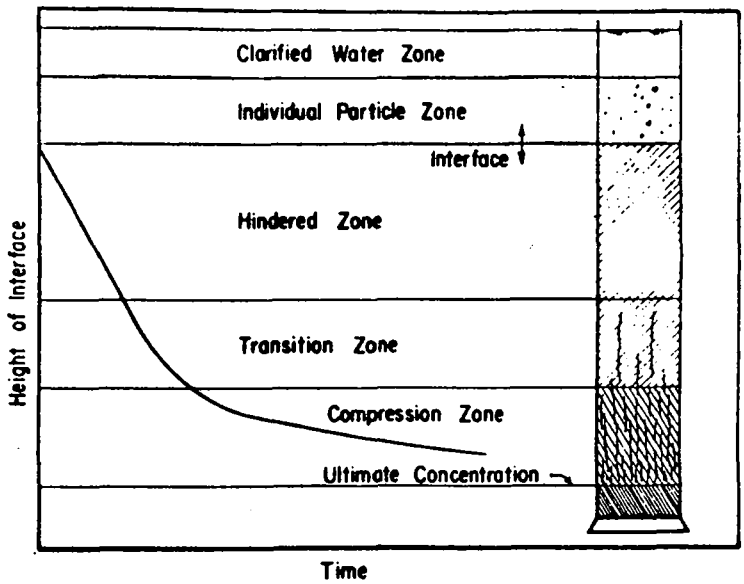


FIGURE 8-5. TIME SEQUENCE OF SETTLING AND THICKENING CLASSES IN BATCH SETTLING OF A FLOCCULENT SUSPENSION*

conditions where sludge particles are supported by one another. The matrix has become so dense that there is little void space between individual flocs or particles. In this condition, floc at the bottom of the vessel deforms and slips under compressive stress forcing out liquid which seeps through the structure providing subsidence. Subsidence results in the slow movement of the interface. It is this phenomenon that occurs in the sludge blanket at the bottom of a clarifier or in a thickener.

Mechanical rakes used to move the sludge play an important role in compaction. Stirring provided by the rakes increases the seepage of liquid from the bottom sludge layers and also provides "jiggling" to obtain closer packing. Continuous thickeners frequently give higher sludge densities than batch measurements at the same holding times.

Our discussion of sedimentation and thickening to this point provides an adequate basis for the modelling of "ideal" clarifiers. This term was used by Camp to indicate that the hydrodynamics of clarifiers is not considered. Unfortunately, hydrodynamics is important and it operates

*Figure taken from reference (6) with the kind permission of the publisher.

(6)Eckenfelder, W.W., Jr., and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970)

to reduce clarifier efficiency. Hydrodynamics refers to interrelated phenomena of density currents, nonuniform influent distribution and overflow withdrawal, and turbulent mixing in basins.

To deal with nonuniform flow, we must first introduce the idea of particle trajectories or settling paths. Figure 8-6 shows the trajectories of two particles settling in an ideal basin. Both particles originate at the top of the inlet region, but one is larger or denser and settles with a terminal velocity v_o. The fluid velocity is u so the paths of the particles are vectorially determined by v_o and u for the first particle and by v_s and u for the second. Obviously, a sufficient depth must be attained at the outlet if the particle is not to be swept out of the basin in the overflow. It is evident from the diagram (Figure 8-6) that this depth depends on both v and u.

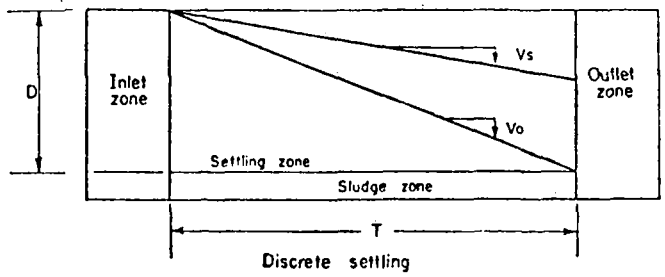


FIGURE 8-6. SETTLING PATH IN AN IDEAL BASIN*

If there is maldistribution of the flow, a portion of the fluid will have a velocity $u' > u$ and particles expected to settle will be swept out. An equal portion of the flow, of course, must have a velocity $u'' < u$, but this will not compensate for the solids swept out. In the same way, there will be a loss of clarifier efficiency if the fluid has a vertical velocity component in a portion of the basin. Both flow situations occur to a greater or lesser extent in clarifiers.

Density currents are an important source of maldistribution of flow. The fluid entering a clarifier will be denser than the clarified liquid and will sink. Significant velocities can be attained as easily

*Figure taken from reference (3) with the kind permission of the publisher.

verified by dye tests when a saline solution is added to a basin. The downflow will be deflected by the sludge blanket towards the outlet. This can result in unexpectedly high velocities along the surface of the sludge blanket and causes scour.

Wind forces on a clarifier surface and convective currents from heat transfer at the surface also induce currents in basins[7]. This induced flow causes mixing and may contribute to maldistribution of flow in the basin. Currents from these sources may also be responsible occasionally for bottom scour.

Camp[5] estimates that flow in basins will have open channel Reynolds Numbers in excess of 500 so that the velocity profile (assuming a uniform inlet vertical velocity profile) will be turbulent. This means that some turbulence will be generated at the sludge blanket. If the velocity above the blanket is sufficiently large, settled solids will be resuspended. This is the scour phenomenon.

The shear exerted on a surface can be calculated from the velocity profile in the neighborhood of the surface. If this is equated to the static forces in the surface resisting movement, a formula for the scour velocity may be derived. Camp[5] gives,

$$v_{sc} = \sqrt{\frac{8\, g\, \beta}{f}\ (\rho/\rho_w)\, d_p} \qquad (8\text{-}5)$$

where v_{sc} is the critical scour velocity for resuspension of solids of diameter d_p and specific gravity ρ/ρ_w. β is a constant peculiar to the sludge, f is the friction factor for open channel flow and g is the acceleration of gravity. We encounter eqn. (8-5) again in Chapter 12 where it is used for the design of grit chambers.

Although undoubtedly the turbulence level is low, it is unavoidable. Very little is known about the scale and intensity of turbulence in a clarifier. Mixing and dispersion tests have been made repeatedly, but

---

[7] Takamatsu T., and Naito, M., "Effect of Flow Conditions on the Efficiency of a Sedimentation Vessel", Water Research, 1, 433-450 (1967)

these tests are not able to distinguish adequately between large scale circulation and turbulence. However, the effect of turbulence on sedimentation is quite well understood. Turbulence causes mixing. If mixing occurs in a system where concentration or density gradients exist, material will be transferred from the more dense to the less dense regions. If we let J_T be the flux of suspended matter transferred by turbulent mixing and D_M be a dispersion coefficient characterizing the intensity of mixing, then at a point in a clarifier,

$$J_T = - D_M \frac{dM}{dy} \qquad (8\text{-}6)$$

In this relation y is a coordinate direction and M is the solids concentration in, say, mg/l. The minus sign simply tells us that the transfer is <u>into</u> the less dense region.

Concentration gradients in clarifiers are caused by sedimentation. Consider an ideal basin as shown in Figure 8-7. Removal of suspended matter changes the concentration along the horizontal axis as shown in the figure. Along the vertical axis, the situation is identical to what would be observed in a settling column experiment. This is also shown in the figure.

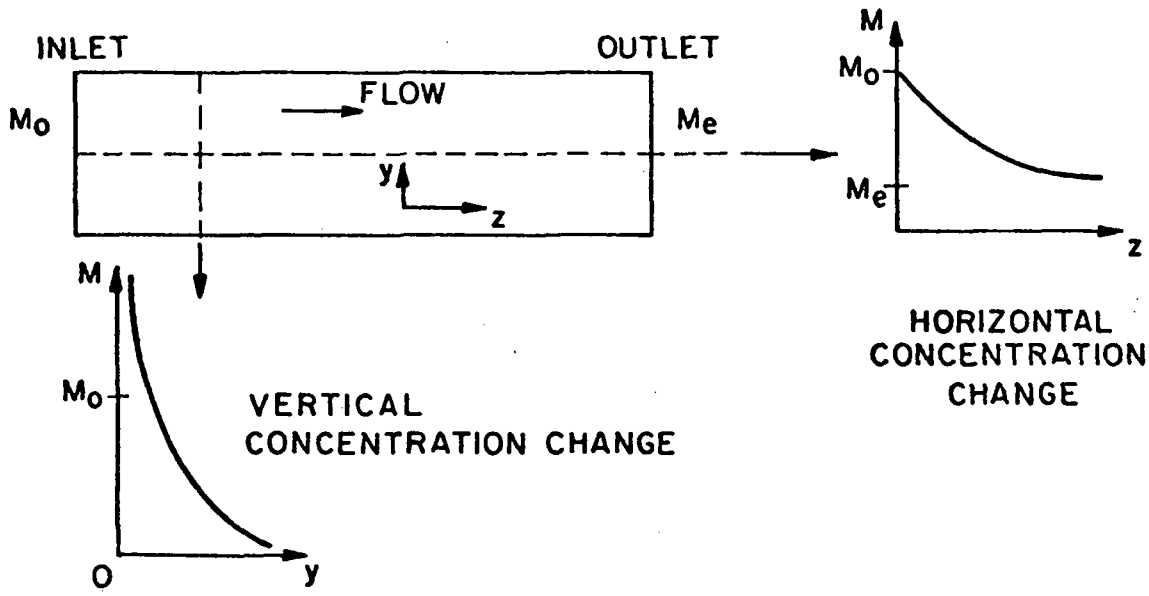


FIGURE 8-7. SOLIDS CONCENTRATION GRADIENTS IN IDEAL BASINS

The significance of Figure 8-7 with respect to the flux equation (eqn. (8-6)) is that any turbulent mixing decreases the concentration gradients. This means that clarification efficiency will be reduced. Quantitative analysis of this mixing effect is possible, in principle.

Dispersion coefficients normally will be different in the horizontal and vertical directions. Thus, the influence of turbulence at a point in a basin can be represented by

$$D_{M_z} \frac{\partial^2 M}{\partial z^2} - u \frac{\partial M}{\partial z} + D_{M_y} \frac{\partial^2 M}{\partial y^2} - \bar{v}_t \frac{\partial M}{\partial y} = 0 \qquad (8\text{-}7)$$

where u is the fluid velocity in the basin and $\bar{v}_t$ is the characteristic settling velocity of the suspended matter. Eqn. (8-7) cannot be solved in the absence of the functional dependence of D_M and u on y and z. Unfortunately, this type of information is not available.

Research into basin hydrodynamics for the last few decades has centered upon tracer studies of residence time distributions in basins. We have introduced this subject in Chapter 7 and we refer to that discussion for definitions. Dyes or radioactive substances normally serve as tracers. They are injected immediately upstream of a clarifier and the concentration of the tracer is detected in the overflow.

Figure 8-8[8] compares hypothetical results of tracer tests for two idealized basins to a result where some mixing and some short circuiting occur. The normalized concentration (C_o is the concentration that results if the tracer is mixed into the basin) at the basin outlet is plotted against dimensionless time ($t\ Q/V$) where V is the effective volume allowing for the sludge layer. The line (curve B) results if the basin is "ideal", that is, the influent is evenly distributed across the vertical plane at the inlet and moves across uniformly towards the outlet. All of the fluid is in the basin the same time, thus causing a spike in the figure. The other extreme is where the fluid in the basin is well

---

[8] Rebhun, M and Argaman, Y., "Evaluation of Hydraulic Efficiency of Sedimentation Basins", J. Sanitary Eng. Div., Proc. A.S.C.E., SA5, 37 (1965)

mixed (curve A). Curve C shows an intermediate case.

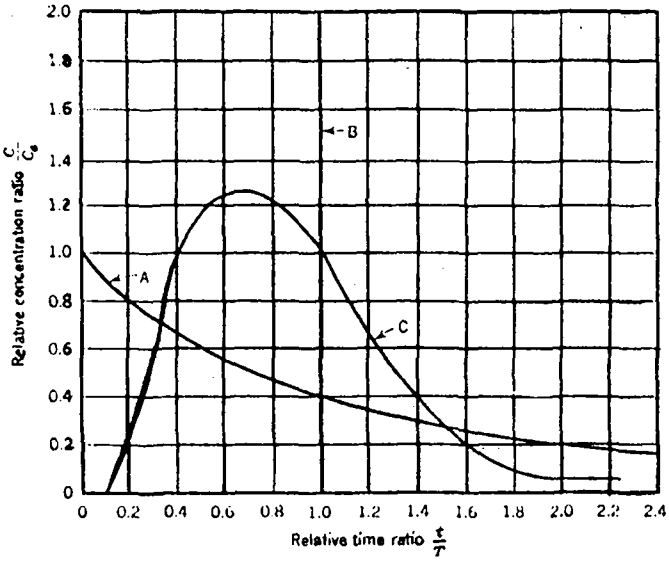


FIGURE 8-8. RESIDENCE TIME DISTRIBUTIONS FOR ZERO MIXING, PLUG FLOW (B), COMPLETELY MIXED (A), VESSEL AND A PARTIALLY MIXED VESSEL WITH SOME SHORT CIRCUITING*

Figure 8-9 shows data for center and peripheral feed clarifiers[1]. The significance of the shapes is that they indicate that short circuiting occurred. The figure also suggests that for the inlet design used, peripheral feed causes less short circuiting. (Its maximum is closer to the theoretical detention time). Figure 8-10 shows data taken by Thomas and Archibald[9] on a rectangular clarifier. The tracer distribution is interesting because it demonstrates two mixing phenomena often found in clarifiers. The mean residence time (mean time in the figure), which is the first moment of the normalized distribution:

$$\bar{t} = \frac{\int_0^\infty t\, C\, dt}{\int_0^\infty C\, dt} \qquad (8\text{-}8)$$

*Figure taken from reference (8) with the kind permission of the Journal.

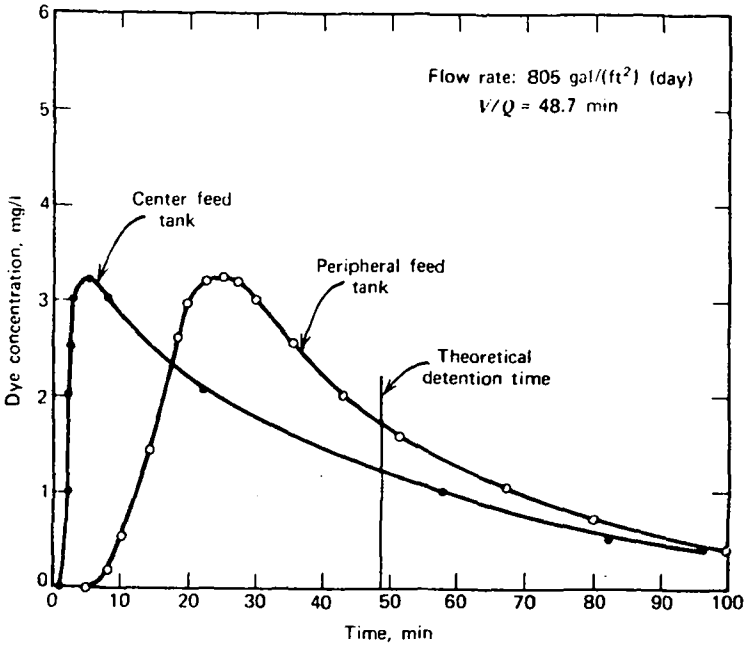


FIGURE 8-9. COMPARISON OF TRACER TESTS FOR CENTRAL AND PERIPHERAL FEED CLARIFIERS*

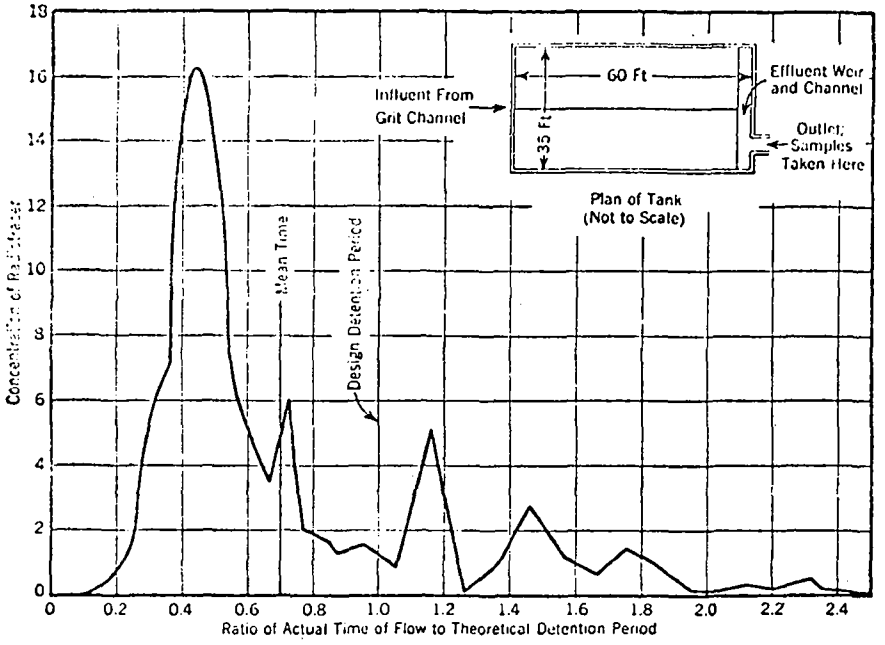


FIGURE 8-10. TRACER OUTLET CONCENTRATION PROFILE FOR A RECTANGULAR CLARIFIER**

*Figure taken from reference (1) with the kind permission of the publisher.

**Figure taken from reference (9) with the kind permission of the Transactions.

should be equal to the detention time (τ). In the relation t is the residence time corresponding to a tracer concentration C in the clarifier. However, in Figure 8-10 $\bar{t} < \tau$. This is possible only if some of the vessel volume is not "irrigated" by the influent, that is, if "dead space" occurs (It could also be explained if the volume of the sludge in the clarifier was not subtracted from the clarifier before τ was calculated).

The second phenomenon is the periodic, diminishing peaks after $t/\tau > 1.1$. These peaks are the result of a large scale recirculation in the basin. This type of pattern, shown in Figure 8-11[7], arises from short circuiting, or either wind or density driven currents. Residence time distribution curves taken on rectangular clarifiers similar to Figure 8-10 have been published by Wills and Davis[10].

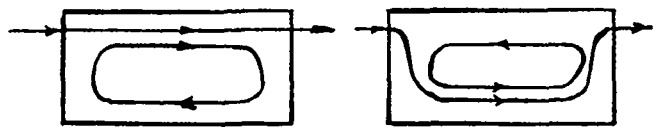


FIGURE 8-11. RECIRCULATION PATTERNS IN CLARIFIERS*

Interpretation of tracer or residence time distribution curves has become reasonably formalized in the Sanitary Engineering literature as they have been applied to the design of clarifier inlet and outlet devices. Figure 8-12 taken from Thirumurthi[11] illustrates various characterizations of the curves by times which have been used for inter-

*Figure taken from reference (7) with the kind permission of the Journal.

(9) Thomas, H.A., Jr., and Archibald, R.S., "Longitudinal Mixing Measured by Radioactive Tracers", Trans. Am. Soc. of Civil eng. 117, 839 (1952)

(10) Wills, R.F. and Davis C., "Flow Patterns in a Rectangular Sewage Sedimentation Tank", Adv. in Water Pollution Research, Volume 2, Pergamon Press (London, 1964)

(11) Thirumurthi, D., "A Break-through in the Tracer Studies of Sedimentation Tanks", J.W.P.C.F., 41, No. 11, R405 (1969)

pretation. For example, t_p/τ is used by Camp[5] to identify the severity of short circuiting, while Villemonte and Rohlich[12], among others, use $(\bar{t} - t_p)/\bar{t}$ as a short circuiting index. Short circuiting is absent when the index is zero.

Attempts have been made by some authors to derive dispersion coefficients from the tracer curves. The formula used for this purpose

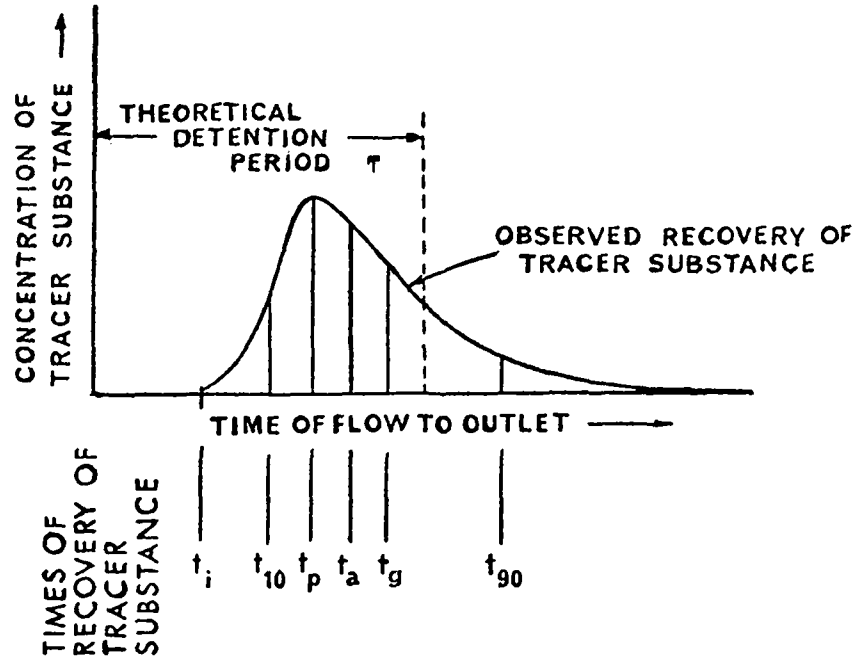


FIGURE 8-12. CHARACTERIZATION OF TRACER CURVES BY TIMES*

depends on how tracer is introduced into a clarifier and how it is detected as well as the point at which injection and detection occur. For example if pulse injection and continuous monitoring at points <u>within</u> a clarifier are used, the dispersion coefficient, D, may be calculated from the simple relation,

$$\frac{\sigma^2}{\bar{t}^2} = \frac{2}{N_{Pe}} + \frac{8}{N_{Pe}^2} \qquad (8\text{-}9)$$

*Figure taken from reference (11) with the kind permission of the Journal.

where N_{Pe} is the Peclet Number ($= \frac{uL}{D}$) and u is the velocity in a clarifier of length or characteristic dimension L. If the dispersion coefficient is to be used as a measure of turbulent mixing, as has been proposed, use of eqn. (8-9) assumes that gross circulation patterns (short circuiting for example) are absent. This assumption is rarely justified.

8.4 Primary Clarifier Models

In discussing models for clarifiers, we have chosen to consider the primary and final clarifier separately. This is justified because zone settling frequently occurs in final clarifiers, while discrete settling is the dominant mode in the primary unit. The performance of the secondary clarifier is also heavily dependent on the upstream biological unit. Nonetheless, some of the models we will discuss in this section will be applicable to final as well as to primary clarifiers.

We pointed out in the previous section that separation in a clarifier is governed primarily by the velocity through the unit and the settling velocity of the suspended matter. Other phenomena discussed, such as mixing, modify the basic separation-velocity relationship. Camp, in his classic treatment of settling, writes for the "ideal" basin[5],

$$f_R = 1 - P_{crit.} + \frac{1}{v_o} \int_o^{v_o} v \; p\,(v)\; dv \qquad (8\text{-}10)$$

In this expression f_R is the fractional removal (as weight) by sedimentation of any specified class of suspended solids. P_{crit} is the cumulative distribution by weight of solids whose settling velocity is greater than v_o. It is the weight fraction of the solids whose settling velocity is sufficiently great so that the solids settle through at least the depth h, the effective depth of the clarifier, during the detention time τ in the basin. $p(v)\,dv$ = the fraction of the solids whose settling velocities lay between v and $v + dv$. The velocity v_o is often referred to as the overflow rate

$$v_o = Q/A_{set} \qquad (8\text{-}11)$$

where Q is the volumetric flow rate and A_{set} is the surface area of the clarifier. For a rectangular basin $A_{set} = WL$ where W and L are the basin width and length, while for a circular basin, $A_{set} = \frac{1}{4} \pi d_{set}^2$ where d_{set} is the diameter of the clarifier.

The suspended solids in the clarifier overflow will be

$$M_e = M_o (1 - f_R) \tag{8-12}$$

Equation (8-10) can be rewritten for different settling situations[4]. If the suspension has a single settling velocity (particle size is within a very narrow range)

$$f_R = \frac{v \tau}{h} \phi (t) \tag{8-13}$$

where h is again the effective settling depth (usually the depth to the top of the sludge blanket) and $\phi (t)$ is a two valued weighing function:

$$\begin{aligned} \frac{\tau v}{h} &< 1, \quad \phi (t) = 1 \\ \frac{\tau v}{h} &> 1, \quad \phi (t) = \frac{h}{v\tau} \end{aligned} \tag{8-14}$$

The criterion of the weighing function is actually v/v_o, the ratio of the settling velocity to the overflow rate.

For zone settling

$$f_R = \frac{v_z \tau}{h} (1 - P_f) \phi (t) \tag{8-15}$$

where v_z = the settling velocity of the zone interface, and P_f = the fraction of the solids remaining in suspension after zone settling has occurred. These remaining solids settle at a velocity (v_d) less than v_z, so

$$f_R = \frac{v_z \tau}{h} (1 - P_f) \phi(t) + \frac{v_z v_d \tau^2}{h} \left(\frac{\phi(t) - 1}{h - v_z \tau}\right) \qquad (8\text{-}16)$$

If size rather than settling velocity is used, eqn. (8-10) can be written

$$f_R = 1 - P_{crit.} + \frac{\tau}{h} \int_o^{d_{p_{crit.}}} v \; p(d_p) \, d(d_p) \qquad (8\text{-}17)$$

where d_p is the particle size (usually an equivalent spherical diameter).

It has been demonstrated that the models can be extended to partially allow for circulation or short circuiting[4]. If we assume that the residence time distribution (tracer curve) results entirely from short circuiting and not from small scale turbulence, the distribution can be introduced directly into a relation for f_R. Letting $f_R(t)$ be given by which ever equation among eqns. (8-10), (8-13), or (8-15) to (8-17) is appropriate, assuming t is a detention time, the non ideal clarifier fractional removal, $\bar{f}_R$, is

$$\bar{f}_R = \int_o^\infty f_R(t) \, E(t) \, dt \qquad (8\text{-}18)$$

In this equation, $E(t)$ is a form of the residence time distribution whereby $E(t)dt$ is the fraction of the influent which leaves the basin after having spent a time between t and $t + dt$ in the basin. It is often referred to as an exit age distribution.

As an example of the use of eqn. (8-18), consider a zone settling system, in which eqn. (8-15) applies. Replacing τ by a variable detention time t and introducing eqn. (8-15) as $f_R(t)$ into eqn. (8-18), we obtain,

$$\bar{f}_R = \frac{v_z}{h} (1 - P_f) \int_o^\infty t \, \phi(t) \, E(t) \, dt \qquad (8\text{-}19)$$

for the fractional removal in a non ideal clarifier with zone settling.

Equation (8-18) assumes that the influent is subdivided into columnar elements extending from the surface to the sludge blanket which move intact to the outlet with individual residence times conforming to the distribution. Although the model is not realistic, it does give better results than Camp's ideal basin treatment.

Settling velocity data will be obtained experimentally for most wastes. The procedure for this measurement is quite well known, however, we will review it just briefly and then show how a clarifier model may be built directly from such data.

Settling velocities are measured by filling a column whose depth is the effective settling depth in a basin (usually 6 to 8 ft.) with a test waste. The column is normally of the order of 10" in diameter to provide a sufficient sample for gravimetric solids determination and to minimize wall effects. Taps are located at intervals vertically (ca. every 2 ft.) along the column. Measurements are conducted by thoroughly mixing the waste in the column up to time zero, halting the agitation and at time intervals thereafter withdrawing waste samples to measure the suspended solids concentrations. A plot is prepared of the concentrations (or more conveniently the fraction of solids removed) for each depth and time interval such as shown in Figure 8-13. The circles represent percentages of solids removed for depths and times shown on the

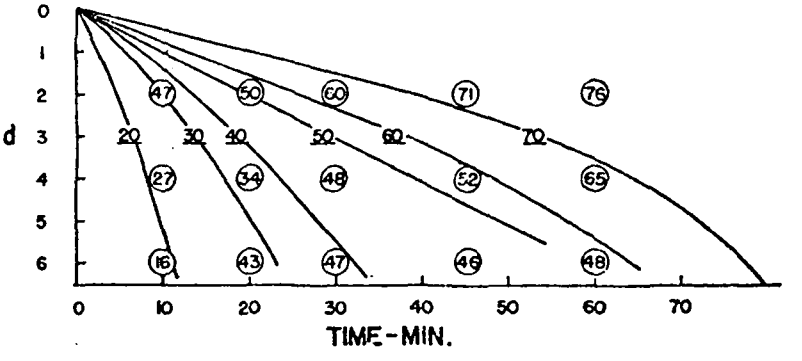


FIGURE 8-13. ESTIMATION OF SETTLING VELOCITIES AND FRACTIONAL REMOVAL VS. TIME FROM COLUMN SETTLING DATA*

*Figure taken from reference (3) with the kind permission of the publisher.

axes of the figure. The lines represent constant percent removed and are found by interpolation. Settling velocities (ft/min) are their slopes. Curvature of the 70% line indicates some flocculation may be occurring with this slow settling matter because the slope increases with time. The cumulative fraction of the suspended matter P(v) with a settling velocity equal or less than v may be obtained by subtracting the fractional removal from one. Figure 8-14 shows a plot of P(v) (as percent) vs. v prepared from Figure 8-13. The slopes at different settling velocities results in p(v), the frequency distribution, which would be used in eqn. (8-10). Normally, analysis of column settling data would be performed separately from a simulation or design run and P(v) or p(v) vs. v would be supplied as a function or as a table.

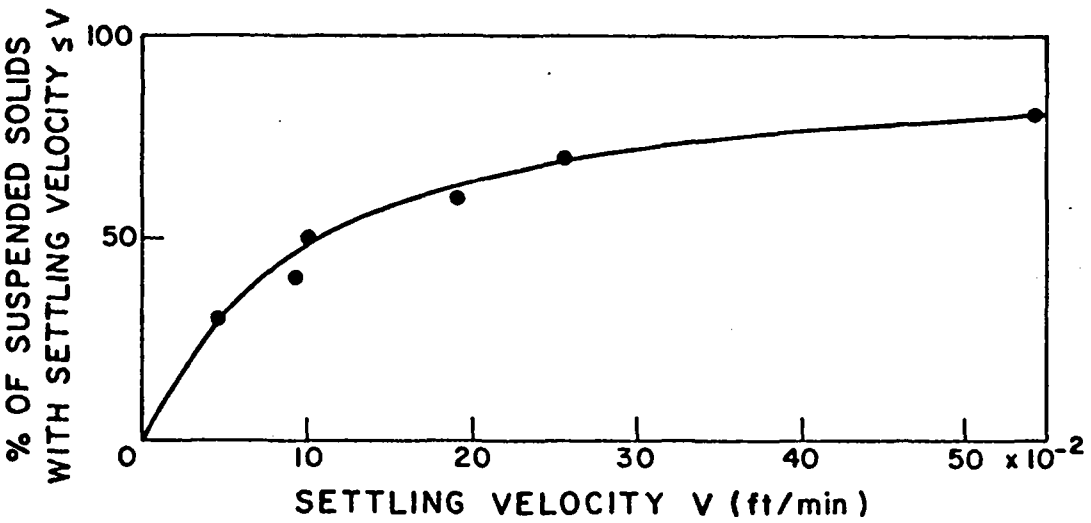


FIGURE 8-14. CUMULATIVE FRACTION OF SUSPENDED SOLIDS (AS %) WITH SETTLING VELOCITY EQUAL OR LESS THAN v (DATA IN FIGURE 8-13)

The interface settling velocity, v_z, for zone settling used in eqns. (8-15) and (8-16) may also be obtained from column measurements. The interface is usually quite distinct so that concentration measurements are not needed.

Experimental data, such as shown in Figure 8-13, may be used directly to relate f_R or $\bar{f}_R$ with the overflow velocity (v_o). If the column used for the settling test has been chosen to correspond to the

effective height, $f_R(t)$ can be obtained directly from a figure such as Figure 8-13 by taking a suitably weighted average of the fraction removed measurements for each of the depths used at different times. The averages ($f_R(t)$) would be as shown in Figure 8-15. The settling time in the column is related to the overflow rate v_o by $t = h/v_o$.

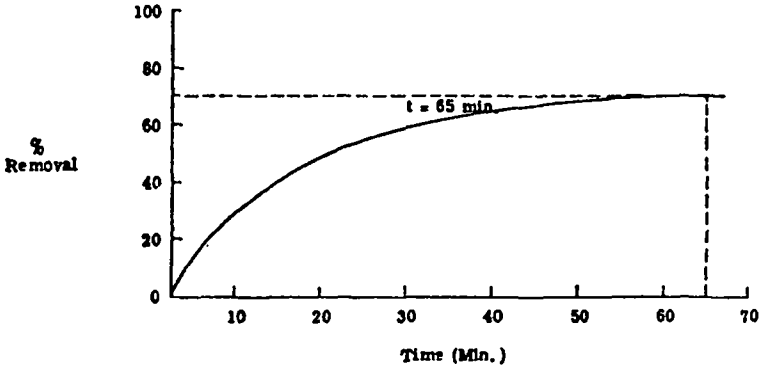


FIGURE 8-15. PERCENT OF SOLIDS REMOVED IN A 6 FOOT DEEP COLUMN AS A FUNCTION OF TIME*

Fitting the curve or using tabulated data, $f_R(t)$ can be substituted in eqn. (8-18) to give $\bar{f}_R$. Villemonte et al.[12] and Wallace[13] applied eqn. (8-18) with f_R determined as just shown to oil-water separators and to sedimentation basins.

Figure 8-16 shows a WATCRAP-PACER program[14] which calculates suspended solids and suspended BOD in a clarifier overflow using vessel dimensions, influent flow rate and settling test data (see Figure 8-13) in

*Figure taken from reference (3) with the kind permission of the publisher.

[12] Villemonte, J.R., Rohlich, G.A., and Wallace, A.T., "Hydraulics and Removal Efficiencies in Sedimentation Basins", Adv. in Water Pollution Research 2, 381, Pergamon Press (London, 1967)

[13] Wallace, A.T., "Design and Analysis of Sedimentation Basins", Water and Sewage Works, 114, R-219 (1967)

[14] Singh, D.P., "Steady State Simulation of the Kitchener Waste Treatment Plant", M.A.Sc. Thesis, Dept. of Chem. Eng., University of Waterloo (Waterloo, Ontario, 1970)

raw form. The subroutine illustrates the use of the AEN vector in SEPSIM to read tabular data into a subroutine. Program statements illustrate table look up procedure and linear interpolation. Detention time is obtained from settler volume and the volumetric flow rate. A look up procedure interpolates in the fraction removal data table to give the removal at three depths. These are averaged to give the overall basin removal. The same fractional removal is used for all classes of suspended solids.

```
      SUBROUTINE PWISTL
C
C THIS SUBROUTINE CALCULATES THE SIZE OF A CLARIFIER OR PREDICTS
C CLARIFIER PERFORMANCE ON THE BSIS OF SETTLING DATA OBTAINED
C IN A QUIESCENT COLUMN
C THE SUBROUTINE WAS ORIGINALLY WRITTEN BY D.P.SINGH AS A PART
C OF AN M.A.SC. THESIS FOR THE DEPT. OF CHEMICAL ENGINEERING,
C UNIVERSITY OF WATERLOO.
C PROGRAMME WRITTEN IN SEPTEMBER, 1969, REVISED OCTOBER,1969,
C FURTHER REVISION BY P.L.SILVESTON IN 1973
C
C SETTLING DATA IS INTRODUCED THRU THE AEN VECTOR.. THE PROGRAM CALCULATES
C THE MEAN RESIDENCE TIME IN THE CLARIFIER AND LOOKS UP IN THE
C TABULATED DATA THE FRACTION OF SOLIDS REMOVED CORRESPONDING
C TO THAT DETENTION TIME. VALUES ARE OBTAINED FOR THREE DEPTHS.
C THESE ARE AVERAGED TO GIVE THE FRACTIONAL REMOVAL OF SUSPENDED
C SOLIDS IN THE CLARIFIER. ALL CLASSES OF SOLIDS ARE ASSUMED
C TO SETTLE IN THE SAME WAY. NO CHANGE IN DISSOLVED SPECIES
C IS ASSUMED TO OCCUR
C
C                    STREAM VECTOR
C         1. STREAM NO.
C         2.
C         3. VOLUMETRIC FLOW
C         4. SUSPENDED SOLIDS (AS CONC|N)
C         5. DISSOLVED B O D
C         6. SUSPENDED B O D
C         7. TOTAL B O D
C         8. VOLATILE SUSPENDED SOLIDS
C         9. PH
C        10.TOTAL SUSPENDED SOLIDS
C        11. TEMPERATURE
C        12. INERT SUSPENDED SOLIDS
C        13.
C        14. TOTAL VOLATILE SUSPENDED SOLIDS
C
C                    EQUIPMENT PARAMETERS VECTOR
C         1. EQUIPMENT NO.
C         2.
C         3. CLARIFIER DIAMETER IN FT.
C         4. EFFECTIVE HEIGHT OF CLARIFIER IN FT.
C         5. NO. OF VESSELS USED
C         6.
C         7. SPLIT RATIO (FRACTION OF INFLUENT LEAVING AS OVERFLOW)
C         8.
C         9. J WHERE IS THE FIRST DATA POINT IN THE AEN VECTOR
C        10. NUMBER OF TIME DATA POINT IN AEN VECTOR
C
C                    AEN VECTOR
C         1. EQUIPMENT NO.
C         2. LENGTH OF AEN VECTOR
C         3. LOWEST HEIGHT AT WHICH % REMOVAL DATA TAKEN (2 FT.)
C         4. MIDDLE HEIGHT AT WHICH % REMOVAL DATA  TAKEN (4 FT)
C         5. GREATEST HEIGHT AT WHICH % REMOVAL DATA TAKEN (6 FT)
C         6. HEIGHT OF COLUMN
C         7. TO 14. TIME VECTOR
C        15. TO 22. % REMOVAL AT 6 FT.
C        23. TO 30. % REMOVAL AT 4 FT.
C        31. TO 38. % REMOVAL AT 2 FT.
C        39. MAXIMUM % REMOVAL IN COLUMN
C
C         SEPSIM COMMON AND DIMENSION STATEMENTS HAVE BEEN DELETED
C         FROM THIS EXAMPLE
C
C AVOID DIVISION BY ZERO
```

```
      IF(STRMI(1,3))2,2,3
    2 STRMI(1,3)=1.
    3 CONTINUE
C
C INITIALIZE THE DUMMY VECTOR
      DO 1 I=1,19
    1 PAPER(1,I)=0.0
      PAPER(1,1)=(22.*(EN(NE,3)**2))/28.
      PAPER(1,2)=PAPER(1,1)*EN(NE,4)
      PAPER(1,3)=PAPER(1,2)*EN(NE,5)
C
C PAPER(1,4) CALCULATES RESIDENCE TIME IN MINS.
C FACTOR 0.008986 CONVERTS FT**3*DAY/M.G TO MIN-1
      PAPER(1,4)=PAPER(1,3)*0.008986/STRMI(1,3)
      M=EN(NE,9)
      N=EN(NE,9)+EN(NE,10)-1
C
C THIS DO LOOP FINDS THE NEAREST RESIDENCE TIME IN TIME VECTOR
      DO 100 J=M,N
      IF(PAPER(1,4) .GT. AEN(1,J))GO TO 100
      GO TO 101
  101 M=J+EN(NE,10)
  100 CONTINUE
C
C PAPER(1,7) CALCULATES % REMOVED OF SS AT 6 FT.
      PAPER(1,5)=(AEN(1,M)-AEN(1,M-1))/(AEN(1,J)-AEN(1,J-1))
      PAPER(1,6)=PAPER(1,4)-AEN(1,J-1)
      PAPER(1,7)=(PAPER(1,5)*PAPER(1,6))+AEN(1,M-1)
      M=M+EN(NE,10)
C
C PAPER(1,9) CALCULATES % REMOVED OF SS AT 4 FT.
      PAPER(1,8)=(AEN(1,M)-AEN(1,M-1))/(AEN(1,J)-AEN(1,J-1))
      PAPER(1,9)=(PAPER(1,8)*PAPER(1,6))+AEN(1,M-1)
      M=M+EN(NE,10)
C
C PAPER(1,11) CALCULATES % REMOVED OF SS AT 2 FT.
      PAPER(1,10)=(AEN(1,M)-AEN(1,M-1))/(AEN(1,J)-AEN(1,J-1))
      PAPER(1,11)=(PAPER(1,10)*PAPER(1,6))+AEN(1,M-1)
C
C Z1,Z2,Z3 CALCULATE THE AVERAGE HTS.
      Z1=(AEN(1,3)+AEN(1,4))/2.
      Z2=(AEN(1,4)+AEN(1,5))/2.
      Z3=(AEN(1,3)+AEN(1,6))/2.
C
C D1,D2,D3 CALCULATE THE DIFF. OF % SS REMOVED
      D1=ABS(PAPER(1,8)-PAPER(1,7))
      D2=ABS(PAPER(1,11)-PAPER(1,9))
      D3=ABS(AEN(1,38)-PAPER(1,11))
C
C TOPT CALCULATES % SS (TOTAL) REMOVED
      TOPT=PAPER(1,7)+(Z2*D1/EN(NE,6))+(Z1*D2/EN(NE,6))
     1+(Z3*D3/EN(NE,6))
      SUM=100.-TOPT
C
C CALCULATE OVERFLOW AND UNDERFLOW
      STRMO(1,3)=STRMI(1,3)*EN(NE,7)
      STRMO(2,3)=STRMI(1,3)*(1.-EN(NE,7))
C
C ASSUME THAT ALL SUSPENDED COMPONENTS ARE REMOVED AT ONE SETTLING RATE
      DO 11 I=4,14,2
   11 STRMO(1,I)=STRMI(1,I)*SUM
C
C ASSUME THERE IS NO REMOVAL OF DISSOLVED COMPONENTS AND NO CHANGE IN
C     IPH,TEMP.
      STRMO(1,5)=STRMI(1,5)
      STRMO(1,9)=STRMI(1,9)
      STRMO(2,5)=STRMI(1,5)
      STRMO(2,9)=STRMI(1,9)
      STRMO(1,11)=STRMI(1,11)
      STRMO(2,11)=STRMI(1,11)
      STRMO(1,7)=STRMO(1,5)+STRMO(1,6)
C
C UNDERFLOW CONC.  ARE CALCULATED BY MATERIAL BALANCE.
      DO 12 I=4,14,2
   12 STRMO(2,I)=((STRMI(1,3)*STRMI(1,I))-(STRMO(1,3)*STRMO(1,I)))/
     1STRMO(2,3)
      STRMO(2,7)=STRMO(2,5)+STRMO(2,6)
C
      RETURN
      END
```

FIGURE 8-16. PRISTL SUBROUTINE (PRIMARY CLARIFIER) USING SETTLING TEST DATA

If a basin is carefully designed to avoid gross short circuiting and recirculation, the remaining mixing can be attributed to turbulence. We discussed in the previous section how turbulence hinders sedimentation. An early expression for f_R in the presence of turbulence was developed by Camp[5] based on Dobbins' research. The expression is too complicated for use. Takamatsu and Naito have reexamined the problem[7]. They simplify it by separating the turbulence effect on settling velocity from the problem of lateral dispersion. The model can be written as

$$\frac{d^2c}{d\eta^2} - N_{Pe}\frac{dc}{d\eta} - N_{Pe}\,\psi\,c^{\gamma} = 0 \qquad (8\text{-}20)$$

where c represents the dimensionless concentration in a cell extending from the surface to the sludge interface ($c = \bar{M}/M_o$), N_{Pe} is the Peclet No. ($= uL/D_z$), $\eta = z/L$, $\gamma = 1 - e^{-BD_y}$ and $\psi = 1 - Ae^{-\phi/D_y}$: B, A and ϕ are model parameters which must be established by data. The boundary conditions are

$$\frac{dc}{d\eta} = N_{Pe}(1-c) \qquad \text{at } \eta = 0 \qquad (8\text{-}21)$$

$$\frac{dc}{d\eta} = 0 \qquad \text{at } \eta = 1 \qquad (8\text{-}22)$$

Integration must be used to establish c at $\eta = 1$ which is the dimensionless solids concentration in the overflow. Equations (8-20) to (8-22) compose a boundary value problem which may be difficult to solve.

As an approximation, Takamatsu and Naito suggest that the cell is well mixed vertically and they obtain a relatively simple solution:

$$f_R = 1 - \frac{N_{Pe}(\alpha - \beta)\,e^{\alpha + \beta}}{\alpha^2 e^{\alpha} - \beta^2 e^{\beta}} \qquad (8\text{-}23)$$

where α, β are the roots

$$\alpha, \beta = \frac{N_{Pe}}{2}\left[1 \pm \sqrt{1 + \frac{4\psi\lambda}{N_{Pe}}}\right] \qquad (8\text{-}24)$$

Five parameters, B, A, ϕ, D_y, D_z must be evaluated from basin data and settling test data must be at hand to obtain $\lambda = v/v_o$ in order to use eqn. (8-23). It is not a convenient method for estimating f_R.

In a primitive analysis, Thirumurthi[11] considers just dispersion along the mean flow direction (z axis) in a basin. However, the dispersion in this case can result from the circulation pattern as well as from turbulence. The relationship which can be deduced from the assumptions used by Thirumurthi is[16]

$$\bar{f}_R = f_R + (k\bar{t})^2 D (f_R - 1) \qquad (8\text{-}25)$$

In this expression f_R is the fraction removed predicted by eqns. (8-10), (8-13), (8-15) or (8-16), (8-17) or directly from Figure 8-15. It is the fraction removed assuming an ideal basin. Thirumurthi assumes that settling is a first order phenomena.

The assumption that settling of a class 1 suspension could be modelled as a kinetic phenomena was explored by Singh[14]. Singh found that a first order kinetic model satisfactorily reproduced the performance of a full-scale primary clarifier and proposed an interesting stochastic model for a clarifier on this basis. The 1st order expression is

$$1 - f_R = e^{-kA_{set}/Q} \qquad (8\text{-}26)$$

or in terms of the overflow rate

$$1 - f_R = e^{-k/v_o} \qquad (8\text{-}27)$$

---

[16] Stepko, W.E., "Comparison of Mathematical Models of a Continuous Sedimentation Basin", M.A.Sc. Thesis, Dept. of Chem. Eng., Univ. of Waterloo (Waterloo, 1970)

We have recently found that the 1st order model is satisfactory because the settling curve of a waste may be closely fitted by an exponential expression.[17] Indeed k in eqn. (8-26) or (8-27) may be evaluated from a curve such as Figure 8-14 through the expression

$$P(v) = e^{-k/v} \left(1 + \frac{k}{v}\right) \tag{8-28}$$

If k is evaluated from settling data through eqn. (8-28), f_R obtained from eqns. (8-26) or (8-27) will be the fractional removal of suspended solids in an ideal basin. Basin performance, $\bar{f}_R$, may be found by substituting f_R in either eqn. (8-18) or eqn. (8-25).

Equations (8-26) or (8-27), however, model full-scale clarifiers satisfactorily if k is evaluated from plant data. In an independent study Fitz[18] was able to correlate the performance of a laboratory scale clarifier with the same equations. Mixing in the basins, thus, may be incorporated in k.

Two empirical models for primary settlers are in use. The first was proposed by Smith[19]; its development was discussed in Chapter 7. The Smith model is

$$f_R = A\, e^{-\alpha v_o} \tag{8-29}$$

Smith suggested that $A = 0.82$ and $\alpha = 3.6 \times 10^{-4}$ if the units of v_o are gallons (U.S.)/day/ft^2. Either eqn. (8-29) or eqn. (8-26) have been used in the simulation of Ontario waste treatment plants carried out at the University of Waterloo over the past few years[20]. The coefficient

[17] Sakata, N. and Silveston, P.L., "Exponential Approximation for Settling Rate", Unpublished Manuscript (1973)

[18] Fitz, L.W., "The Use of Tracers in Sedimentation Basins", M. Eng. Thesis, McMaster University, Hamilton, Ontario (1969)

[19] Smith, R., "Preliminary Design and Simulation of Conventional Waste Water Renovation Systems Using the Digital Computer", Water Pollution Control Research Series WP-20-9 F.W.P.C.A./U.S.D.I. (Washington, 1968)

[20] see, for example, Silveston, P.L. "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research, 6, 1101 (1972)

α is not universal but changes for each waste treatment plant. For example $\alpha = 0.86 \times 10^{-4}$ for the Kitchener, Ontario W.T.P. Goering[21] also found that Smith's values of α and A were not satisfactory.

Voshel and Sak's[22] empirical model for a primary clarifier has been used by Fan and his research group at Kansas State University. The model is

$$f_R = \frac{1 - A\,(M_o)^{\alpha}}{(v_o')^{\beta}} \qquad (8\text{-}30)$$

and Fan et al.[23] suggest $A = 0.568$, $\alpha = 0.27$ and $\beta = 0.22$ if the units of M_o (suspended solids in the influent) are mg/l. and mgd (U.S.)/ft^2 for v_o' (overflow rate). If a polymeric flocculating agent is used in the clarifier at a dosage of 1 mg/l., the constants are $A = 0.779$, $\alpha = 0.17$ and $\beta = 0.13$.

Most investigations and modelling of primary clarifiers have dealt only with suspended solids. Some of the solids contribute to the BOD as well as to the levels of phosphorus and nitrogen in the waste. Clarification therefore will reduce both BOD and nutrients in the overflow. The question is whether the reduction in the suspended matter contributions to BOD and nutrients are the same fraction as that of the suspended matter as a whole. Smith[19] recommends that the same fractional reduction calculated for suspended solids be used to compute the reduction in suspended solids contribution to BOD. Our studies of Ontario treatment plants suggests this is not satisfactory. For the Kitchener W.T.P., we find that α in eqn. (8-29) is 0.86×10^{-4} for suspended solids, but is 1.5×10^{-4} for suspended BOD assuming that suspended solids account for

---

[21] Goering, S.W., "A Computer Model of the Sewage Treatment Process of Boulder Colorado", M.Sc. Thesis, Dept. of Chem. Eng., Univ. of Colorado (1972)

[22] Voshel, D. and Sak, J.G., "Effect of Primary Effluent Suspended Solids and BOD on Activated Sludge Production", J.W.P.C.F. 40, Part 1, 203 (1968)

[23] Chen, G.K., Fan, L.T. and Erickson, L.E.,"Computer Software for Wastewater Treatment Plant Design", J.W.P.C.F. 44, 747 (1972)

70% of the waste BOD$^{(20)}$. We have not had sufficient data to test the reduction of the suspended solids contribution to nutrients as a function of the overall suspended solids reduction.

Figure 8-17 shows a listing of a subroutine employing eqn. (8-29), but with different values of α for BOD (S_*) and suspended solids (M). Fractional reduction of volatile suspended solids is assumed to be the same as the fractional reduction of total suspended solids. The program is written using the SEPSIM "language" as discussed in Chapter 7.

```
      SUBROUTINE PRISTL
C
C   SMITH MODEL FOR PRIMARY SETTLER.
C  DIGSTR AND PRISTL MODELS OBTAINED FROM PAPER BY R.SMITH,W.CP.C.S.,
C   WP-20-8,CINCINNATI,OHIO.,MARCH,1968.
C
C  SMITH HAS PROPOSED THE FOLLOWING RELATIONSHIP,
C
C                            FRPS=0.82*EXP(-GPS/X)
C
C  WHERE,GPS=OVERFLOW RATE FOR SETTLER(GPD/FT.**2)
C        X=CHARACTERISTIC PARAMETER
C        FRPS=FRACTION OF SOLIDS ENTERING SETTLER WHICH ARE REMOVED
C        FROM THE MAIN STREAM AND PASS INTO UNDERFLOW.
C
C  SMITH ALSO DEFINES A QUANTITY,URPS, AS THE RATIO OF INLET SOLIDS
C  CONCENTRATION TO UNDERFLOW SOLIDS CONCENTRATION.
C
C  THE PROCESS STREAM VECTOR IS AS FOLLOWS,
C     1. STREAM NUMBER.
C     2. STREAM FLAG.
C     3. FLOW RATE(MGD).
C     4. SUSPENDED SOLIDS CONCENTRATION.
C     5.DISSOLVED BOD CONCENTRATION(MG/L).
C     6. SOLID BOD CONCENTRATION(MG/L).
C     7. TOTAL BOD CONCENTRATION(MG/L).
C     8. VOLATILE SUSPENDED SOLIDS CONCENTRATION(MG/L)
C
C  THE EQUIPMENT VECTOR IS AS FOLLOWS,
C
C     3. DIAMETER OF SETTLING TANK(FT.)
C     4. NO. OF TANKS.
C     5. X(BOD)
C     6. A CONSTANT(0.82)
C     7.URPS
C     8. X(SS)
C     9. A CONSTANT(0.82)
C     10. URPS
C
C*********SEPSIM COMMON AND DIMENSION DECK*********
C
C     SUM ALL FLOWS IN.
      PAPER(1,1)=0.0
      DO 1 I=1,NIN
 1    PAPER(1,1)=PAPER(1,1)+STRMI(I,3)
      DO 3 J=4,NSLMAX
      K=J-2
      PAPER(1,K)=0.0
      DO 4 I=1,NIN
 4    PAPER(1,K)=PAPER(1,K)+STRMI(I,J)*STRMI(I,3)
 3    CONTINUE
C
C     CALCULATE OUTFLOWS.
      PAPER(2,J)=PAPER(1,1)
      DO 6 I=4,NSLMAX
      K=I-2
```

```
C
C     WEIGHTED MEAN CONCENTRATION.
      PAPER(2,I)=PAPER(1,K)/PAPER(1,I)
6     CONTINUE
C
C  START OF SETTLER CALCULATIONS.
C
C  FIND CROSS-SECTIONAL AREA OF ONE TANK.
      PAPER(1,1)=(3.1416)*(EN(NE,3)**2)/4.
C
C  MULTIPLY BY NO. OF TANKS.
      PAPER(1,2)=PAPER(1,1)*EN(NE,4)
C
C  FIND GPS-OVERFLOW RATE.
      PAPER(1,3)=PAPER(2,3)*1.E+06/PAPER(1,2)
C
C  FIND EXPS(PAPER(1,6))
      PAPER(1,4)=-PAPER(1,3)/EN(NE,5)
      PAPER(1,5)=EXP(PAPER(1,4))
      PAPER(1,6)=EN(NE,6)*PAPER(1,5)
      PAPER(1,7)=1.-PAPER(1,6)
C
C  PAPER(1,8) IS THE RATIO OF UNDERFLOW TO TOTAL FLOW.
      PAPER(1,8)=PAPER(1,6)/EN(NE,7)
      PAPER(2,9)=-PAPER(1,3)/EN(NE,8)
      PAPER(2,9)=EXP(PAPER(2,9))
      PAPER(2,9)=EN(NE,9)*PAPER(2,8)
      PAPER(2,10)=PAPER(2,9)/EN(NE,10)
      PAPER(2,10)=(PAPER(2,10)+PAPER(1,8))/2.
C
C  SET NO. OF ENTRIES IN EQUIPMENT VECTOR FROM THIS SUBROUTINE
      EN(NE,2)=10.
      KEY(NE)=7
      DATA (NAMEN(7,I),I=1,10)/'NO. ','NTRY','DIA','NTES','BOD.',
     *'CST.','UNPS','S.S.','CST.','UNPS'/
C
C  OUTPUT CALCULATIONS.
      STRMO(2,3)=PAPER(2,3)*PAPER(2,10)
      STRMO(1,3)=PAPER(2,3)-STRMO(2,3)
      DO 70 I=4,K,2
      VAR=PAPER(2,9)
      IF(I.EQ.6)VAR=PAPER(1,6)
      STRMO(1,I)=PAPER(2,I)*(1.-VAR          )*PAPER(2,3)/STRMO(1,3)
      STRMO(2,I)=PAPER(2,I)*VAR          *PAPER(2,3)/STRMO(2,3)
 70   CONTINUE
      STRMO(1,5)=PAPER(2,5)
      STRMO(2,5)=PAPER(2,5)
      STRMO(1,7)=STRMO(1,6)*STRMO(1,5)
      STRMO(2,7)=STRMO(2,6)*STRMO(2,5)
C
      RETURN
      END
```

FIGURE 8-17. MODEL SUBROUTINE FOR A PRIMARY CLARIFIER

We recommend eqn. (8-26) for modelling primary clarifiers where k is either evaluated from measurements on full-scale basins or through eqn. (8-28) from column settling data. If RTD data is available, eqn. (8-18) can be utilized if k is obtained from settling data. Settling column experiments should be repeated using BOD and nutrient measurements so as to obtain separate k's for suspended solids contributions to BOD, phosphorus and nitrogen.

8.5 Thickener Models

In this section we will deal with models for full-scale sludge

thickeners as well as for thickening that occurs in the sludge blanket of settlers. A problem immediately arises. Whereas the influent is introduced at one point in a thickener, it is spread over the entire surface of the sludge layer at the bottom of a clarifier. We will follow a recent study by Tracy and Keinath[24] who assume that this makes no difference in the thickening operation. If we assume steady state in the thickener (again neglecting the effect of periodic draw off normally practiced for primary clarifiers), at any plane in the sludge layer

$$J_u = \frac{M_u Q}{A} = (v_z + u)\, M \qquad (8\text{-}31)$$

where J_u is the solids flux which consists of a contribution due to settling (v_z = settling velocity) and one due to the bulk movement of the sludge (u = superficial withdrawal velocity) caused by withdrawing it at the bottom of the thickener. Equation (8-31) applies at the surface of the sludge blanket, thus, if we are interested in a simulation with a specified withdrawal rate Q (ft^3/min)

$$M_u = M_b\, (v_b + Q/A)/Q/A \qquad (8\text{-}32)$$

According to Kynch's theory, the settling velocity at the top of the blanket (v_b) is uniquely determined by the concentration M_b[25]. Thus, if we can relate v_b to M_b or if we have measured values of v_b, eqn. (8-32) provides a simulation model for a thickener.

We pointed out while discussing the theory of thickening that sludge subsidence can be viewed as controlled by flow through a matrix of solids. There have been some attempts to calculate settling velocity theoretically from expressions for the velocity of liquids in packed beds of solids[25]. For chemical sludges,[25]

---

[24] Tracy, K.D. and Keinath, T.M., "Dynamic Model for Thickening of Activated Sludge", Paper, 74th National Meeting, A.I.Ch.E., New Orleans (March, 1973)

[25] Scott, K.J., "Mathematical Models of Mechanism of Thickening", Ind. and Eng. Chemistry Fund, 5, 109 (1966)

$$v = K \frac{(1 - \phi_r M)^3}{M} \qquad (8\text{-}33)$$

has been used where K is a constant and ϕ_r is the ratio of liquid volume bound to a solid particle to the weight of the particle. M is a solids concentration (mg/l.). Other equations use an exponent of 2 instead of 3. If $M \approx M_b$, eqn. (8-33) gives the desired expression for v_b.

Dick and Ewing[26] demonstrate that v_b depends on sludge layer depth for an activated sludge up to depths less than 7.5 ft. They derive an expression for the effect of depth (h),

$$v_b = \frac{h}{Be^{\gamma M_b} + h/(v_b)_{max.}} \qquad (8\text{-}34)$$

where B and γ are constants specific to a sludge. $(v_b)_{max.}$ is the maximum interface settling velocity. This will be an initial velocity. It can be evaluated by settling tests made at more than one depth.

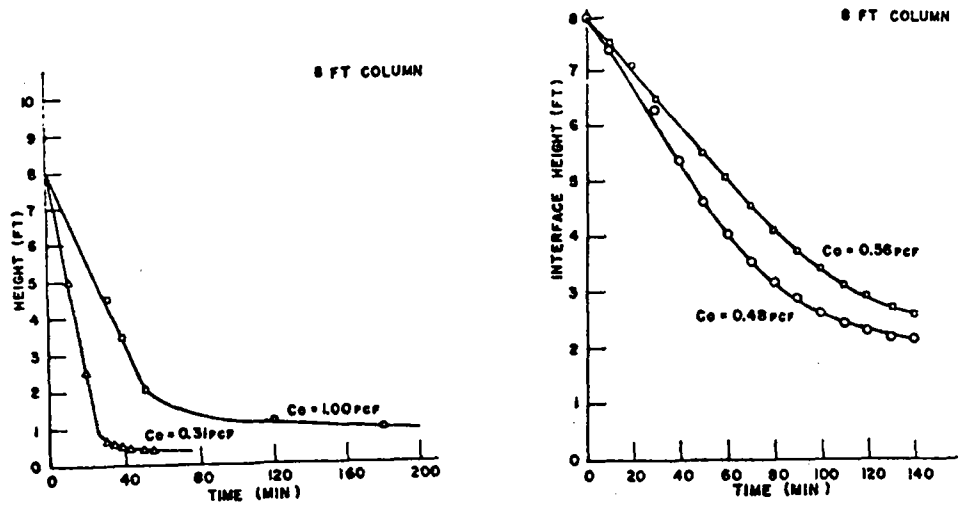
General practice for thickener design is to measure settling velocities as sludge height vs. time. Normally, the measurements will be repeated. Applicability of Kynch's theory to a specific sludge can be checked by establishing whether the experimental sludge height vs. time curve for the lowest sludge concentration can be obtained from v_b measurements at increasing sludge concentrations[26]. Figure 8-18 a), b) show sludge settling curves. The initial velocity is the slope at zero time.

A simple empirical model for underflow concentration, quite similar to eqn. (8-32), has been proposed by Eckenfelder and his students[27,28]

---

[26] Dick, R.I. and Ewing, B.B., "Evaluation of Activated Sludge Thickening Theories", J. Sanitary Eng. Div., Proc. A.S.C.E. 93, SA4, 9 (1967)

[27] Edde, H.J. and Eckenfelder, W.W., Jr., "Theoretical Concepts of Gravity Sludge Thickening and Methods of Scale-up from Laboratory Units to Prototype Design", Tech. Rep't. EHE-02-6701, CRWR-15, Center for Research in Water Resources, Univ. of Texas (1967)



a) PRIMARY CLARIFIER SLUDGE

b) FINAL CLARIFIER (ACTIVATED) SLUDGE

FIGURE 8-18. SUPERNATANT-SLUDGE INTERFACE HEIGHT VERSUS TIME FOR TWO AUSTIN, TEXAS SLUDGES (PCF = LBS/CU. FT.)*

$$M_u/M_o = 1 + \frac{D}{\left(\frac{M_o Q_o}{A_{set}}\right)^n} \qquad (8\text{-}35)$$

where Q_o is the flow to the thickener in suitable units and A_{set} is the surface area for the thickener. For the sludge blanket in a clarifier, $M_o Q_o$ would be the mass (lbs) of dry sludge drawn off/day. D is a constant which relates blanket depth in the full scale unit to the depth in a batch test. It is a strong function of M_o. The exponent characterizes the sludge and is independent of the operation of the thickener. Edde and Eckenfelder[27] report values of n for sewage sludges between 0.25 and 0.75.

A number of models to describe thickening of compressed sludge have been proposed. The problem is that the so-called compression zone

*Figure taken from reference (27).

[28]Eckenfelder, W.W. Jr., and Mancini, J.L., "Thickening of Industrial Sludges", Proc. 5th Texas Industrial Water and Waste Conf. (1965)

forms only a part of the sludge blanket. This is illustrated in Figure 8-19 taken from Eckenfelder[3].

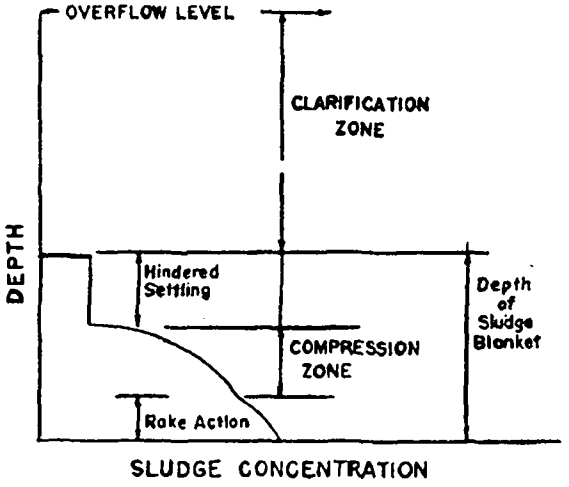


FIGURE 8-19. SOLIDS CONCENTRATION PROFILE IN A CLARIFIER*

The compression zone models are useful as approximation if we recognize that they will contain constants which must be evaluated by fitting operating data. Thus, the "error" built in by applying the models to the entire sludge blanket rather than the compression zone can be taken up in the constant(s).

The depth of the blanket in a thickener can be estimated from a formula proposed by Eckenfelder and Mancini[28]

$$h = \frac{B\tau_{bl}}{\bar{M}} \left(\frac{M_o Q_o}{A_{set}} \right) \qquad (8\text{-}36)$$

where τ_{bl} is the holdup time in sludge blanket, $\bar{M}$ is the mean of the influent and underflow sludge concentrations and B is a constant. For a clarifier, the loading term is the mass of sludge withdrawn in the underflow per unit time and unit clarifier surface area.

*Figure taken from reference (3) with the kind permission of the publisher.

On the assumption that subsidence is a first order phenomena[29], the relationship between sludge concentration and detention time is

$$\frac{M_\infty - M}{M_\infty - M_c} = e^{-\beta(t - t_c)} \qquad (8\text{-}37)$$

where M_c is the critical solids concentration, that is the concentration at the beginning of the compression zone, M_∞ is the maximum solids concentration, t_c is the holdup time of sludge in the thickener before it enters the compression zone and t is the time in the zone to reach a concentration M. Using the form of eqn. (8-37), an approximate model for the underflow in a thickener or a clarifier would be

$$\frac{M_\infty - M_u}{M_\infty - M_b} = B' e^{-\beta' \tau_{bl}} \qquad (8\text{-}38)$$

where B' and k' are constants dependent upon the sludge and the thickener operation. Edde and Eckenfelder[27] eliminate M_∞ and show that full-scale thickener data is well correlated by

$$M_u = \frac{M_b}{1 - B' M_b h e^{-\beta' \tau_{bl}}} \qquad (8\text{-}39)$$

In the above equation, the constants B', β' must be established from operating data.

Models are not widely used for thickener design. For simulation, we recommend the Eckenfelder and Edde equation, eqn. (8-35). The constants n, D in the equation must be evaluated from plant data. Other relations require information such as detention time and height or v_b which may not be available.

8.6 Final Clarifier Models

Progress on modelling final clarifiers has been rapid only in

---

[29] Roberts, E.J., "Thickening - Art or Science", Mining Eng., 1, 61-64 (1949)

the last decade. We will review in this section just the empirical models which have been suggested for this unit. Models based on settling test data, discussed in a previous section, are applicable to final clarifiers as well as primary units.

Smith and Eilers[30] quote a study by R.V. Villiers for the relation

$$1 - f_R = \frac{A\,(v_o')^n}{M_o^m\,(\tau_{act})^p} \qquad (8\text{-}40)$$

In this expression, M_o is the mixed liquor suspended solids (mg/l.) fed to the clarifier, v_o' is the overflow rate as gpd/ft^2 and τ_{act} is the holdup time in the aerator in hours. From bench scale experiments, Villiers estimated the following values $A = 556$, $n = 0.49$, $m = 1.8$ and $p = 0.44$.

Planz[31] correlated f_R data against loading. His correlation may be expressed as

$$1 - f_R = Cv_o \qquad (8\text{-}41)$$

where C is a constant whose value depends on the activated sludge handled as well as the units used for v_o.

Fan and his co-workers[32] have made use of a model proposed by Takamatsu and Naito in their studies; namely,

$$M_e = p(M_o)^{\alpha}\, e^{-\beta\,\tau_{set}} \qquad (8\text{-}42)$$

---

[30] Smith, R. and Eilers, R.G., "A Generalized Computer Model for Steady State Performance of the Activated Sludge Process", FWQA Report No. TWRC-15, Cincinnati Water Research Laboratory, Cincinnati, Ohio (1969)

[31] Planz, P., "The Sedimentation of Activated Sludge in Final Settling Tanks", J. Int. Assocn. of Water Pollution Research, 2, No. 1, 80 (1968)

[32] Fan, L.T., Chen, G.K.C., Erickson, L.E. and Naito, M., "Effects of Axial Dispersion on the Optimal Design of the Activated Sludge Process", Water Research 4, 271 (1970)

where τ_{set} is the holdup time in the clarifier and p, α and β are constants. Values used in Fan's study were $p = 2.1$, $\alpha = 0.5$. In an earlier paper[33], the relation used is somewhat more complex,

$$M_e = M_o - \frac{\bar{v}L}{h}(1 - 0.81\, e^{-1.2D_z})\, pM_o^{\alpha} \qquad (8\text{-}43)$$

or

$$f_R = \frac{p\bar{v}L\, M_o^{\alpha - 1}}{h}(1 - 0.81\, e^{-1.2D_z}) \qquad (8\text{-}44)$$

In these equations $\bar{v}$ is the mean settling velocity of the activated sludge, L is the tank length (a rectangular tank is assumed), h is the effective depth and D_z is a dispersion coefficient which can be crudely estimated from tracer curves as described in the section on Theory.

Recently, a U.S. report[34] has proposed a group of empirical models based on full-scale plant tests. For the overflow,

$$M_e = \frac{B(v_o')^n\, (S_oQ_o/MV)_{act}^{m}}{(M_o)^p\, (\tau_{act})^r} \qquad (8\text{-}45)$$

where the term $(S_o^*Q_o/MV)_{act}$ is the BOD loading in the aerator, e.g. lbs. of BOD/day/lb. of MLSS, and M_o, v_o' and τ_{act} are as defined previously. BOD loading and holdup time in the aerator (τ_{act}) are included to allow for sludge age which determines the settling characteristics of the sludge.

The underflow from a final clarifier is frequently assumed to be given by the sludge volume index:

$$M_u = \frac{10^6}{SVI} \qquad (8\text{-}46)$$

---

[33] Naito, M., Takamatsu, T. and Fan L.T., "Optimization of the Activated Sludge Process-Optimum Volume Ratio of Aeration and Sedimentation Vessels", Water Research 3, 433 (1969)

[34] Rex Chainbelt Inc., "A Mathematical Model of a Final Clarifier", Water Pollution Control Research Series No. 17090 FJW, E.P.A. (Washington, D.C., 1972)

where M_u is in units of mg/l. The index is the volume in millilitres (ml.) occupied by 1 gm. of sludge after a settling time of 30 minutes in usually a 1 l. graduate. It is given by the formula

$$SVI = \frac{\% \text{ settleable solids (30 min.)} \times 10{,}000}{M_o}$$

where the units of the suspend solids (MLSS) influent to the clarifier are mg/l. The index is sometimes referred to as the Mohlman SVI. Equation (8-46) is the basis of the Rex Chainbelt formula. SVI data from full-scale final clarifier were correlated against the fraction of volatile suspended solids in the MLSS and the BOD loading as lbs. BOD/day/lb. MLSS to give

$$SVI = C\left(\frac{X_e}{M_e}\right)^{\alpha}_{act} \left(\frac{S_o Q}{MV}\right)^{\beta}_{act} \tag{8-47}$$

Consequently,

$$M_u = \frac{C'}{(X_e/M_e)^{\alpha}_{act} \left(\frac{S_o Q}{MV}\right)^{\beta}_{act}} \tag{8-48}$$

The Rex Chainbelt report[32] suggest $C = 540$, $C' = 1850$, $\alpha = 4.4$ and $\beta = 0.21$.

In our SEPSIM and WATCRAP-PACER studies at Waterloo, only the Villier relation (eqn. (8-40)) was tested. It was found to be unsatisfactory. f_R was either specified and thereby treated as a model parameter or it was estimated using the simple kinetic models discussed in the primary clarifier section. M_u was always calculated as a fixed multiple of M_o. Smith and Eilers report that the Planz and Rex Chainbelt models also are not satisfactory[30]. In this curious situation in which none of the models proposed is universal, we recommend that settling data models (section 8.5) should be used for design. Since it is well established that the sludge age (controlled by operation of the aerator) has an important influence on settling in the final clarifier, we recommend

using eqns. (8-45) and (8-48) for simulation. The constants in the equations, however, should be determined from plant data.

8.7 Design Models

The objective in design is to achieve some specified performance at the least possible cost. In principle this should be accomplished through optimization involving all variables in the system. So many variables are involved in even simple systems that this is a staggering task without digital computers and a difficult one even using them. Instead of attempting to achieve a global optimization, designers break up waste treatment systems into units. Each unit is designed more or less independently of the rest of the system. To "break" the system in this way, a performance must be specified for each unit. The individual units are themselves complex so current design practice is to break these down into components through specifying the performance of each component. Specifications are based frequently on extensive experience so that this fragmented design procedure often achieves a surprisingly good sub optimal system.

We will refer to the specification just described as design parameters and use (DP) to represent them. Use of design parameters does not completely remove economic considerations from design. Cost considerations still determine which rake system to use for sludge collection even though the decision on clarifier size and slope of the bottom will be made using design parameters without direct reference to cost.

Turning now to the subject of this chapter, we will discuss clarifiers first. Considering the function of clarifiers, the logical design parameter would be M_e, the concentration of suspended solids in the overflow. In Canada, the design of treatment plants is controlled by provincial authorities. Such control is usually exercised through specifications for the process units. Ontario, for example, makes use of "Standards for Sewage Works" prepared by the Upper Mississippi River Board of Public Health Engineers and the Great Lakes Board of Public Health Engineers. The specifications for clarifiers are stated in terms of overflow rate as shown in Table 8-1.

TABLE 8-1. ONTARIO OVERFLOW RATE SPECIFICATIONS FOR CLARIFIERS

Unit	Size (MGD)	Overflow Rate (gpd (U.S.)/ft^2)
Primary Treatment	< 1	600
	> 1	can exceed 600
Secondary Treatment		
Primary Unit	---	1,000
Final Unit (act. sludge)	> 2	1,000
	< 2	800
(trick. filter)	---	800

Weir loading limits are given as well as clarifier depths. The consequence of these specifications is that M_e functions as a "weak" design parameter.

Nonetheless, it is advisable to check the performance of clarifiers either through simulation using the v_o specification to see if M_e values are reasonable or by using M_e as a design parameter and checking if the v_o calculated exceeds the specification. M_e is "weak" in the sense that an overriding specification may be encountered.

The models in the clarifier sections were set up for simulation. If, however, v_o is wanted rather than M_e, the models can be solved for v_o instead of for f_R or M_e. For example, eqn. (8-27), the simple kinetic model, can be solved for v_o to give

$$v_o = \frac{kh}{\ln (M_o/M_e)} \tag{8-49}$$

which would be a "design" model. Rearrangement of the settling velocity models, such as eqns. (8-10) or (8-15), to solve for v_o is also possible, All these models contain h, the effective depth, which then must be specified as a design parameter.

Once v_o is available, the surface area of the clarifier is

easily calculated from the design flow rate. Weir length and design do not appear in clarifier models. They must be set by experience within the limits specified by the "standards".

Overflow performance dominates clarifier design. For final clarifiers, however, the underflow solids concentrations are important and M_u may serve as a second design parameter. Unfortunately the empirical model for M_u, eqn. (8-48), is of little use for clarifier design because it is written in terms of variables operative in the aerator. Thus, the model must be considered in aerator design. Thickener equations are written in terms of M_u and sludge blanket variables. Equation (8-39), for example, relates M_u to blanket height and holdup time. Treating holdup time as a design parameter, permits an estimate to be made of the blanket height and, with height available A_{set} can be checked to see if it is reasonable. Sludge holdup time and M_u, therefore, under some conditions could fix clarifier surface area in place of the v_o specification or M_e.

Thickener models can be used to calculate thickener surface areas as we have just indicated. Like clarifiers, thickener depths are constrained by practice so depth is not an important design parameter. In practice, thickeners are not designed from mathematical models but rather directly from blanket height vs. time data or initial interface velocity vs. solids concentration data. The procedures estimate a critical settling velocity and use the solids concentrations at the critical point to calculate a limiting mass flux or they estimate the flux graphically. The flux sets the thickener area. Although these procedures could be computerized, the resulting subroutines would be tedious to develop and probably quite long. For most purposes, the graphical operations could be performed apart from a computer run. Only the flux or the settling velocity obtained would be entered. The thickener area from this starting point can be calculated through a few simple statements.

9 ACTIVATED SLUDGE SYSTEMS

The activated sludge process is by far the most frequently employed method of secondary treatment in Canada, both in terms of the number of installations and in terms of the total volume of wastes treated. Developed in 1914 in the U.K. from fill and draw aeration - a batch process - it has undergone considerable change. A variety of designs for contacting the waste and biomass having widely different contact times are currently used. Many of these designs are recent; the result of a large and continuing research effort on the basic process. Curiously the name - activated sludge - is drawn from the 1914 discovery that the sludge remaining in the aeration tank after drawing is "active" and if left in the tank accelerates the oxidation of the next batch.

In most treatments of the process, the secondary clarifier is discussed together with the biological reactor. From a modelling standpoint, the two parts of the process are quite different. Thus, we have separated them and we discuss clarifiers in Chapter 8.

Many phenomena are important in activated sludge systems ranging from cellular biology to hydrodynamics. Although in some cases the behaviour of the process is governed by just a few physical or biological processes, we must look at all the phenomena for the purposes of general modelling. In this chapter, we review briefly the operation of activated sludge systems; we then turn to the phenomena occurring in the process, and finally we list and discuss models for different steps in the process. The sum of the step models constitute the model for the entire process. Our objective in the chapter is solely the presentation of the models. The "introductory material" is intended to provide background for the choice of a particular model among a group of possible models, understanding of what the model represents, and, of course, understanding for the proper application of the model. All of the "introductory" material has been taken from standard texts[1-4], as indeed have many of the models.

---

[1] Eckenfelder, W.W., Jr. and O'Connor, D.J., "Biological Waste Treatment", Pergamon Press (New York, 1961).

[2] Eckenfelder, W.W., Jr. and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970).

9.1 Operation

The function of the activated sludge system is to remove colloidal and soluble biodegradable organic matter from a waste stream. It can be a most effective system. Reduction of the remaining BOD after clarification of 85 to 90 percent is routine. The system operates through a suspended biomass which feeds on the wastes, converting a portion to cellular matter and oxidizing the remainder. Through these steps, some of the organic nitrogen is released as nitrites or nitrates, and some of the organic phosphorus is solubilized.

In the conventional process, waste water and return sludge enter at one end of a long narrow tank. This mixture, called the mixed liquor, flows longitudinally through the tank in a spiral pattern induced by the diffused air aeration system. Modern designs introduce partitions into the tank with flow either over or through subsurface openings. This splits the process into stages. Mechanical aerators have replaced the diffused air systems. Figure 9-1 shows a typical activated sludge system with partitioned tanks.

Modifications of the basic process are shown in Figure 9-2. The basic differences occur in the point at which the primary effluent is introduced into the aeration tank and mixed with the return sludge, mixing characteristics in the tank and whether aeration of the return sludge prior to contact with the incoming waste is used.

Aeration of the return sludge has been practiced for many years. Originally, reaeration was used to keep the return sludge aerobic. A small tank was used, and in some cases, digester supernatant was introduced into this tank instead of directly into the main contactor. Contact stabilization is a reaeration system. However, this variant is based on observations that the soluble fraction of the organic material in waste water is almost entirely removed after just short contact times. Therefore, in this variant, the primary effluent is mixed with the return

---

(3) "Biological Waste Treatment", Notes for a course at the University of Waterloo (July, 1967).

(4) Eckenfelder, W.W., Jr. and McCabe, Joseph (Editors), "Advances in Biological Waste Treatment", MacMillan Co. (New York, 1963).

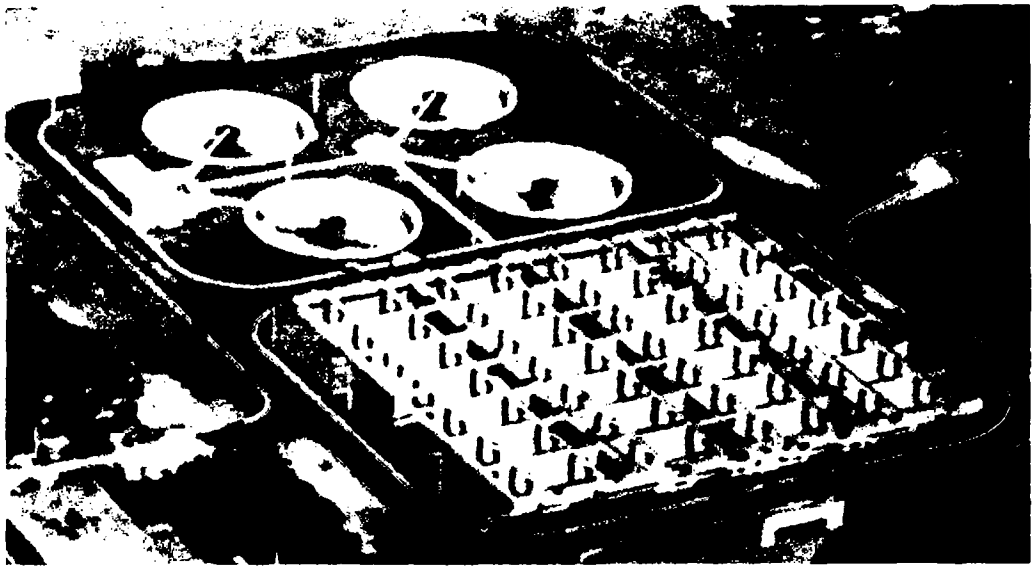


FIGURE 9-1. EMPTY PARTITIONED ACTIVATED SLUDGE TANKS SHOWING A STAGED PARALLEL ARRANGEMENT

reaerated sludge for about thirty minutes to two hours. This is long enough to reduce soluble organic matter to a desired effluent concentration. Colloidal and particulate matter are also incorporated into the activated sludge floc particles in the contact zone. The sludge solids are separated in the final clarifier and the concentrated sludge is reaerated prior to its return for an additional two to four hours in the stabilization or reaeration tank. In some plants, the stabilization zone and the contact zone are not physically separated (see Figure 9-2).

Step aeration distributes the waste across the tank (Figure 9-2), and, in this way, permits operation at the highest BOD reduction rates. Consequently, BOD removal per unit aerator volume is high. Level of BOD in the effluent, however, tends to be higher and nitrification does not take place.

The completely mixed variant is used extensively in laboratory-scale units to evaluate the parameters which affect the activated sludge process. Recently, this variant has been installed for the treatment of municipal and industrial wastes. In the system, the concentration of oxygen and of the substrate is uniform throughout the tank. Control of the oxygen level is improved, and the system is relatively resistant to shock

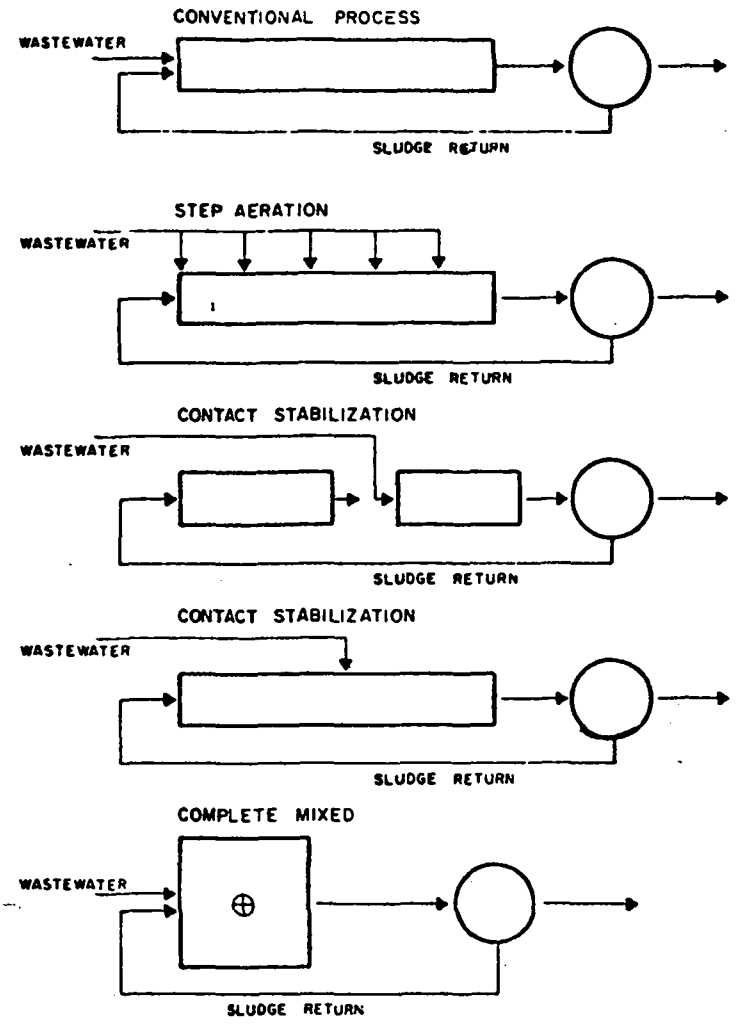


FIGURE 9-2. CONTACTING VARIATIONS OF ACTIVATED SLUDGE SYSTEM*

loading since the influent is distributed uniformly throughout the tank.

Extended aeration is a modification of the basic activated sludge process which is characterized by relatively low organic loadings. Contact time is long so that the sludge produced during biodegradation is also stabilized. Nonbiodegradable solids tend to accumulate so some sludge must be wasted periodically. A flow sheet would show just a contactor if sludge is wasted to the receiving stream, or it would look like

*Figure taken from reference (6).

the conventional process (Figure 9-2) except that the underflow from the clarifier is not recycled.

Comparison of the variants as full-scale plants is practically impossible because conditions of the sewage or plant operation are never identical. Laboratory scale comparisons of contact stabilization with the conventional process at the same loading rates show essentially the same effluent BOD levels[5].

A wide variety of aeration devices are now in use. Older installations employ porous plate diffuser or pipe sparger with fine holes. Air is compressed and is forced through the plate or holes generating a cloud of fine bubbles. Locating the diffusers eccentrically (see Figure 9-3 - bubble aeration) initiates an air lift which results in a spiral flow pattern. This pattern mixes the vessel contents and keeps

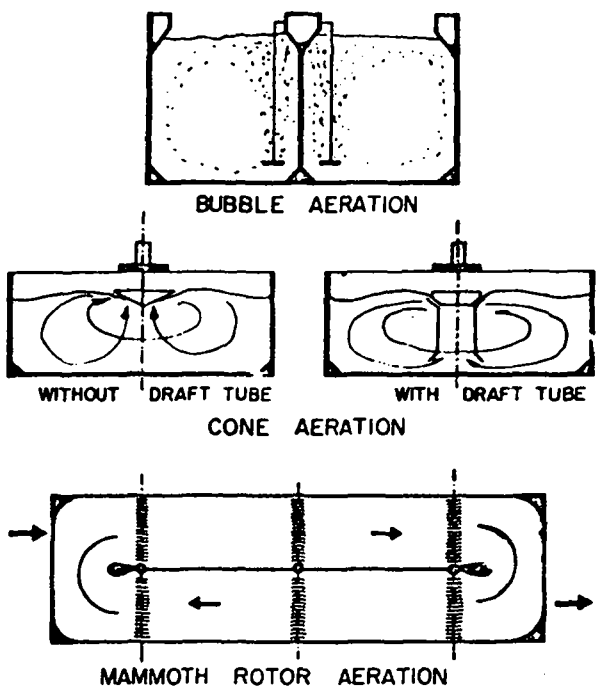


FIGURE 9-3. TYPICAL AERATION SYSTEMS OF ACTIVATED SLUDGE UNITS*

(5) "Water Pollution Research", Dept. Scient. and Indust. Research, H.M. Stationary Office (London, 1967), also 1968.

* Figure taken from reference (6).

the biomass suspended. Depletion of oxygen in the fine bubbles makes the gas phase mass transfer resistance important. The need for compressors raises capital and operating costs. However, use of oxygen in place of air appreciably improves the performance of these systems and may keep existing units in operation despite higher operating costs.

Newer units use turbine or pump-type aerators or surface devices. Two types of surface devices are shown in Figure 9-3. The efficiency of the cone aerator is controlled by the depth of immersion of the rotor, r.p.m., and the use or absence of draft tubes. Maintaining a good suspension can be a problem with surface aerators. A high level of turbulence is required. Consequently, the device must be designed to deliver some minimum horsepower per unit volume of the tank. Draft tubes are often used to improve mixing and prevent sludge deposits.

Brush aerators may be of the mammoth type shown in Figure 9-3. The more popular choice is a cage-type rotor. This rotor forms a sheet-like spray with excellent oxygen transfer properties.

Pump aerators work on the Bernoulli principle. Air is drawn into the liquid in the "eye" of the pump. Intimate mixing occurs in the casing and the discharge nozzle. An alternative arrangement is to use a turbine (for mixing) and a coarse holed ring sparger as shown in Figure 9-4. The turbine shatters the large bubbles leaving the sparger to form the desirable bubble cloud.

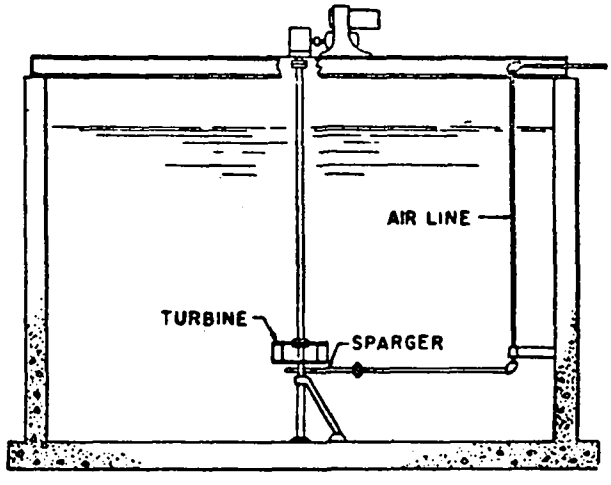


FIGURE 9-4. TURBINE-SPARGER AERATION*

*Figure taken from reference (4) with the kind permission of the publisher.

"Design Guides for Biological Wastewater Treatment Processes"[6] quotes oxygen transfer efficiencies (lbs O_2 transferred/HP-hr) for cone-type aerators that are 50 - 100 percent higher than values for plate or sparger diffusers.

9.2 Theory

From the previous section, one can surmise that the phenomena involved in the activated sludge system are hydrodynamics which controls mixing, mass transfer of oxygen and a myriad of physical and physiological phenomena controlling the composition of the biomass and the rate at which it consumes organic matter. We will begin with a discussion of the biomass and how it functions to remove wastes. We will consider mixing next and finally deal with oxygen transport.

Eckenfelder[7] succinctly describes the removal process.

"BOD removal from a waste by a biological sludge may be considered to occur in two phases, an initial high removal of suspended, colloidal, and soluble BOD, followed by a slow progressive removal of soluble BOD. Initial BOD removal is accomplished by one or more mechanisms, depending on the physical and chemical characteristics of the organic matter. These are:

(a) Removal of suspended matter by enmeshment in the biological floc. This removal is rapid and is dependent upon adequate mixing of the waste with sludge.

(b) Removal of colloidal material by physiochemical adsorption on the biological floc.

(c) A biosorption of soluble organic matter by the microorganisms. There is some doubt as to whether this removal is the result of enzymatic complexing or a surface phenomenon and whether the organic matter is held to the bacterial surface or within the cell as a storage product or both. The amount of immediate removal of soluble BOD is directly proportional to the concentration of sludge present, the sludge age, and the chemical

---

[6] "Design Guides for Biological Wastewater Treatment", Water Pollution Control Research Series, 11010 ESQ, 08/71, U.S. Environmental Protection Agency (Washington, D.C., 1971)

[7] Eckenfelder, W.W., Jr., "Biological Treatment of Waste Water", Adv. in Hydroscience, Vol. 3, Academic Press (New York, 1966)

characteristics of the soluble organic matter."[7]

The floc that accomplishes the functions mentioned above is a complex bio system consisting primarily of bacteria. Many of these contain a slimy outer surface which permits them to attach one to another and thereby form the floc structure. These bacteria were at one time referred to as Zooglea Ramigera, but it is not a single species. Bacteria that predominate in the floc are Bacillus and Micrococuss which are sugar feeders. Proteus, again a sugar feeder, is present as well as Escherichia and Pseudomonas. Nitrosomonas and Nitrobacter which feed on ammonia salts and nitrites are found. Algae, such as Clorella, are also present in the floc. If the pH drops appreciably below 7, fungi become prevalent, and yeasts appear.

Higher organisms are present in the floc giving rise to predation, commensalism, synergism, etc. Protozoa are attached to the floc grazing on the bacteria, but they may also ingest colloidal matter entrapped in the floc. Rotifers are also found. They too are capable of feeding on matter in the floc as well as predation. The highest organisms encountered in a healthy aerobic sludge are blood and sludgeworms.

Disregarding the predatory chain for the moment, the floc organisms convert the waste materials as indicated in Figure 9-5. End products can range from carbon dioxide and water, ammonia, nitrites or nitrates, phosphates to simple organic molecules such as organic acids and amines. A crude estimate is that about one-third of soluble BOD consumed is employed to supply energy required by the microorganism while the remainder is converted into cellular matter. The process can be written:

$$\text{Organic material} + O_2 + NH_3 + P \xrightarrow{\text{bacteria}} \underset{(C_5 H_7 NO_2)_{10}P}{\text{New Cells}} + CO_2 + H_2O \quad (9\text{-}1)$$

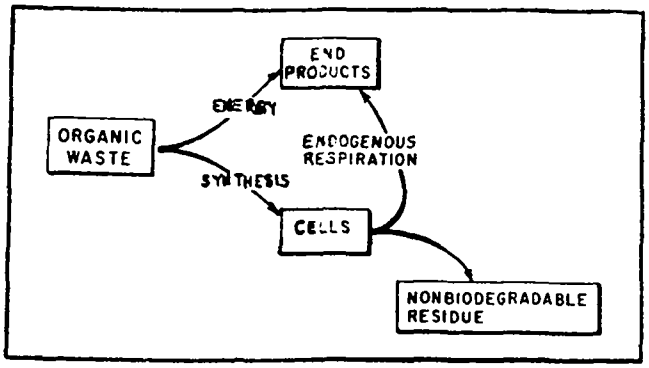


FIGURE 9-5. CONVERSION SEQUENCE IN THE SLUDGE FLOC *

Cell composition is represented as $(C_5H_7NO_2)_{10}P$.

With a specific substrate such as glucose, the two ways of waste conversion can be represented stoichiometrically as,

Respiration

$$C_6H_{12}O_6 + 6\ O_2 \longrightarrow 6\ CO_2 + 6\ H_2O \qquad (9\text{-}2)$$

Synthesis

$$5\ C_6H_{12}O_6 + 6\ NH_4^+ \longrightarrow 6\ C_5H_7NO_2 + 18\ H_2O + 6\ H^+ \qquad (9\text{-}3)$$

Assuming a yield coefficient of 0.5 moles microorganisms/mole glucose:

$$C_6H_{12}O_6 + 0.5\ NH_4^+ + 3.5\ O_2 \longrightarrow 0.5\ C_5H_7NO_2 + 3.5\ CO_2 + 5\ H_2O + 0.5\ H^+ \qquad (9\text{-}4)$$

The three reactions mentioned in the quotation from Eckenfelder occur rapidly once the biomass and primary effluent are mixed together (Figure 9-6). Biosorption of soluble organic matter is probably best treated as an equilibrium phenomenon so that some of the matter remains in the liquid phase. Biosorption will be selective whereby substances

* Figure taken from reference (3).

will be preferentially removed. It is widely accepted that most of the enmeshed and adsorbed suspended and colloidal matter must undergo sequential breakdown into smaller soluble molecules to be assimilated into the bacterial cells. Extra cellular enzymes excreted, perhaps, by the cells are assumed to be responsible for the breakdown. Eckenfelder believes that the rate of synthesis, that is, cell growth and reproduction, is controlled by the breakdown steps[7].

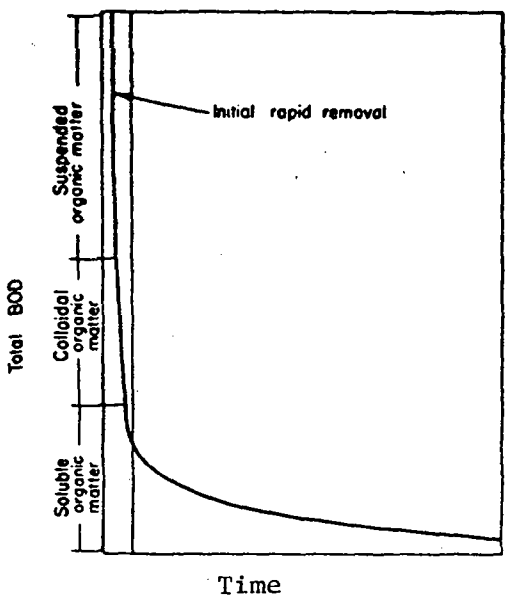


FIGURE 9-6. REMOVAL OF BOD FROM DOMESTIC SEWAGE BY THE ACTIVATED SLUDGE PROCESS*

We are not able to distinguish among the soluble species present in the mixed liquor. Indeed, we can only measure the sum of the species and even this only imprecisely as total organic carbon or BOD. Thus, the interaction of equilibrium biosorption and production of soluble matter by breakdown makes it appear as though organic matter is removed by some simple rate process at least after the initial sharp drop in BOD due to adsorption. This behaviour is shown in Figure 9-6 and by the S curve in Figure 9-7.

Soluble organic matter initially removed from solution or obtained from breakdown is assimilated by the cell as a surface complex or as a cellular storage product. This material is then used by the cell

---

* Figure taken from reference (7) with the kind permission of the publisher.

for synthesis. Initially, when concentrations of BOD are high, the rate of synthesis is not limited by substrate availability so that a constant and, indeed, maximum rate of cellular growth is obtained.

When the cell mass reaches a maximum (B in the figure), the sludge floc still contains unassimilated organic carbon. Cell composition can be approximated as $C_5H_7NO_2 \cdot (CH_2O)_x$. Cell synthesis continues at a maximum rate until the excess CH_2O (Carbohydrate) in the cell is depleted by conversion into cellular mass. Cell composition then is approximately $C_5H_7NO_2$. Cell nitrogen continues to build up after cell mass stops increasing because of this carbohydrate conversion.

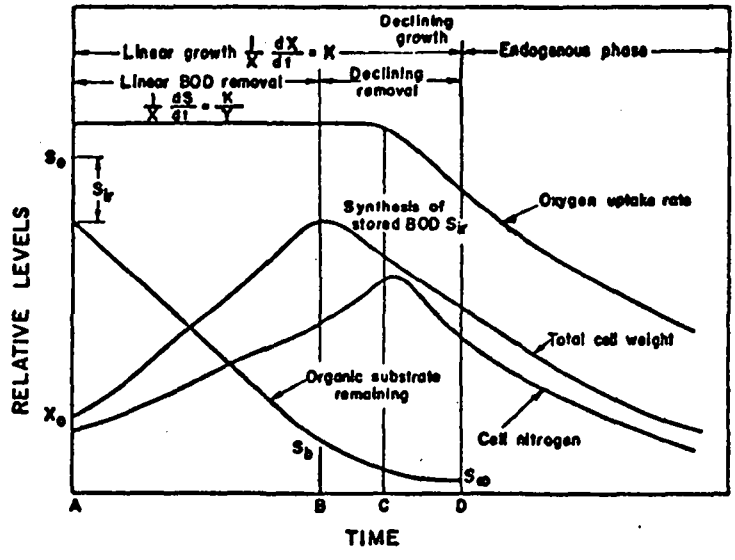


FIGURE 9-7. SCHEMATIC REPRESENTATION OF BOD REMOVAL, SLUDGE GROWTH, AND SLUDGE OXIDATION.*

Beyond D, autooxidation results in a decrease in both cell weight and cell nitrogen. The concentration of BOD, S_∞, is the equilibrium concentration from solubilization of cellular constituents in autooxidation. This is the region of endogenous respiration. The cells are

*Adapted from reference (7) with the kind permission of the publisher.

now consuming cell protoplasm to meet their respiratory energy requirements. Once the available protoplasm is sufficiently reduced, the cells die. Autooxidation may be represented as,

$$(C_5H_7NO_2)_{10}P + O_2 \longrightarrow CO_2 + H_2O + NH_3 + \text{Polysaccharide-like material} \qquad (9\text{-}5)$$

Figure 9-7 also shows the rate of oxygen utilization. The rate depends on cell synthesis and respiration. While the cells are growing, up to C in the Figure, synthesis dominates. During this phase, there is adequate organic matter so the synthesis rate proceeds at its maximum value for the substrate-cell system. The oxygen utilization rate is constant. Once the synthesis rate decreases and respiration becomes dominant, the utilization rate drops.

Cell synthesis requires nutrients and trace minerals of various types. The latter are normally available in most any waste. However, nutrients occasionally must be supplied with industrial wastes.

Ammonia utilization for synthesis is shown in eqns. (9-1), (9-3) and (9-4); ammonia is also released in autooxidation as shown in eqn. (9-5). Autotrophic bacteria, specifically Nitrosomonas, consume ammonia and discharge nitrites as waste products. Nitrites in turn are consumed by Nitrobacter to form nitrates. Nitrates can be used as well as NH_3 for cell synthesis.

The complete nitrogen cycle is shown in Figure 9-8. If autooxidation occurs, the net effect of the autotrophic species is to convert ammonia and organically-bound nitrogen to nitrates. Most variants of the active sludge process accomplish a high level of nitrification.

Autooxidation discharges phosphorus as ortho-phosphate; consequently, the activated sludge process also converts organically-bound phosphorus to phosphate.

Widespread interest in nutrient removal has led to research on modification of the activated sludge process to achieve phosphorus-nitrogen removal. Facultative species in the floc are capable of using nitrates as an oxygen source giving off nitrogen and a small amount of N_2O as waste products. Thus, denitrification can be accomplished once autooxida-

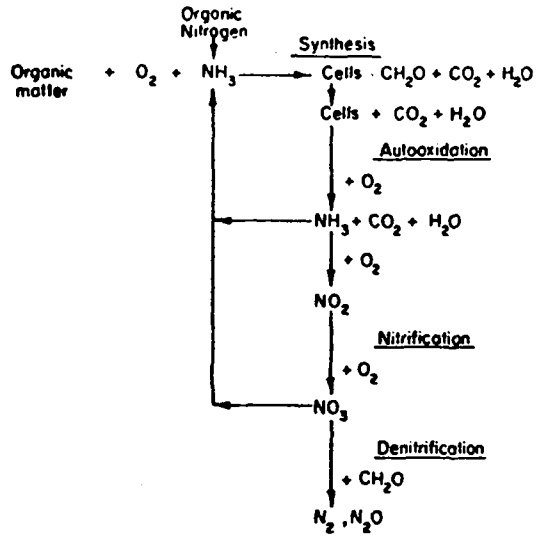


FIGURE 9-8. N_2 CYCLE IN BIOLOGICAL OXIDATION PROCESSES*

tion has occurred by letting the biomass go anaerobic. Bypassing of a portion of the primary effluent to this stage provides substrate for the facultative organisms. Nitrogen gas generated, unfortunately, tends to float the floc and interferes with clarification.

Clarification or secondary settling is an important element of the activated sludge system. A high biomass concentration should be maintained in the aerator so sludge recovery is necessary. With roughly two-thirds of the BOD removal through cell synthesis, cells must be removed from the effluent and wasted if the BOD reduction is to be realized. Clarification depends on effective flocculation of the sludge, and a density and sludge structure which will provide rapid settling and thickening. Eckenfelder[7], quoting a 1963 Ph.D. thesis, states that flocculation results from the production of a polysaccharide slime layer on the "Zooglea Ramigera" whose sticky surface causes adherence of adjoining organisms. Flagelettes are also entrapped. Apparently, slime formation does not occur in the maximum growth rate region (A-C in Figure 9-7). "Starvation" conditions are required so good flocculation is associated with the declining growth stage (region C-D); that is, higher sludge age and low food - to biomass ratios.

*Taken from reference (7) with the kind permission of the publisher.

Low density or "bulking" sludges are associated with the presence of high levels of filamentous fungi and algae in the biomass. High dissolved oxygen and substrate levels in the biomass promote the growth of fungi and algae. On the other hand, anaerobic conditions can lead to a dispersed floc with some wastes. If autooxidation proceeds appreciably, carbohydrate material associated with the bacteria is completely consumed, and the floc disperses. Figure 9-9 summarizes these floc condition effects. Scales are not given (with the exception of sludge loading where domestic sewage is assumed), since they depend on the waste and acclimatization of the biomass.

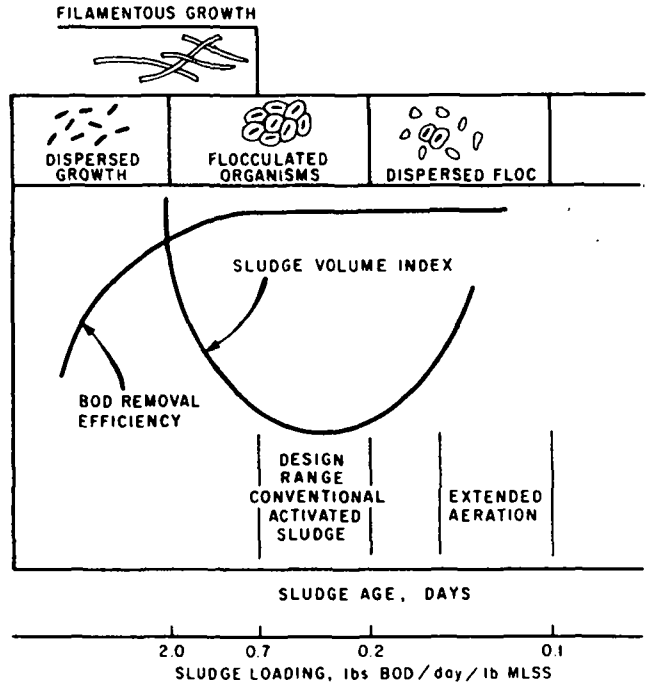


FIGURE 9-9. BEHAVIOUR OF SLUDGE CONDITION INDICATORS WITH OPERATING PARAMETERS *

Sludge age, in Figure 9-9, is the ratio of the mixed liquor suspended solids (MLSS) in the aerator to the weight of sludge wasted per day. Sludge density is measured by the Sludge Volume Index (SVI) defined as the volume (ml.) occupied by 1 gm of dry sludge after thirty minutes of settling.

To reach high BOD removal levels in activated sludge units, short-circuiting of raw primary effluent through the aerator must be

* Figure taken from reference (3).

avoided. The size of units will be smaller if there is no backmixing, that is, mixing of the low BOD effluent with the incoming waste. Both conditions are met if the flow moves through the tank as a slug. This type of flow is known as plug flow. We met the concept in the previous chapter. Plug flow is a limiting and ideal case of contacting pattern, that is, type of macro mixing. The other limiting case is complete mixing, also called perfect backmixing. In the latter case, the BOD level and MLSS concentrations would be uniform throughout the aerator.

The degree of macromixing is easily measured by adding a slug of an inert, non-consumed tracer at the inlet of the vessel and observing the tracer concentration in the outlet as a function of time (see Chapter 8). The behaviour we would observe is shown in Figure 9-10 for perfect backmixing, plug flow and for an intermediate level of macromixing. Theta (θ) is dimensionless time. It is the ratio of time of the observation to the nominal holding time (τ) where $\tau = V/Q$. V is tank volume while Q is flow rate, both expressed in the same volumetric units. If a unit amount of tracer is injected at the start of the experiment, the concentration of tracer leaving at each time is a form of the residence time distribution function known as the exit age distribution ($E(t)$ or $E(\theta)$). It expresses the probability that an element of fluid entering a vessel at zero time will leave between times t and $t + \Delta t$.

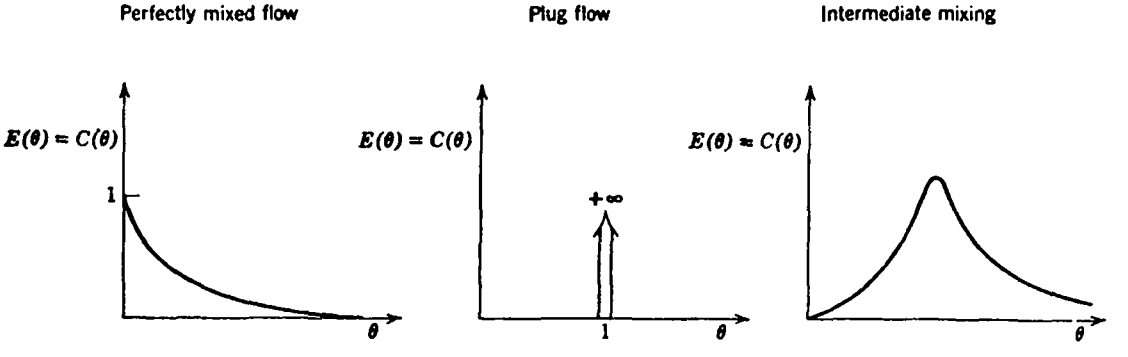


FIGURE 9-10. TRACER CURVES FOR VARIOUS CONTACTING PATTERNS OR MACROMIXING CASES*

*Figures taken from reference (8) with the kind permission of the publisher.

(8) Himmelblau, D.M. and Bischoff, K.B., "Process Analysis and Simulation", John Wiley (New York, 1968)

Flow through vessels will be normally represented by the intermediate case shown in Figure 9-10. Poor contacting patterns such as short-circuiting (by-passing) and dead space (that is, the presence of poorly irrigated regions in the aerator) can be identified from the shape of the exit age distribution as may be seen in Figure 9-11.

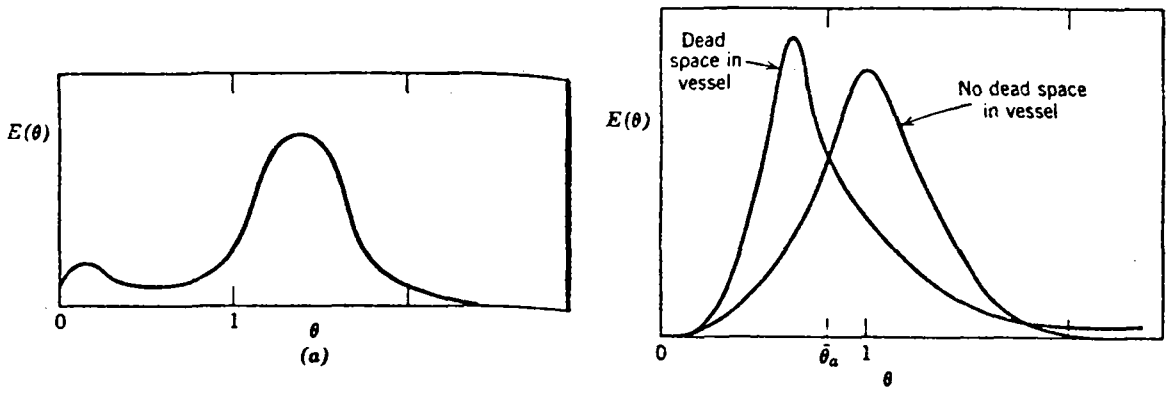


FIGURE 9-11. TRACER CURVES SHOWING THE EXISTENCE OF SHORT CIRCUITING (a) AND REGIONS OF LOW CIRCULATION (DEAD SPACE) (b)*

Intermediate macromixing cases, which are normally encountered, can be handled in two ways: 1) a continuous model in which backmixing is represented by a dispersion coefficient, D (ft^2/hour); 2) a staged model is which each stage is perfectly backmixed. Both D and the number of stages (n_s) measure the level of mixing. If $D = 0$ or $n_s = \infty$, there is effectively no backmixing and the tracer curve becomes identical to the plug flow case in Figure 9-10. Since both types of models may be used to represent mixing, there must be a relation between n_s and D. This relation is,

$$\frac{1}{n_s} = 2\left(\frac{D}{uL}\right) - 2\left(\frac{D}{uL}\right)^2 \left[1 - \exp\left(-\frac{uL}{D}\right)\right] \qquad (9\text{-}6)$$

If D/uL is small, the second term can be neglected, so

*Figure taken from reference (8) with the kind permission of the publisher.

$$n_s \approx \frac{1}{2} \left(\frac{uL}{D} \right) \qquad (9\text{-}7)$$

where L = length of the vessel; u is the mean velocity through the vessel.

In modern partitioned aerators each cell has one or more mechanical aerators which provide a high level of mixing. Measurements in the Kitchener treatment plant[9] indicate each stage can be taken as perfectly backmixed. Thus, a staged model for the aerator would seem to resemble the real situation. However, the continuous model might be chosen for computational reasons. Mixing between stages seems to exist so that the number of stages in the model will always be less than the number of real cells in a cascade.

Macromixing expresses large-scale mixing patterns. The velocity of the fluid referred to stationary coordinates and the level of mixing, both at a point are also important. Velocities must be sufficient to keep the biomass in suspension. This is rarely an important consideration with diffuser or sparger systems which generate spiral flow; only in bad design resulting in poorly irrigated regions do such problems arise with mechanical aerators. Fine mixing or micromixing, on the other hand, is important. This type of mixing results in transport of dissolved oxygen from the gas-water interface to the floc-water interface where it is utilized by microorganisms. It is also the mechanism responsible for circulating substrate-laden water to the floc.

Micromixing is associated with the fine scale turbulence at a point in a vessel. Turbulence is induced by fluid motion past surfaces or motion where direction changes. The theory is far too complex to summarize in the space we have available. Since turbulence is a mode of energy dissipation, it is probably best correlated by work input/volume of fluid. For design, there is a minimum value of power input per volume of cell necessary to achieve a sufficient level of micromixing.

---

[9] Silveston, P.L., "Use of Residence Time Distributions for Design of Aerobic Waste Treatment Units", Proc. 1st Annual Symp. Water Pollution Res., (Univ. of Waterloo, 1966).

Oxygen requirements in the activated sludge process depend, as already indicated, on the rate of cell synthesis and upon the cell respiration requirements. Transport of oxygen to the individual organisms is a complex, multi-step process. These steps are transport: i) through a gas film at the air-water interface; ii) through a water film surrounding a bubble or bordering a surface into the bulk of the liquid; iii) through the liquid from the region of the gas-water interface to a floc; iv) through a water film surrounding the floc; v) diffusion in the floc to an individual cell where oxygen is actually consumed. Even though not all of the steps must be considered, the resulting expression would be still too difficult to employ. Instead, an empirical approach is taken. The rate of transfer of oxygen from air to the water by analogy to transfer of charge in a potential field is written

$$\mathcal{R} = K_L A \, (C_g - C_L) \tag{9-8}$$

where $\mathcal{R}$ is the pounds of oxygen transfer per unit time; A is the effective area of the gas-liquid interface; K_L is a mass transfer coefficient and $C_g - C_L$ is the concentration driving force. The driving force must be expressed in a single set of units, such as mg/l even though gas and liquid phases are involved. To do this, a solubility relation for oxygen in water is invoked:

$$p_{O_2} = HC_g \, . \tag{9-9}$$

where p_{O_2} is the partial pressure of oxygen in air, C_g is the oxygen concentration in the liquid at equilibrium and H is a proportionally constant often called Henry's Law constant. From eqn. (9-9) at one atmosphere and $20^{\circ}C$, $C_g = 9.2$ mg/l. Thus the maximum driving force for oxygen transfer to water is less than 10 mg/l. This is low and means that oxygen transport flux will be small. If the oxygen requirement is large, then the area of the gas-liquid interface must be made very large. High interfacial area is a key factor in the choice of diffusers

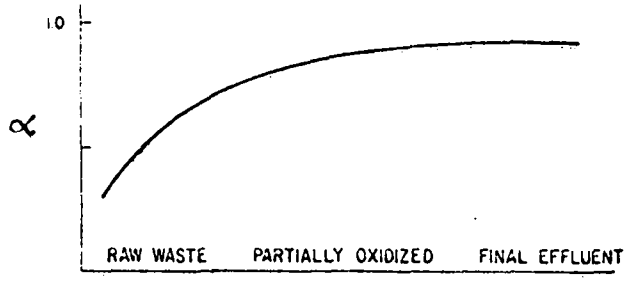
and surface aerators for this reason.

The small driving force simplifies the analysis of oxygen transfer somewhat. Transport through the air side film (step i)) will be relatively fast since air is 20% oxygen. Thus, this step can be neglected. Similarly, the turbulence level in an aerator is usually sufficiently high so that transport through the bulk of the liquid via mixing processes is rapid. Consequently step iii) can also be neglected. Turbulence also prevents large flocs from forming. Small flocs, then, in a well mixed aerator will exhibit large surface areas so that even though the driving force for step iv) is small, the net transport will be large. Small flocs also mean short diffusion paths to reach the interior of the floc making step v) unimportant. For these reasons, the important step for oxygen transport in many types of aeration systems is step ii) - transport through the liquid side film.

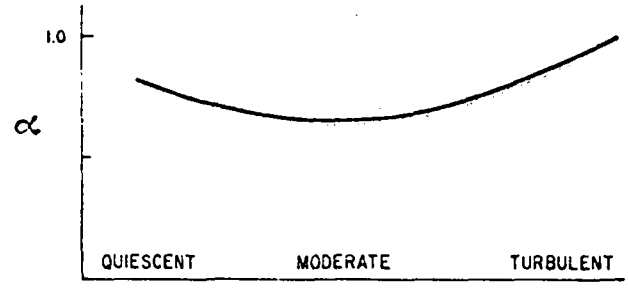
A good deal of attention has been paid to the presence of surface active agents (soaps) in waste and their depression of the mass transfer coefficient K_L. Surface active agents probably influence K_L by thickening the film at the gas-water interface and damping out turbulence near the interface rather than by adding an interface "resistance" to oxygen transport. The theoretical analysis of the effect of these agents is just about impossible so the common practice is to introduce a correction factor α into Equation (9-8) to allow for surface active agents. This factor depends on mixing intensity (HP/ft^3) as well as the extent of BOD reduction as shown schematically in Figure 9-12.

The area A in Equation (9-8) and the mass transfer coefficient K_L are difficult quantities to measure. Normally, these are replaced by design parameters. For example, A for diffusers or spargers will depend on the rate of bubble formation, mean bubble size, and the mean path a bubble follows until it breaks the surface. Bubble rate and size depend on the air rate (scfm/volume) and on sparger depth, while mean path will depend on aerator vessel dimensions.

In surface aerators, area is created by splashing or forming a water sheet as well as by causing bubble formation in the liquid phase. The splashing and sheet mechanism account for as much as 60% of the oxygen



(a) BOD REDUCTION



(b) HP/VOLUME

FIGURE 9-12. INFLUENCE OF BOD REDUCTION AND TURBULENT INTENSITY ON CORRECTION OF OXYGEN TRANSFER FOR SURFACE ACTIVE AGENTS IN WASTE*

transfer for some types of equipment[3]. Area and K_L have been found to be dependent on the horsepower of the aerator, depth of rotor immersion, rotor design and diameter. In the discussion of models which follows, we will examine expressions for oxygen transfer of the type just mentioned.

9.3 General Considerations For An Activated Sludge Process Model

A computer model must represent the function of a process unit by quantitatively specifying all changes in streams crossing the unit. The function of the activated sludge aerator is to remove BOD from a waste stream. In addition, the organic nitrogen and ammonia levels are reduced, some organic phosphorus is converted into soluble phosphate, and the suspended solids are enormously increased (mainly by adding return sludge).

*Figure taken from reference (2) with the kind permission of the publisher.

Consequently, an aerator model must contain relations giving:

a) reduction in BOD

b) nitrogen conversion

c) phosphorus conversion

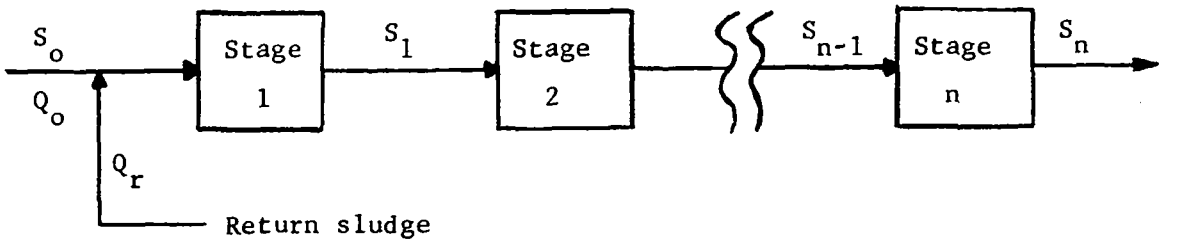
d) change in mixed liquor suspended solids.

Performance of the aerator depends on the oxygen level maintained and upon the waste and biomass contacting pattern. Consequently, a mixing description must be introduced into the model and the model must also contain statements giving the oxygen transport.

The designer is primarily interested in the size of the unit, the number of impellers (or diffuser plates) and the horsepower required. The number of impellers - if mechanical - will depend on the number of cells and their size. Horsepower also will depend on size. Return sludge flow and wasting rate are particularly important design parameters. In a design model subroutine, therefore, relations must be provided to calculate size, number of cells, and mechanical horsepower.

9.4 Mixing Models

Intermediate levels of backmixing are usually found in activated sludge systems. This condition can be modelled as a cascade of ideally backmixed vessels, usually of equal size. The aerator can be represented as:



In the diagram, S stands for substrate concentration and Q for volumetric flow. A mass balance on substrate over the n^{th} stage yields:

$$S_{n-1} Q - S_n Q - R_s V_n = 0 \qquad (9\text{-}10)$$

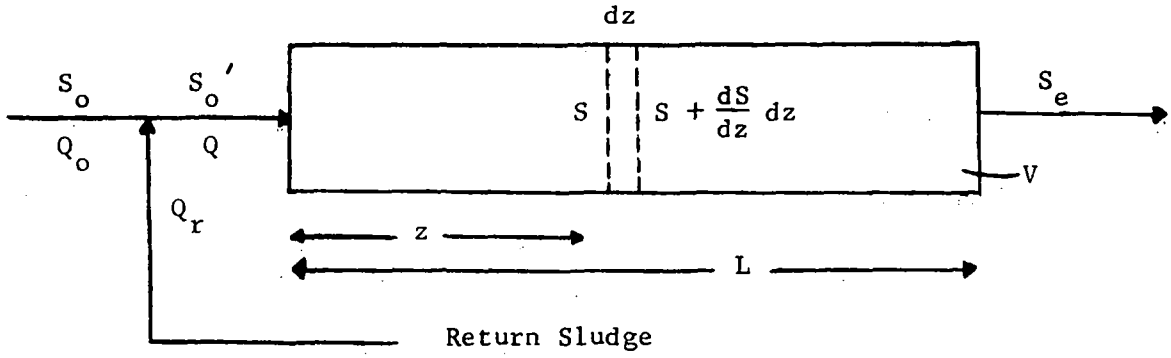
in which V_n is the volume of the n^{th} vessel, and R_S is the rate of

substrate removal per volume of the aeration vessel (written with a positive sign). Q and V_n must be expressed in the same volumetric units. Solving,

$$S_n = S_{n-1} - \tau_n R_S \tag{9-11}$$

This relation holds for any stage in the cascade. Usually the cascade is assumed to consist of equally sized stages. In this case $\tau_n = V_n/Q$, the nominal holding time per stage, will be the same for each stage. If the aeration vessel is partitioned, the number of stages (n_s) could be the number of successive cells in a train, and V_n would be simply the volume of a cell. Aeration vessels are built with four to eight partitions in a vessel so there could be between 5 and 9 cells in a unit. However, we cautioned earlier that n_s should be taken as less than the number of cells to allow for backmixing between successive cells.

Even if the aeration vessel is partitioned, a continuous model can be used by introducing a dispersion coefficient. A substrate balance on a differential slice (vertical cross-section) of the vessel:



gives

$$D \frac{d^2S}{dz^2} - u \frac{dS}{dz} - R_S = 0 \tag{9-12}$$

where z is the coordinate in the direction of net flow in the vessel, u is the net superficial velocity (Q/A_x), and D is a dispersion coefficient (ft^2/h).

As discussed in Chapter 7, one boundary condition for this second order, ordinary differential equation is,

$$S_o u_p = S'_o u - D \left(\frac{dS}{dz}\right)_{z=0} \qquad (9\text{-}13)$$

where u_p is the velocity in the conduit and assumes that no substrate is carried into the vessel with the return sludge. Equation (9-13) states that at the vessel entrance the flux of substrate into the reactor splits into a convective flux (u) and a diffusive flux (D). The other boundary condition is,

$$\left(\frac{dS}{dz}\right)_{z=L} = 0 \qquad (9\text{-}14)$$

If R_S is linear and homogeneous (so that eqn. (9-12) is not coupled with the disappearance or the formation of another material), the analytical solution of eqns. (9-12 to 9-14) is given in chapter 7 as eqn. (7-29). For wastes, R_S is rarely linear or homogeneous, so numerical solutions via an appropriate integration routine will be necessary to find S_e (simulation) or determine V to give the design substrate reduction. Use of a Runge-Kutta method for the integration was illustrated in section 7.5 of chapter 7.

Research at McMaster University[10] on rectangular aerators with spiral flow induced by spargers or diffusers indicates that

$$D = 3.11\ W^2\ (q_{Air})^{0.346} \qquad (9\text{-}15)$$

where D is in ft^2/hour, W is the vessel width in ft. and q_{Air} is air introduced through the spargers per unit volume of the aerator (scfm/1000 ft^3). The effect of vessel geometry and dimension is so important that eqn. 9-15 should be used only in the absence of tracer data. As

---

[10] Murphy, K.L., "Significance of Flow Patterns and Mixing in Biological Waste Treatment" in Canale, R.P. (Editor), "Biological Waste Treatment", Interscience Publ. (New York, 1971)

indicated in section 9.2, tracer measurements are the usual source of dispersion coefficients. If from such measurements either D or n_s is available, the other parameter can be obtained through eqns. (9-6) or (9-7).

9.5 Rate of BOD Removal

Rapid assimilation of suspended organic matter by the sludge floc on contact with the primary effluent means that BOD associated with suspended matter in the waste can be ignored in formulating simulation or design models for most activated sludge systems (contact stabilization may be an exception). Consequently, our models in this section will be developed in terms of soluble BOD (S^*).

The most widely quoted model for BOD removal is based on the Monod equation. This approach has largely replaced the older two-phase model. We will examine both models and introduce other variants that have been proposed.

Equilibrium biosorption of soluble matter by the floc, slow utilization of substrate and selectivity for different components of the waste combine to make the removal of soluble BOD_5 in a continuous, steady state system closely resemble the removal of a single substrate by a single, well acclimatized microorganism colony. For this type of system Monod [11] found that the increase in cell mass could be described by

$$\mu = \hat{\mu} \left(\frac{S^*}{k_m + S^*}\right) - b \qquad (9\text{-}16)$$

where μ expresses the rate of change of cell mass per unit weight of cells. In eqn. (9-16) $\hat{\mu}$ is the maximum specific growth rate (day^{-1}), k_m is a saturation constant and corresponds to a substrate level when $\hat{\mu} = 0.5\,\mu$, while b is the endogenous respiration rate (day^{-1}). The units of S and k_m are arbitrary, although they are often given as mg/l. Figure 9-13 shows how the specific growth rate μ varys with S^* according to the equation.

---

[11] Monod, J., "The Growth of Bacterial Cultures", Ann. Rev. of Microbiology, 3, 371 (1949)

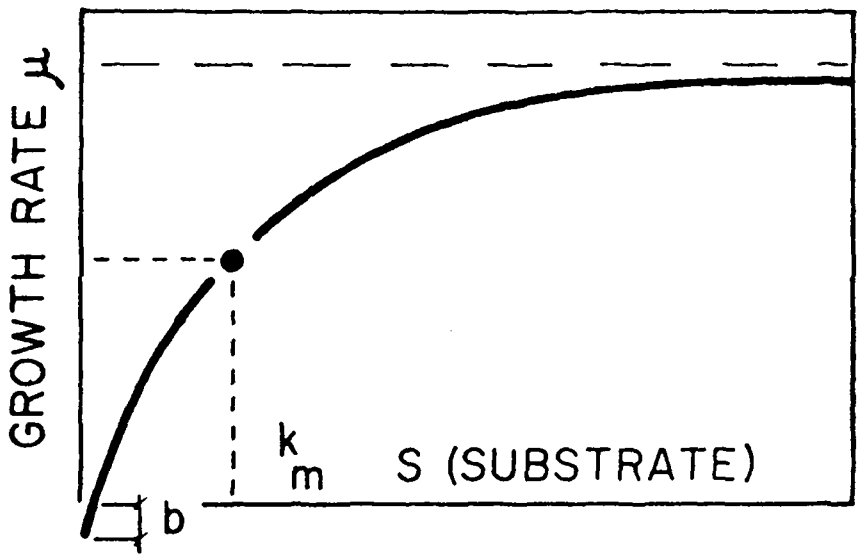


FIGURE 9-13. GROWTH OF CELL MASS AS A FUNCTION OF A GROWTH LIMITING SUBSTRATE AS OBSERVED BY MONOD ("b" REPRESENTS A CELL MASS DECREASE DUE TO ENDOGENOUS RESPIRATION)*

Some confusion in the name used for Eqn. (9-16) exists. It is often referred to as the Michaelis-Menten equation, although usually with "b" removed. Michaelis and Menten originally proposed Eqn. (9-16), without "b", in 1913 to describe the kinetics of enzymes on substrates. Monod in the '40's used their formulation to describe the growth of a colony feeding on a glucose substrate. A number of researchers in the '50's and '60's showed that the model could be applied to bio-oxidation of wastes.

Substrate removal rate has been found to be proportional to the growth rate of the cell mass. At high cell growth rates, the proportionality is constant so

$$\frac{dX}{dt} = - Y \frac{dS^*}{dt} \qquad (9\text{-}17)$$

Y is referred to as a yield coefficient. Since

$$\mu \equiv \frac{1}{X} \frac{dX}{dt} \quad \text{and} \quad - \frac{dS^*}{dt} = R_S,$$

* Figure taken from reference (3).

$$R_S = \frac{\mu M}{Y} = \frac{X}{Y}\left(\hat{\mu}\frac{S^*}{k_m + S^*} - b\right) \qquad (9\text{-}18)$$

Some authors[7] leave out endogenous respiration and write

$$R_S = k_S \frac{S^* X}{k_m + S^*} \qquad (9\text{-}19)$$

where $k_S = \frac{\hat{\mu}}{Y}$

Smith and Eilers[12] suggest $\hat{\mu} = 4.8\ day^{-1}$, $k_m = 150$ mg/l. and $Y = 0.5$ (lbs volatile suspended solids/lb BOD_5) for domestic sewage at 20° c. With these values, $k_S = 9.6\ day^{-1}$. Course notes[3] tabulate values for the yield coefficient Y and for Y′, the oxygen requirement per unit of BOD removed. These are shown in Table 9-1. Table 9-2 from the same source gives values of the endogenous respiration constant b.

TABLE 9-1. BIOMASS YIELD COEFFICIENTS AND OXYGEN REQUIREMENT COEFFICIENTS FOR VARIOUS WASTES[3]

Waste	Y	Y'
Spent sulfite liquor	0.55	0.40
Waste paper repulping and semichemical	0.76	0.38
Mixed pulp and paper		0.48
Kraft pulping and bleaching	0.5	0.65-0.8
Board mill		0.33-0.40
Wallboard	0.7-0.78	0.37-0.48
Synthetic fiber	0.38	0.55
Refinery	0.70	0.56
Brewery	0.93	0.44
Pharmaceutical	0.77	0.35
Domestic sewage	0.49-0.64	0.52

[12] Smith, Robert, and Eilers, R.G., "A Generalized Computer Model for the Steady State Performance of the Activated Sludge Process", Division of Research, Report, F.W.P.C.A., U.S. Dept. of the Interior (October, 1969)

TABLE 9-2. ENDOGENOUS RESPIRATION CONSTANTS

Substrate	b (day^{-1})	Temp. ^{o}C
Dairy Waste	0.30	25
Sewage (<500 mg/l MLSS)	0.345	<11 ^{o}C
Sewage (6000 mg/l MLSS)	0.20	<11 ^{o}C
Sewage (<500 mg/l MLSS)	0.295	>13 ^{o}C
Sewage (6000 mg/l MLSS)	0.25	>13 ^{o}C
Sewage	0.075	20 ^{o}C
Sewage	0.055	15 ^{o}C

The two-phase model is based on observations of growth in batch cultures (Figure 9-14). It is assumed that a similar curve applies to the complex, multiple colony systems in the biomass feeding on waste streams. In a continuous system, however, the introduction of acclimatized biomass means that the lag region will not be encountered. In the constant growth region the specific growth rate (μ) is constant, however,

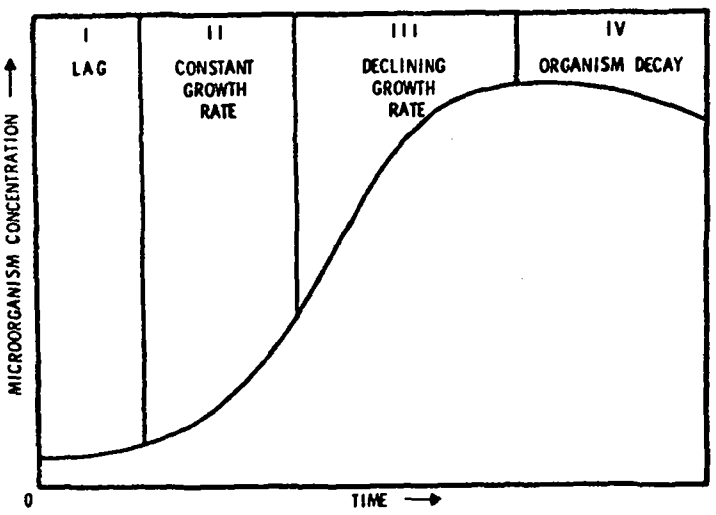


FIGURE 9-14. GROWTH OF MICROORGANISMS IN A BATCH REACTOR

the increase in the number of cells or the cell mass is a logarithmic function. Thus, the region is often referred to as the log growth phase or just simply as phase I. The specific growth rate declines once a critical substrate level is attained and the rate becomes a function of substrate concentration. Figure 9-15 plots the log of microorganism density versus time and the linear portion of the curve is evident. In terms of

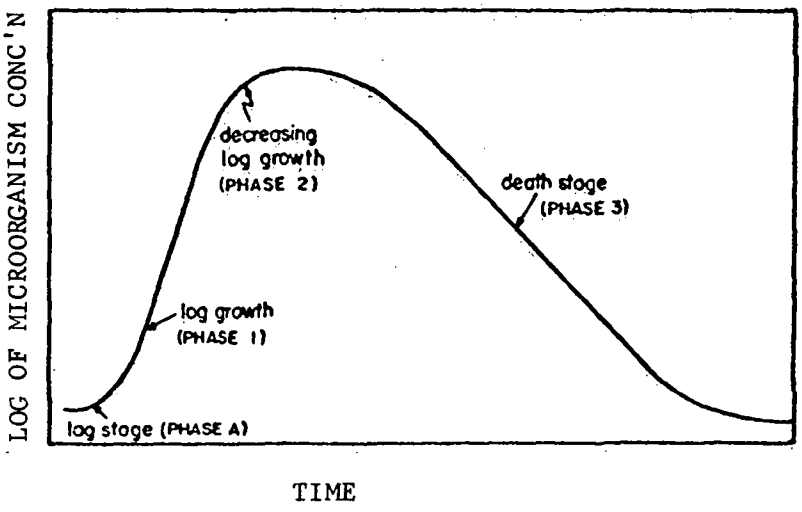


FIGURE 9-15. LOG OF MICROORGANISM CONCENTRATION AS A TIME FUNCTION IN A BATCH REACTOR*

BOD: "The two-phase theory states that the rate of BOD removal per unit of cells will remain constant to a limiting BOD concentration (log-growth phase) below which the rate will become concentration-dependent (declining growth phase) and decrease (The rate of cell growth may continue at a maximum longer than the rate of BOD removal due to assimilation of stored BOD). The rate of BOD removal during the declining growth phase may follow first order kinetics or, in the case of a complex waste mixture, a retardant reaction as various waste components are removed at different rates."(7)

Growth of the biomass for the log growth phase is

*Adapted from reference (4) with the kind permission of the publisher.

$$\frac{dX}{dt} = k_{tp}X \tag{9-20}$$

k_{tp} is the rate constant for the two phase model. Using eqn. (9-17) and the definition of R_S

$$R_S = \frac{k_{tp}X}{Y} \tag{9-21}$$

This form results from eqn. (9-19) if $S^* >> k_m$.

Below a critical substrate level, the growth rate becomes a function of the substrate concentration. This is phase II. According to Eckenfelder[7], various choices for the S^* dependence result in the following rate of substrate removal expressions:

$$R_S = \frac{k'_{tp} X S^*}{Y} \tag{9-22}$$

$$R_S = \frac{k''_{tp} X (S^*)^2}{Y} \tag{9-23}$$

Equation (9-19) also can be used. Of course, eqn. (9-22) drops from eqn. (9-19) if $k_m >> S^*$.

Although eqns. (9-21) and (9-22) are simple models, careful investigations have suggested that the two phase approach is less satisfactory than the Monod equation. This is shown by Figure 9-16 which is taken from a paper by Eckenfelder[7].

Fan and his co-workers at Kansas State University[13, 14] and Takamatsu and co-workers in Japan[15] use eqn. (9-22) but add a term for

---

[13] Fan, L.T., Chen, G.K.C., Erickson, L.E. and Naito, M., "Effects of Axial Dispersion on the Optimal Design of the Activated Sludge Process", Water Research, 4, 271-284 (1970)

[14] Chiu, S.Y., Erickson, L.E., Fan, L.T., and Kao, I.C., "Kinetic Model Identification in Mixed Populations Using Continuous Culture Data", Biotech. and Bioeng., 14, 207-231 (1972)

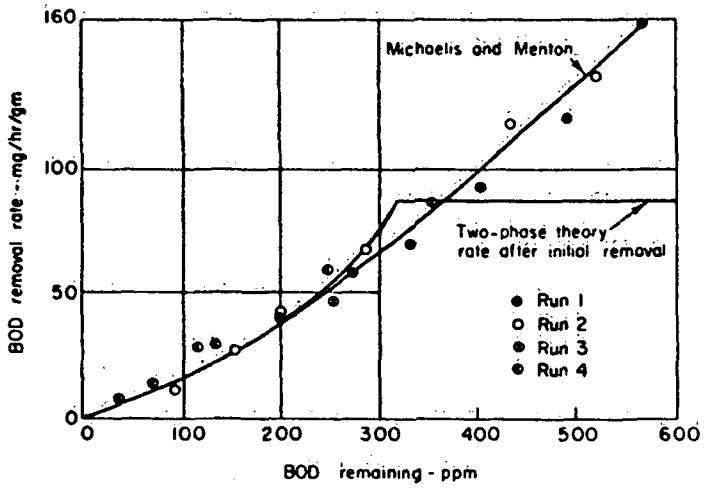


FIGURE 9-16. COMPARISON OF THE MONOD MODEL AND THE TWO-PHASE THEORY FOR PETROLEUM REFINERY WASTE WATERS TREATED BY THE ACTIVATED SLUDGE PROCESS*.

endogenous respiration, presumably to allow for an increase in soluble BOD through cell lysis

$$R_S = k'_S \; X \; S^* - b \; X \qquad (9\text{-}24)$$

Naito et al.[15] suggest $k'_S = 0.0005$ hr^{-1} ppm sludge solids^{-1} and $b = 0.0035$ ppm BOD/ppm sludge solids - hr.

An attractive model, proposed by Eckenfelder in "Advances in Biological Waste Treatment[4], assumes that the waste is composed of a group of J identifiable substances or substrates so that

$$S^* = \sum_{i=1}^{J} S^*_i$$

Each substance is removed at a rate R_S whose form is given by eqn.

*Figure taken from Reference (7) with the kind permission of the publisher.

[15] Naito, M., Takamatsu, T. and Fan, L.T., "Optimization of the Activated Sludge Process - Optimum Volume Ratio of Aeration and Sedimentation Vessels", Water Research, 3, 433-443 (1969)

(9-22) and which is independent of other substrates present. The model is best expressed vectorially:

$$\underline{R_S} = X [\underline{k}] \cdot \underline{S}^* \qquad (9\text{-}25)$$

In this expression $\underline{R_S}$ is a column vector of substrate removal rates, $\underline{S}^*$ is a column vector of BOD_5 associated with each substance and $[\underline{k}]$ is the coefficient matrix, which to conform with eqn. (9-22) must be diagonal.

Assuming plug flow through the aerator leads to a simple exponential relationship -

$$S_e^*/S_o^* = \sum_{i=1}^{J} f_{S_i} \exp [-k_i \bar{X} \tau] \qquad (9\text{-}26)$$

where f_{S_i} = fraction of the entering soluble BOD contributed by the i^{th} substance in the waste, $\bar{X}$ is the mean level of active biomass (as mg/l.) in the aerator and τ is the detention time. If the aerator is assumed to be completely backmixed, the expression equivalent to eqn. (9-26) is

$$S_e^* = S_o^* - \tau \Sigma R_{S_i} \qquad (9\text{-}27)$$

where R_{S_i} can be obtained from the vector equation (eqn. (9-25)).

The BOD removal model represented by eqn. (9-25) is capable, in principle, of representing the aerobic oxidation of any wastes. Accuracy of the model can always be improved by adding additional terms. There is no reason that each term must be identified with a specific component in the waste. Eckenfelder[4] demonstrates successful use of the integrated model (eqn. (9-26)) to describe BOD removal for a variety of industrial wastes assuming 3 or in some cases just 2 components. However, eqn. (9-26) has a serious drawback because macromixing has an appreciable effect upon k_i. Thus, treatability studies cannot be used to evaluate k_i and the model is limited to simulation.

Additional cell growth models have been proposed and each of

these can be rewritten to describe BOD removal. Table 9-3 summarizes these models giving one or more sources for each. A study by Chiu et al.[14] employing a continuous laboratory activated sludge system started with a plant sludge innoculation, but utilizing an artificial sewage based on glucose found that the Moser equation (9-30) was marginally superior to the Monod equation (9-18) and the Contois equation (9-31). The two phase model (eqns. 9-21 and 9-22) was found to be poor.

The practice is to use the Monod equation. Thus, we recommend eqn. (9-18) for expressing the rate of BOD removal in activated sludge systems. Three constants appear in the model so it should be capable of fitting most data. Recommended alternatives are eqn. (9-19) if a simpler model is desirable or eqn. (9-26) for similation if two or three terms are used.

TABLE 9-3. FURTHER BOD REMOVAL MODELS BASED ON BACTERIAL CELL GROWTH RELATIONS

Model	Relation	
Teissier[14] Schulze[12]	$R_S = \frac{\hat{\mu} X}{Y} (1 - e^{-S^*/k_t})$	(9-28)

Chiu et al.[14] suggest that $k_t = 63.9$ mg/l., $\hat{\mu} = 0.66$ hr^{-1} and $Y = 0.57$, while Smith and Eilers[12] indicate that $0.39 \leq \hat{\mu} \leq 0.55$ hr^{-1} and $35 \leq k_t \leq 138$ mg/l.

Contois[14]

$$R_S = \frac{\hat{\mu} X S^*}{Y (B X + S^*)} \qquad (9\text{-}29)$$

Chiu et al. propose $\hat{\mu} = 0.67$ hr^{-1}, $Y = 0.57$ and $B = 0.046$.

Moser[12, 14]

$$R_S = \frac{\hat{\mu} X}{Y} (1 + k_X / S^{*\lambda}) \qquad (9\text{-}30)$$

Chiu et al. give $\hat{\mu} = 1.15$ hr^{-1}, $Y = 0.56$, $\lambda = 0.175$ and $k_X = 2.36$ (mg/l.)$^{\lambda}$ based on mixed culture and an artificial sewage based on glucose.

9.6 Sludge Production Models

Modelling of sludge production in activated sludge systems can begin either with the Monod equation (eqn. (9-16)) or with the various expressions for substrate removal given in the previous section. Using the definition of specific growth rate, we obtain,

$$R_X = \mu X \tag{9-31}$$

Basing sludge production on substrate removal gives,

$$R_X = -Y R_S \tag{9-32}$$

However, if the R_S expression does not allow for a BOD contribution from endogenous respiration (such as eqns. (9-19) to (9-23), (9-25) and (9-28) to (9-30), a term bX must be added to eqn. (9-32).

In section 9.5, we assumed that X in the rate expression could be the mixed liquor suspended solids. In treating sludge production we must distinguish between classes of sludge. From here on, X is the active biomass in mg/l., not the mixed liquor suspended solids (MLSS). The convention is to assume that the active biomass is measured by the volatile suspended solids. We will follow this convention. We will use subscripts on X to denote classes of biomass and let M represent sludge concentration.

Auto oxidation produces nonbiodegradable cell debris as well as degradable cell matter. The simplest approach is to assume that the degradable matter is soluble. The degradable material results in the limiting effluent BOD_5 predicted by eqn. (9-18). This limiting value may be estimated by letting $R_S = 0$; some authors refer to this value as the ultimate activated sludge effluent and designate the value as S^*_∞.

The production of nonbiodegradable cell debris introduces another rate term. Assuming that this debris appears as suspended matter,

$$(R_M)_{nb} = -b' X \tag{9-33}$$

The rate term b' is usually given as a fraction of b. Eckenfelder and Ford[2] suggest 23% of the cell debris is nonbiodegradable. Smith and Eilers[12], on the other hand, quote 18%. Consequently $0.18 \leq b'/b \leq 0.23$.

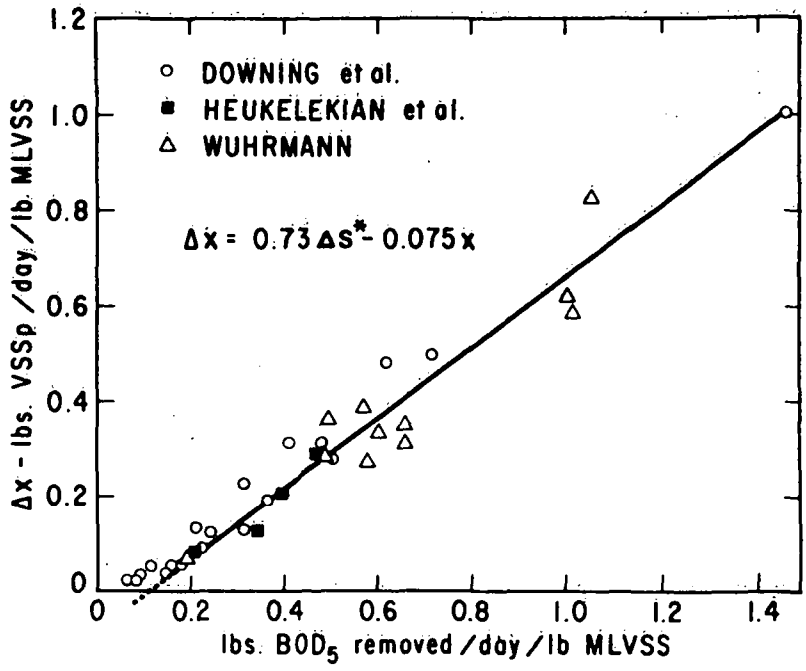


FIGURE 9-17. ESTIMATION OF THE YIELD COEFFICIENT*

If eqn. (9-31) or (9-33) is introduced into the cascade model, eqns. (9-11), in place of R_S and S is replaced by X or M_{nb}, solving eqn. (9-11) for X or M_{nb} will give the level of MLVSS and MLSS in each stage of an aerator model. Making like changes in eqn. (9-12) and using the boundary conditions (eqns. (9-13) and (9-14)) will provide on integration the variation of MLVSS and MLSS along the length of the aerator.

The solution is not quite as simple as the previous paragraph suggests. If a staged model for the aerator is used (eqn. (9-11)) and we assume that performance is independent of oxygen supply, we see from the expressions for R_S and R_X that S^*_n can be calculated from eqn. (9-11) only if $(X)_n$ is known, while $(X)_n$ can be calculated only with

* Figure taken from Reference (3).

S^*_n known. Thus the two forms of eqn. (9-11) must be solved simultaneously. If the continuous model, eqn. (9-12), is used, two similtaneous ordinary differential equations must be solved because of the considerations just mentioned.

An alternate approach to the solution for S_n^* for the cascade model is to use successive approximation. Assume X_n in the expressions for R_S is $(X)_{n-1}$ and calculate S^*_n. ΔX can be estimated from the change in S^* over the stage. X_n for the next approximation is $(X)_{n-1} + \Delta X$ and the procedure can be repeated until S^*_n converges.

If the variation of MLVSS is small across the aerator, a similar procedure can be used with the continuous model (eqn. (9-12)) and the solution for S_e^* can be greatly simplified. The procedure for eqn. (9-12) is to assume for a first approximation that $\bar{X} = X_o$. Integration of the eqn. (9-12) with $\bar{X}$ substituted for X yields a first approximation of S_e^*. Using this approximation, the increase in X across the aerator, ΔX, can be calculated. For the second approximation, $\bar{X} = X_o + \frac{\Delta X}{2}$, and the procedure may be repeated until S^*_e converges.

To use these alternative procedures, relations to predict ΔX (and ΔM_{nb}) are needed. One such relation is

$$\Delta X = Y (S_o - S_e^*) - b \bar{X} \tau \qquad (9\text{-}34)$$

Another uses the concept of sludge age. Sludge age, G, is defined as the mean residence or "life" time of sludge in the system. Thus

$$G \equiv \frac{\bar{X}V}{Q_W X_r + Q(X_e)_{set}} \qquad (9\text{-}35)$$

where $\bar{X}$ is the mean MLVSS in the aerator, Q_W is the sludge wasting rate in mgd, while X_r is the return sludge concentration (usually the clarifier underflow concentration) and X_e is the clarifier overflow concentration. Equation (9-35) can also be written in terms of MLSS (M). Sludge age may be specified as a design parameter. At steady state,

sludge wasted must be the sludge produced so

$$G = \frac{\bar{X}\,V}{\Delta X\,Q} = \frac{\bar{X}}{\Delta X}\,\tau \qquad (9\text{-}36)$$

Substitution for ΔX gives,

$$\frac{1}{G} = Y\,\frac{(S_o - S_e^*)}{\tau\,\bar{X}} - b/\tau \qquad (9\text{-}37)$$

If we use MLSS instead of MLVSS to express sludge age, eqn. (9-37) becomes

$$\frac{1}{G} = \frac{Y(S_o - S_e^*)}{\tau\,\bar{M}} - \frac{b - b'}{\tau} + f_{nb}\,\frac{M_o}{\bar{M}\,\tau} \qquad (9\text{-}38)$$

where the $b - b'$ allows for the production of nonbiodegradable matter from cell lysis. The final term allows for nonbiodegradable solids carried into the aerator with the primary effluent. S_o appears in eqns. (9-34), (9-37) and (9-38) instead of S_o^* because we assumed at the outset that suspended BOD is assimilated on contact with the return sludge and it is therefore quantitatively removed. It is available for cell synthesis is nonetheless. Values for Y, b, b′ will be different for eqns. (9-37) and (9-38). Some values are given in Tables 9-1 and 9-2. f_{nb} is often taken as 0.6[6]. Activated sludge systems operate at about 95% removal of the primary effluent BOD so $S_o - S_e^* = 0.95\,S_o$. Letting $Y = 0.63$ and $b - b' = 0.06$ yields a rather simple expression for sludge age in terms of BOD and MLSS

$$\frac{1}{G} = 0.6\,\frac{(S_o + M_o)}{\tau\,\bar{M}} - \frac{0.06}{\tau} \qquad (9\text{-}39)$$

Design Guides[6] shows that eqn. (9-39) successfully correlate sludge production data from 3 plants treating domestic sewage.

Smith and Eilers treat sludge production in considerable detail in their model[12]. They recognize the difficult modelling problem asso-

ciated with sludge production. "One of the most troublesome and complex problems associated with selecting a model for the activated sludge process is representing properly the character of the solids held in the aerator".[12] They define the problem as follows: "Since new cells (MLASS) are continually produced in the aerator; solids must be removed continuously to hold the aerator solids at a stable value. The rate of sludge wasting is determined by the rate of substrate utilization and the yield coefficient. This required wasting rate then determines the concentration of various classes of solids present in the aerator. The six classes generally assumed to be present are listed below:

1. Active heterotrophs (X) mg/l
2. Active nitrifying bacteria (X_N) mg/l
3. Organic biodegradable solids (M_B) mg/l
4. Organic non-biodegradable solids (M_{nb}) mg/l
5. Organic debris solids, non-biodegradable (M_D) mg/l
6. Inorganic solids (M_I) mg/l."

After the primary clarifier, M_I will be quite small, unless chemicals are added for phosphate removal. If it is small, little error is introduced by neglecting M_I so that MLSS $\approx$ MLVSS.* However, if chemicals are added, a material balance from the addition point to just before the aerator gives

$$M_I = \frac{Q_o}{Q} f_I M_o + f_e W_c/Q + \frac{Q_r}{Q} (M_I)_r \qquad (9\text{-}40)$$

where f_I is the inorganic fraction of suspended solids in the screened degritted sewage, W_c is the chemicals feed rate and f_e is the weight fraction of the chemicals ultimately recovered as a solid. $(M_I)_r$ is the inorganic SS returned in the sludge.

The concentration of nitrifying bacteria (X_N) is usually neglected since it accounts for just 1 to 2% of the MLVSS. The yield coefficient for Nitrosomonas (responsible for ammonia oxidation) is 1/10 of that for the BOD consuming organisms, while the coefficient for Nitrobacter is

*We now distinguish between MLVSS and the active biomass.

1/25. Furthermore ammonia and cell nitrogen concentrations in the aerator are low so the numbers of active nitrifying cells cannot be large.

Smith and Eilers[12] use eqn. (9-34) to calculate X leaving the first stage of their cascade model, but substitute S_o^* for S_o to calculate X leaving subsequent stages. Biodegradable solids at any point M_B are calculated from S^*. If for MLSS, $BOD_5/VSS = 0.8$, then

$$M_B = \frac{1}{0.8} \frac{f_*}{1-f_*} S^* \tag{9-41}$$

where f_* is the fraction of BOD_5 as suspended solid, the nonbiodegradable solids, M_{nb}, associated with the sludge is given by

$$M_{nb} = (M - M_I)\left(1 - \left(\frac{BOD_u}{COD}\right)_{solid}\right) \tag{9-42}$$

The principle in eqn. (9-42) is that the biodegradable portion of the sludge is measured by the ratio of the ultimate BOD to the COD of the sludge. If biodegradability is to be measured by BOD_5, it can be used instead of BOD_u in eqn. (9-42). Smith and Eilers suggest $BOD_u/COD = 0.9$. The increase in nonbiodegradable sludge may also be formulated in a way similar to eqn. (9-33) to give

$$\Delta M_{nb} = \Delta M_D = b' \bar{X} \tag{9-43}$$

The nonbiodegradable sludge entering the first stage in the cascade model is

$$(M_{nb})_o = (1 - f_B)\, M_o \frac{Q_o}{Q} + f_{nb} (M_{nb})_r \frac{Q_r}{Q} \tag{9-44}$$

For the first and all subsequent stages,

$$(M_{nb})_n = (M_{nb})_{n-1} + b' \bar{X} \tag{9-45}$$

In each iteration (M_{nb_n}) will change until it gradually converges on its presumed value. Equation (9-42) could be used to suggest a starting value.

At any point in the aerator, the sludge concentration (MLSS) must be

$$M = X + M_B + M_{nb} + M_I \tag{9-46}$$

The BOD contribution of the suspended matter may be calculated from eqn. (9-41). It is, of course, much lower than the potential BOD of the MLSS when the cells are dead.

Application of the Smith and Eiler's activated sludge model (involving essentially eqns. (9-11) with $n_s = 2$, eqns. (9-18), (9-34), (9-41), (9-42), (9-43) and (9-46)) to 3 separate full scale plants treating domestic sewage gave good results for $b_{20} = 0.18$ day^{-1}, $b'/b = 0.18$, $k_m = 150$ mg/l., $0.4 < Y < 0.75$ lbVSS/lb BOD_5 and $\hat{\mu}_{20} = 4.8$ day^{-1}.

Smith and Eiler[12] suggested the following relations to correct the constants just given to the operating temperature:

$$\hat{\mu} = \hat{\mu}_{20} \ (1.047)^{T-20} \tag{9-47}$$

$$\hat{\mu}_N = (\hat{\mu}_N)_{20} \ (1.123)^{T-20} \tag{9-48}$$

$$b = b_{20} \ (1.047)^{T-20} \tag{9-49}$$

In eqn. (9-48), $(\hat{\mu}_N)_{20} = 0.33$.

The state of the modelling of sludge production in an aerator can only be characterized as primitive. Sophistication is hardly warranted. Consequently, we recommend that only X and M_{nb} should be considered in modelling. Equations (9-34) and (9-43) are suggested for this purpose. The biodegradable portion of the sludge can be obtained from eqn. (9-41). Changes in cell concentrations are modest in conventional activated sludge systems so that calculations of S^*_e and X_e through

successive substitution would seem satisfactory.

9.7 Nutrient Removal Models

Nitrification proceeds by the oxidation of ammonia by Nitrosomonas to nitrite and the subsequent oxidation to nitrate by Nitrobacter (Section 9.2). A buildup of nitrite is seldom observed; consequently the rate of ammonia conversion to nitrite controls the rate of nitrification.

Downing et al.[16] use the Monod equation, eqn. (9-19), to describe the rate of ammonia oxidation. The rate term, as before, can be used with the appropriate mixing model (eqn. (9-11) or eqn. (9-12)) to calculate the reduction of ammonia in the aerator. Only inlet ammonia is considered. Ammonia or nitrogen solubilized in cell lysis is neglected. If N_{AM} = ammonia concentration and X_N the concentration of nitrosomonas in mg/l., then,

$$R_{AM} = \frac{\hat{\mu}_N}{Y_N} \frac{X_N N_{AM}}{k_{m_N} + N_{AM}} \qquad (9\text{-}50)$$

Constants suggested by Downing et al.[16] are $\hat{\mu}_N = 0.33\ day^{-1}$, $k_{m_N} = 1.0$ mg/l., $Y_N = 0.05$ lb Nitrosomonas/lb-N in NH_3.

The Nitrosomonas concentration can be determined by multiplying R_{AM} by Y_N and substituting in one of the mixing models. Just as for BOD removal two simultaneous equations must be solved to obtain the profile of N_{AM} and X_N through the aerator. Alternatively an integral relation can be used based on sludge yield. For a stage in the cascade model the relation is

$$(X_N)_n = (X_N)_{n-1} + Y_N \left[(N_{AM})_{n-1} - (N_{AM})_n \right] \qquad (9\text{-}51)$$

Using this equation, N_{AM} and X_N can be calculated in any stage or at the end of the aerator. A suitable starting value for $(X_N)_o$ is 1% of X.

Denitrification can occur in the aerator if the dissolved oxygen

---

[16] Downing, A.L., Painter, H.A. and Knowles, B.A., "Nitrification in the Activated Sludge Process", J. of Inst. of Sewage Purification, Part 2, 130-157 (1964)

level is allowed to drop to a low level at the end of the vessel. Unfortunately, relationships for evaluating denitrification are not yet available.

Organically bound nitrogen and phosphates entering the aerator as suspended matter are handled most conveniently by assuming the suspended matter is completely incorporated into the sludge. The sludge leaving the aerator will contain organically bound nutrients. The amounts may be estimated by assigning values for the weight percent nitrogen as N and phosphorus as P in the sludge. Eckenfelder and Ford[2] tabulate sludge compositions. For activated sludges, the weight percent nitrogen as N ranges from 2 to 5%, while phosphorus as P ranges from 1.5 to 5%. Exact values for use in simulation or design must come from field measurements.

Soluble phosphates should decrease due to assimilation of phosphorus for cell synthesis. The decrease must be estimated from a phosphorus balance over the aerator which yields

$$\Delta P^{*} = -\Delta P_{*} = -f_{P}\,\Delta M \qquad (9\text{-}52)$$

where f_P is the weight fraction of phosphorus in the sludge.

9.8 Oxygen Consumption

All the models we have employed for BOD removal, biomass growth, etc. assume that rates are substrate limited. Relationships for the effect of dissolved oxygen (DO) levels on BOD removal or cell synthesis kinetics do not seem to be available. As a consequence, O_2 consumption and supply are primarily design considerations. In simulation, one could check predicted DO levels against measured levels; but since the models for O_2 supplied to an aerator are crude, agreement of DO levels would have to be considered fortuitous.

Because the kinetics are assumed to be independent of DO, the O_2 requirement can be calculated from an integral relation. Oxygen is necessary for cell respiration, biomass growth and ammonia oxidation. Writing a balance with R_{O_2} = rate of consumption/volume for each stage

$$R_{O_2} = \frac{CY}{\tau}\left[(S^*)_{n-1} - (S^*)_n\right] + bC'\bar{X} +$$

$$\frac{C''}{\tau}\left[(N_{AM})_{n-1} - (N_{AM})_n\right] \qquad (9\text{-}53)$$

Y appears in the BOD term because about 70% of the BOD is synthesized into cell matter. The O_2 requirement, thus, should be related to the yield coefficient. A yield coefficient does not appear for the Nitrosomonas because the cell yield is so low that all the substrate is oxidized for cell metabolism. Since 4 moles of O_2 are required for each mole of ammonia, C'' = 4.6 mg O_2/mg N as a NH_3 consumed. Smith and Eilers[12] find C is between 1.24 and 1.42, where the units of CY are lbs O_2/lb. BOD_5 consumed, and C' = 1.17 with units lbs. O_2/lb. VSS. The "Design Guide"[6] gives CY = 0.53 lbs O_2/lb. BOD_5, bC' = 0.15 lbs O_2/lb. VSS and C'' = 4.6 lbs. O_2/lb N. Elsewhere[7], CY is given between 0.4 and 0.65.

The rate at which O_2 can be supplied as lbs of O_2/volume to an aerator can be estimated only crudely from empirical correlations or from suitably scaled aeration experiments. The latter are conducted with a cobalt catalyzed sodium sulfite solution. This chemical serves as a scavenger for O_2. Steady state or unsteady state experiments[2] can be carried out to measure K_La. If geometric similitude is maintained (cell diameter/impeller diameter, impeller immersion (cell depth, etc.) and the specific power input (HP-hr/ft^3) is kept constant, K_La will be about the same for a full scale unit as for the model. With K_La established the rate at which O_2 can be supplied will be

$$\mathcal{R}_{O_2} = K_La\ (C_g - C_L) \qquad (9\text{-}54)$$

where $\mathcal{R}_{O_2}$ is the pounds of air transferred per cubic foot of the vessel per hour. The units of C are mg./l. while those of K_La are lbs-l./mg-hr-ft^3. In eqn. (9-54) we have replaced the A term (the interfacial area) in eqn. (9-8) by the specific interfacial area (a). Lumping a

together with K_L creates a volumetric mass transfer coefficient.

The volumetric mass transfer coefficient available from experiments is temperature dependent and sensitive to surface active agents in the waste. If $K^o_L a$ is the experimental value assuming 20^oC, the value at a different temperature is

$$K_L a = \alpha\ (1.02)^{20-T}\ K_L{}^o a \tag{9-55}$$

where T is ^oC and α corrects for the waste used. The surface resistance coefficient depends not only upon the waste, but upon the aeration device and operating conditions used. The range is given as $0.65 \leq \alpha \leq 1.33$[3]. Figure (9-12) shows α varies with the HP/ft^3 as well as BOD reduction.

For spargers and plate or tube diffusers, C_g in eqn. (9-54) is the saturation concentration at mid depth. It is a depth function and depends upon the O_2 concentration in the bubbles as well,

$$C_g = C_g{}^o \left(\frac{p_T + 0.018\ h}{14.7} + \frac{f_{O_2}}{.42} \right) \tag{9-56}$$

where $C_g{}^o$ is the concentration in water at atmospheric pressure, p_T is the barometric pressure (psi), h is the sparger depth and f_{O_2} is the volume fraction O_2 in the bubbles breaking the top surface of the tank. It has been found[6] that $K_L a$ is directly proportional to the air rate and to the depth of the sparger or diffuser

$$K_L a = K_L{}^o a\ \frac{q_{air}}{(q_{air})_{Test}}\ \frac{h}{(h)_{Test}} \tag{9-57}$$

The performance of aerators occasionally will be expressed as oxygenation capacity (C_{O_2}) in lbs of O_2/volume of aerator-day. It is related to $K_L{}^o a$ as

$$C_{O_2} = K_L{}^o a\ C_{g_{20}} \tag{9-58}$$

$\mathcal{R}_{O_2}$ can be directly calculated then as

$$\mathcal{R}_{O_2} = \alpha C_{O_2} \frac{C_g - C_L}{C_{g_{20}}} (1.02)^{20-T} \quad (9\text{-}59)$$

where $C_{g_{20}}$ is the saturated DO at 20^oC while C_g is measured at T^oC. Similitude and constant power input are assumed in using eqn. (9-59).

Performance of aeration equipment is also expressed in terms of aeration efficiency, η^o, the lbs. of O_2 supplied per horsepower-hour. This "efficiency" is usually measured with sodium sulfite solutions for a specific application. The efficiency is calculated from this measurement as

$$\eta = \eta^o \alpha \frac{C_g - C}{C_{g_{20}}} (1.02)^{20-T} \quad (9\text{-}60)$$

Aeration efficiency is particularly useful for design.

The rate of oxygen supply also may be estimated from correlations if they exist. A general correlation for diffusers and spargers is[3].

$$\mathcal{R}_{O_2} = \alpha \beta Q_{air}^n \frac{h^{m-1}}{LW^{p+1}} (1.02)^{T-20} (C_g - C_L) \quad (9\text{-}61)$$

where h, W, L are dimensions of the aerator, Q_{air} is the air flow in scfm and β is a constant given in Table 9-4. The exponent m is 0.88 for spargers and 0.72 for Seran tubes while p is about 0.5.

For turbine-sparger ring systems (Figure 9-4), the correlation is[3]

$$\mathcal{R}_{O_2} = \frac{\alpha \beta' \omega_{imp}^x}{V} Q_{air}^n d_{imp}^y (C_g - C_L) (1.02)^{T-20} \quad (9\text{-}62)$$

TABLE 9-4. COEFFICIENTS FOR EQUATION (9-61) FOR DIFFERENT AERATION EQUIPMENT

Aeration Device	β	n
Seran Tubes: 9" Spacing, 14.4 ft. depth 24 ft. wide vessel	0.15 to 0.17	0.81 to 0.92
Spargers: 24" Spacing, 14.8 ft. depth 24 ft. wide vessel	0.081	1.02
Spargers: 9" Spacing, 15 ft. depth 24 to 25 ft. wide vessels, various orifice sizes	0.062 to 0.068	1.02
Plate Tubes: 15 ft. depth 25 ft. wide vessel, single row	0.35	0.49
As above but with double row	0.20	0.80

where ω_{imp} is the turbine rpm, V is vessel volume and d_{imp} is the diameter of the turbine impeller.

A correlation for a bladed surface aerator is given by Kalinske[17]

$$\mathcal{R}_{O_2} = \alpha \beta'' d_{imp} h_{imp} \omega_{imp} (N_{Fr}-1)^z (C_g - C_L) (1.02)^{T-20} \quad (9\text{-}63)$$

where h_{imp} is the height of the impeller blade. N_{Fr} is the Froude number $= \pi d_{imp} N_{imp} / \sqrt{g h_{imp}}$ where g is the force constant = 32.2 lb_f/ lbm ft^2/sec.

The difference between the rate at which O_2 is consumed in the aerator R_{O_2} and the rate at which it is supplied $\mathcal{R}_{O_2}$ determines the rate of change of dissolved oxygen. If the change of BOD_5, ammonia and the active biomass through the aerator are known, eqn. (9-53) may be used

[17] Kalinske, A.A., "Power Consumption for Oxygenation and Mixing" in Eckenfelder and McCabe (Editors), "Advances in Biological Waste Treatment", Macmillan (New York, 1963)

to estimate R_{O_2}, whereas any appropriate equation among eqns. (9-54) or (9-59 to 63) may be used to calculate $\mathcal{R}_{O_2}$. The choice for $\mathcal{R}_{O_2}$ will depend on the nature of the mass transfer information available. If a cascade model is used:

$$(DO)_n = (DO)_{n-1} - \tau_n \left(R_{O_2} - \mathcal{R}_{O_2} \right) \qquad (9\text{-}64)$$

A continuous model for the aerator leads to

$$D \frac{d^2(DO)}{dz^2} - u \frac{(DO)}{dz} - \left(R_{O_2} - \mathcal{R}_{O_2} \right) = 0 \qquad (9\text{-}65)$$

The boundary conditions for the continuous model eqns. (9-13) and (9-14), must also be written in terms of DO. Numerical integration of eqn. (9-65) results in the DO profile along the aerator.

The oxygen concentration is normally kept at 2 mg./l., but it is believed that the various rates are not seriously affected until DO drops to about 0.5 mg./l.

9.9 Models for Other Changes

Nitrification and carbon dioxide from cell respiration will reduce alkalinity, however, wastes are believed to be sufficiently buffered so that pH changes are small. Eckenfelder and Ford[2] indicate 0.5 lbs of alkalinity (as $CaCO_3$) are neutralized per lb. of BOD_5 removed in the aerator. Substrate utilization and cell synthesis kinetics are apparently independent of alkalinity over the normal range encountered in aerators. Consequently the alkalinity profile through the aerator is not necessary for the computation of BOD removal and sludge yield. The overall change in alkalinity A_{Alk} can be obtained from an integral expression

$$(A_{Alk})_e = (A_{Alk})_o - 0.5 \, (S_o - S^*_e) \qquad (9\text{-}66)$$

where alkalinity is measured in mg./l. as $CaCO_3$.

Aeration systems, particularly mechanical aerators, cool the waste being treated by evaporation and by convective heat transfer. The large mass of water held in an aerator, however, will keep the temperature change to little more than a degree. Even so, the sensitivity of rates to temperature means that temperature change must be considered. Unfortunately, temperature change in aerators does not seem to have been analyzed so we can offer only a crude treatment.

Cooling of the waste passing through an aerator occurs through i) evaporation from the water surface into the air and ii) heat transfer due to temperature difference between the waste and the air. Normally i) is the more important of these modes. Because of evaporation, cooling can occur even if the air temperature is greater than the water temperature. Thus, the temperature change must be expressed as the sum not the product of a term containing a humidity driving force and a term containing a temperature difference:

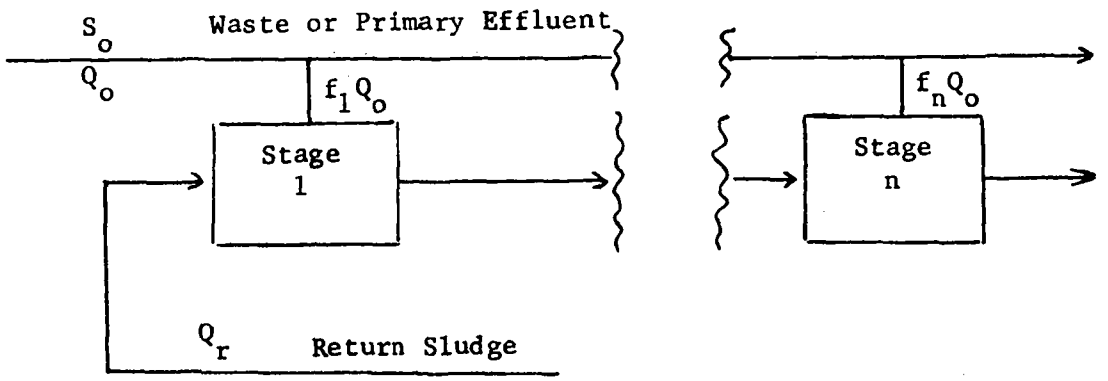
$$T_e - T_o = A\,(T_{air} - T_o) - B\,(\mathcal{H}_o - \mathcal{H}_{air}) \qquad (9\text{-}67)$$

where $\mathcal{H}$ is the humidity in lbs/lb. of dry air and T_o is the temperature at which the mixed liquor enters the aerator. A and B will be some function of $K_L{}^o a$ or $\eta^o\alpha/C_{g_{20}}$ since the same interfacial area is involved in O_2, heat, and H_2O transfer.

9.10 Extension to Step Aeration

The material presented so far in this chapter permits the simulation or design of conventional activated sludge systems. Step aeration and contact stabilization (sludge reaeration) require additional modelling. Reaeration of sludge can be handled by using different sets of coefficients in the various expressions for R_X (such as eqns. (9-34) or (9-38)). Step aeration, however, needs a different contacting model.

Step aeration is most easily represented by a cascade model in which the feed stream splits into streams going to each stage of the cascade. The fraction going to a stage is $f_n Q_o$.



A material balance in terms of substrate around the n^{th} stage gives

$$S_o f_n Q_o + S^*_{n-1} \left(\sum_{n=1}^{n-1} f_n Q_o + Q_r \right) - S^*_n \left(\sum_{n=1}^{n} f_n Q_o + Q_r \right) - R_S V_n = 0 \qquad (9\text{-}68)$$

If $r = Q_r/Q_o$ and $\tau'_n = V_n/Q_o$, the balance can be solved for S^*_n:

$$S^*_n = \frac{S_o f_n + S^*_{n-1} \left(\sum_{n=1}^{n-1} f_n + r \right) - \tau'_n R_S}{\sum_{n=1}^{n} f_n + r} \qquad (9\text{-}69)$$

Similar balances can be made for M, M_{nb}, N_{AM} and P. The balance for X and X_N will be the same as for the conventional activated sludge system because no cells enter with the primary effluent. As before, an alternative to solving the balance equations simultaneously is to write integral equations and solve using successive substitution.

9.11 Design

Process units are designed conventionally through the use of design parameters as we indicated in the previous chapter. These, when taken together with flows and compositions, permit the type of equipment to be specified and the size to be computed. Since the function of an activated sludge system is to remove BOD, the primary design parameter for the system is the fractional removal of BOD (f_S). Measuring aerator

performance using the soluble portion of the BOD, the first design parameter (DP), is defined as

$$f_S = \frac{S_o - S_e^*}{S_o} \qquad (9\text{-}70)$$

This design parameter sets S_e^* and the aerator will be sized to achieve this effluent. There is a trend towards using an effluent level rather than fractional removal for aerator design. In this case, $(DP)_1$, would be simply S^*_e. Table 9-5, for example, shows effluent specifications for conventional activated sludge and extended aeration systems.

Secondary treatment plants are now being designed to achieve 95% BOD removal. Assuming that primary clarifiers account for about 35% of the BOD reduction and, further, that suspended solids escaping from the secondary effluent accounts for half the BOD, f_S must be 0.96 to obtain an overall BOD removal of 95%.

Once size has been established secondary design parameters are needed to choose or compute the number of mechanical aerators (or the diffuser surface area), horsepower, aerator dimensions, cell size (if the aerator is to be staged). Normally after the primary design parameter (f_S in this case) has been invoked, the remaining design parameters are used sequentially. For the activated sludge system, however, sizing of the aerator is complicated by the dependence of the BOD removal on the contacting pattern, sludge age and the oxygen supply rate. These can depend in turn on the secondary design parameters. Frequently an iterative design procedure is necessary.

Secondary design parameters for aerators might be the dimensions of the aerator vessel or compartment, such as height and width $(DP)_2$, the flow per vessel or the number of vessels in parallel $(DP)_3$, and the mean MLSS level $(DP)_4$. The sludge recycle ratio could be specified instead of MLSS as $(DP)_4$. Frequently, the aerator size (as horsepower) per BOD load unit or unit of vessel volume will be a design parameter, however, this parameter is not necessary because power requirement can be computed. The type of aeration equipment (mechanical, diffuser plates, etc.) is chosen

on the basis of cost and not through a "design parameter".

The design procedure for a conventional activated sludge system will be illustrated by two cases i) spiral flow aerator using a sparger or a diffuser, ii) segmented aerator with mechanical aeration. For case i) a continuous model will be used for design, while we employ the cascade model for case ii). Figure 9-19 shows schematically the calculational procedure which might be employed using the continuous model. Figure 9-20 shows the procedure for case ii).

In both procedures we use $(DP)_4$ = r (recycle ratio) instead of MLSS. The first step is to invoke design parameters $(DP)_3$ and $(DP)_4$ to calculate the conditions at the entrance to the aerator. $(DP)_2$ is next used to obtain the velocity if the continuous model is used (case i)) or the detention time in a stage if case ii) is being considered. Although it does not appear in the figures, the primary design parameter, $(DP)_1$, is now used to obtain S_e^*. Figure 9-20 shows simultaneous solution of the stage equation (eqn. (9-11)) for S_n^* and X_n until $S_n^* \leq S_e^*$. This establishes the number of stages required and the detention time in the aerator (τ) can be computed.

Figure 9-19 indicates simultaneous forward integration of eqn. (9-12) for S^* and X. This may be accomplished, for example, by a standard Runge Kutta integration routine. At the end of the aerator with forward integration, a rather difficult boundary condition must be satisfied. Often it is convenient to integrate backwards to avoid this problem. The nature of the problem and the backwards integration technique are discussed in Chapter 7 and a sample FORTRAN program is shown.

With the mathematical operations just indicated complete, the procedure in both figures shows the calculation of the food to organism ratio (F/X). This ratio is checked against constraints and if the constraints are not satisfied, both figures show that the sludge recycle ratio, a design parameter, is adjusted. This operation calls for some discussion.

Conditions exist in the operation of a system which regardless of the size of equipment chosen will prevent the system from achieving

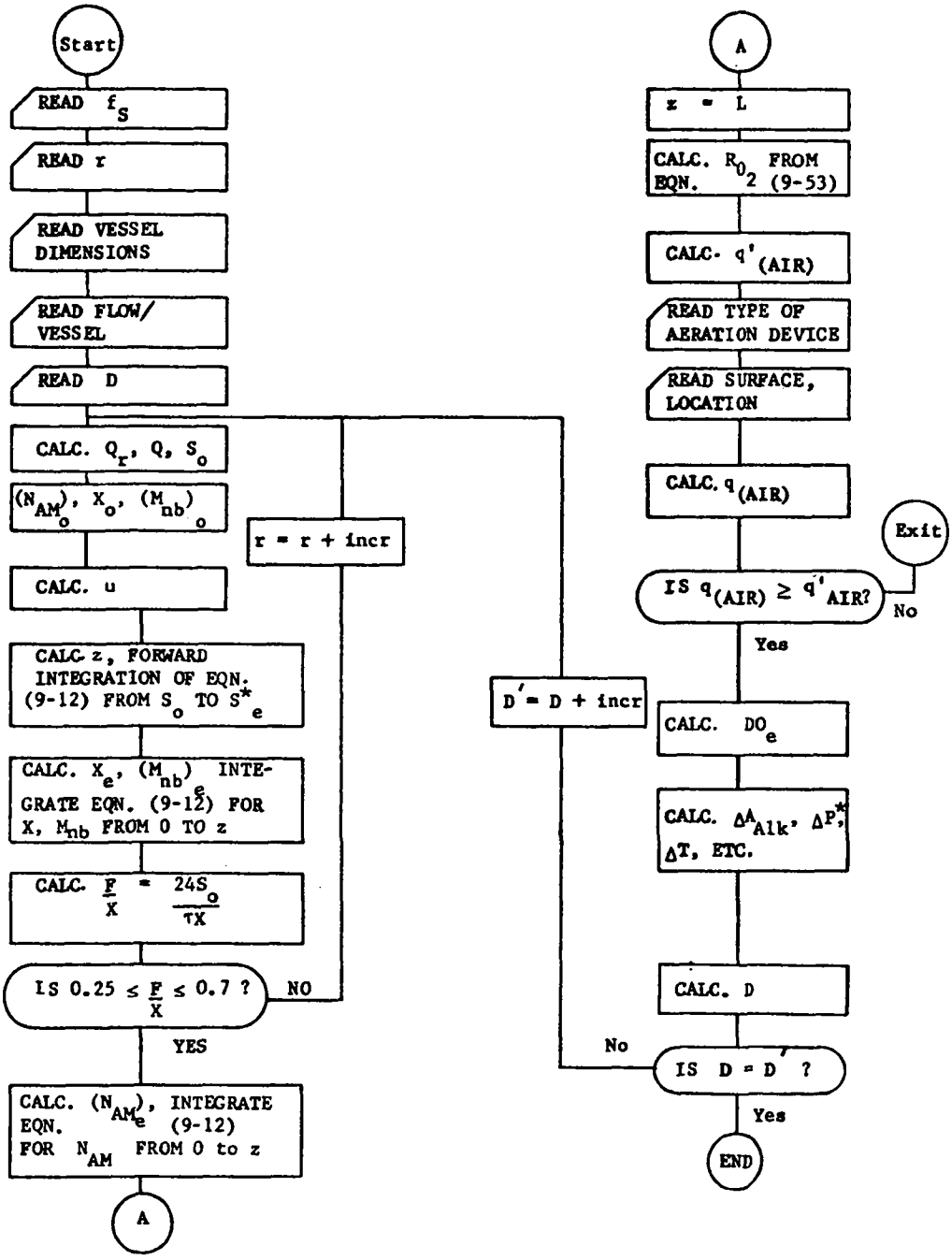


FIGURE 9-18. DESIGN FLOW SHEET FOR A PLANT WITH DIFFUSER AERATION

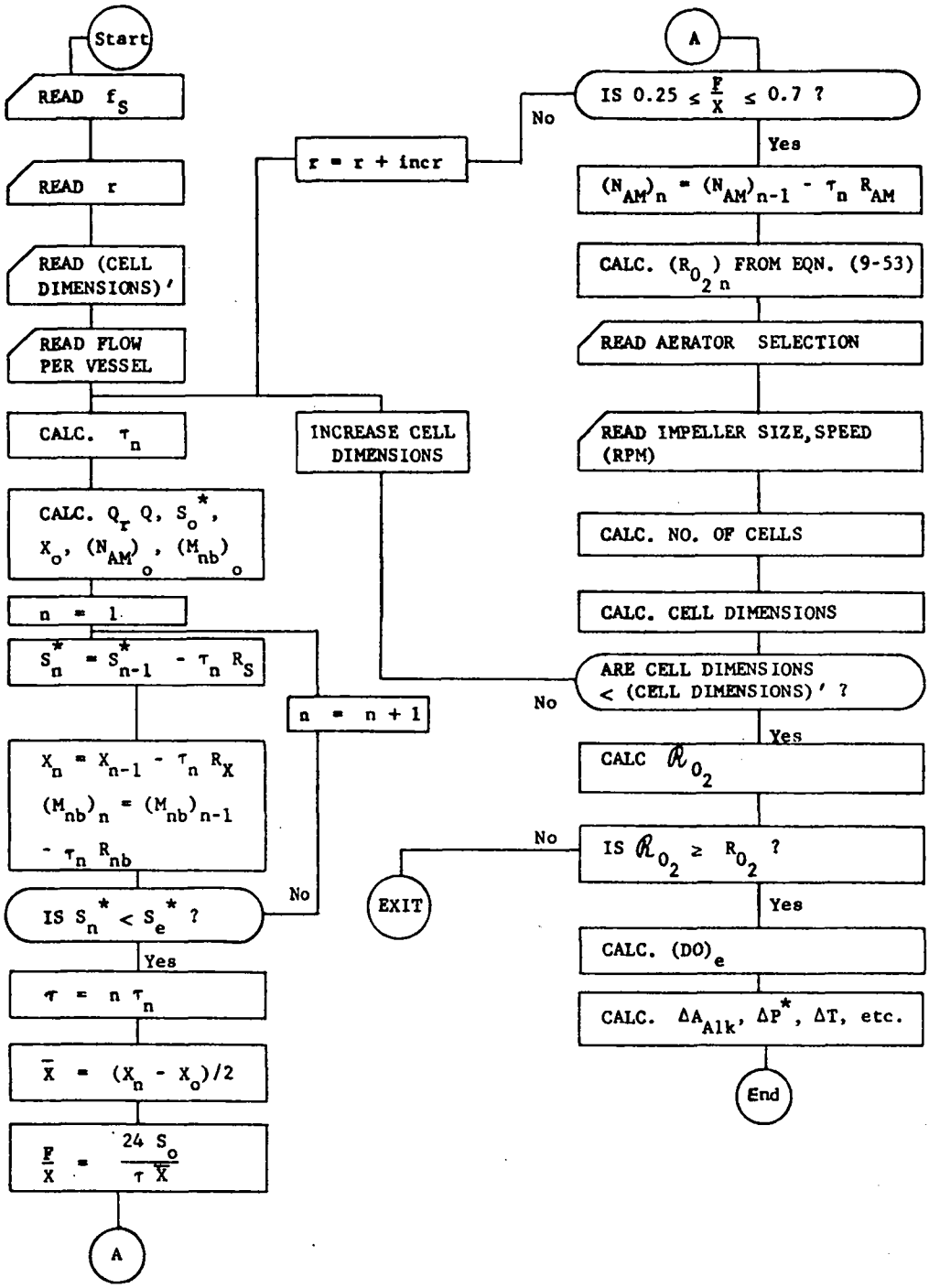


FIGURE 9-19. DESIGN FLOW SHEET FOR A STAGED PLANT WITH MECHANICAL AERATION

its specified performance. These conditions are often expressed as constraints. A simple example of limiting operational conditions is pH. The activated sludge system functions poorly at pH's outside of a range from about 6.5 to 8.0. pH level, thus, acts as a constraint on the design. The F/X constraint, however, arises because of the operation of the final clarifier.

It is well established that sludge age must be held within a fairly narrow range to achieve a rapid settling sludge with good thickening properties. This was evident in the schematic diagram, Figure (9-9), included in the discussion of theory. Figure (9-21) shows much the same information, but data is included. It is evident that the sludge age should not be less than 2 days if the SVI is to be kept near its minimum. This limit corresponds to an organic loading of less than 0.7 for domestic sewage. Sludge ages of 10 days are satisfactory. On the other hand, only in extended aeration are sludge ages greater than 10 days encountered. Thus, the other limit on organic loading for conventional activated sludge is 0.2 lb. BOD_5/day/lb. MLVSS. Organic loading is often referred to as the food to organism (F/X) ratio. By definition

$$F/X \equiv \frac{24\ S_o}{\tau\ X} \tag{9-71}$$

where τ is the detention time in the aerator in hours. The constraint can be stated as $0.2 < F/X < 0.7$.

Once the F/X constraint is satisfied and the length of the aerator is established for case i) and the number of stages for case ii), the oxygen requirement is calculated using eqn. (9-53). The oxygen supplied by the aeration equipment specified is computed next. If the supply is inadequate, the aeration equipment specification is faulty. If the oxygen supply is adequate, the DO level at the end of aerator is determined.

With specific air rate known, the next step in the procedure in Figure 9-19 is to calculate the dispersion coefficient using eqn. (9-15) or an equivalent expression. The assumed dispersion coefficient D' is checked and iteration can occur at this point. A similar procedure may

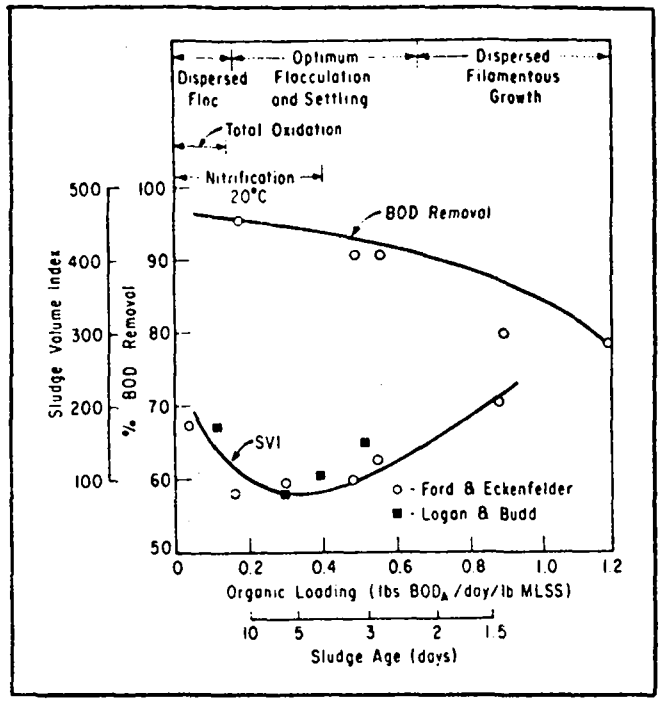


FIGURE 9-20. SLUDGE SETTLING LIMITS ON ORGANIC LOADING*

be seen in Figure 9-20. In this case, the cell dimensions to contain the mechanical aerator specified are computed and compared with the cell dimension set through a design parameter. If the agreement is not satisfactory, iteration on the design parameter must take place.

Sludge recycle is usually in the range $0.5 < r < 2$. This range can be used as a constraint on r set to satisfy the F/X constraint. If the latter constraint forces r to the limits, the procedure would be to vary the flow per aeration vessel, $(DP)_3$, or dimensions, $(DP)_2$. This is not shown in the figures.

Table 9-5 taken from "Design Guide"[6] shows a number of computed parameters of conventional and extended aeration activated sludge systems based on design parameters of effluent BOD (line 1 or 2), MLSS (line 6), and air flow (line 16). The difference between design BOD and suspended solids and the average values reflects the practice of using

* Figure taken from reference (3).

"worst" flows for design. Note that MLSS is used in place of sludge recycle ratio as a design parameter and air flow has been used in place of specifying aeration equipment as shown in Figures 9-19 and 9-20. The BOD load specification could be used in place of the effluent as a design parameter. When both are given they indicate a feed condition as suggested by the 4 columns listed for the conventional process. The table is useful because it serves as a comparison for operating or equipment parameters computed in a simulation or design.

TABLE 9-5. ACTIVATED SLUDGE PROCESS DESIGN CHART

		Dimensions	Extended Aeration	Activated Sludge				
1.	Design BOD Effluent	mg/l	(15)**	20		25	35	50
2.	Average BOD Effluent	mg/l	(10)**	10		12	15	22
3.	Design Suspended Solids Effluent	mg/l	(-65)*	25		30	35	45
4.	Average Suspended Solids Effluent	mg/l	(-15)**	15		16	18	22
5.	Design BOD Load	lb/lb/day	0.065	0.25		0.50	1.0	2.0
6.	Design MLSS	mg/l	3000	3000		3000	3000	3000
7.	BOD Volume Load	lb/10^3 gal/day	1.60	6.25		12.5	25	50
8.	Excess Sludge	lb/lb MLSS/day	0.03	0.22		0.52	1.12	2.32
9.	Oxygen Uptake Rate	lb/lb MLSS/day	0.185	0.370+	0.275++	0.40	0.65	1.15
10.	per gallon tank	lb/10^3 gal/day	4.40	9.30	6.90	10.0	16.20	28.70
11.	Oxygen Concentration, ml	mg/l	1	2	2	2	2	2
12.	Oxygen Transfer	lb/10^3 gal/day	5.20	12.20	9.10	13.20	21.50	38.0
13.	Airflow/gallon tank	cu ft/gal/day	3.60	8.60	6.40	9.30	15.00	26.5
14.	Airflow/lb BOD Appl.	cu ft/lb BOD	2250	1360	1000	740	600	550
15.	Peak (24/18)	cu ft/lb BOD	2250	1820	1350	1000	800	730
16.	Design Airflow	cu ft/lb BOD	2800	2400	2000	1500	1200	1100

Table 9-6 summerizes a set of criteria prepared by OWRC for the operation of their activated sludge systems. They can be considered as design parameters. The design parameters indicated are BOD loading, MLSS, and air supplied rather than effluent BOD, recycle ratio, and aeration equipment specification which were used in Figures 9-19 and 9-20. Sludge quality (age) and DO level also appear as well as pH and temperature. These latter criteria function as constraints as we suggested earlier. The table illustrates that a variety of other design parameters

can be used for activated sludge systems.

TABLE 9-6. OWRC CRITERIA FOR A WELL FUNCTION ACTIVATED SLUDGE SYSTEM

Temperature:	75 to 85°F
pH:	Between 7.0 and 7.5
Air Requirements:	(a) 0.5 to 1.5 cu. feet of free air per gallon of sewage
	(b) 500 to 700 cu. feet per lb. B.O.D. removed when B.O.D. loading 25 to 30 lb. per 100 lb. aerator solids
	(c) 700 to 1750 cu. feet per lb. B.O.D. removed when B.O.D. loading 25 to 12 lb. per 100 lb. aerator suspended solids
Aeration Period:	(a) Diffused air - 5 to 7 hours
	(b) Mechanical - 8 to 10 hours
Sludge Age:	3 to 4 days
B.O.D. Loading:	(a) 25 to 30 lb. of B.O.D. per 1000 cu. feet of aeration tank
	(b) 30 to 40 lb. of B.O.D. per 100 lb. of aerator suspended solids for large plants
	(c) 20 to 30 lb. of B.O.D. per 100 lb. of aerator suspended solids for small plants
Sludge Quantity:	(a) 1500 to 3000 p.p.m. aerator suspended solids for diffused air plants
	(b) 500 to 1200 p.p.m. for mechanical aeration plants
Sludge Quality:	Volatile matter - 60 to 85% of total aerator solids
	Alkalinity - 100 to 200 p.p.m.
	Dissolved Oxygen -
	Content at outlet - 2.0 to 5 p.p.m.
	30-minute settling test - 15 to 25%
	Sludge Volume Index (a) near 100 for diffused air plants
	(b) about 250 for mechanical aeration plants

9.12 Example

Figure 9-22 is a simulation model adapted from Smith and Eilers[12] and used in some of our studies of Ontario waste treatment plants[18]. A staged aerator is assumed. Among others, eqns. (9-11), (9-31), (9-33), (9-44) to (9-49) are employed in the model. Notice that the subroutine is considerably longer than others in the notes, even

[18] Silveston, P.L., "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research 6, 1101-1111 (1972)

though nitrification, O_2 requirement, change in the DO level are ignored. This reflects the complexity of models for the activated sludge system.

Although the subroutine follows the recommendation of translating the STRMI and EN statements into more easily understood symbols we made in Chapter 7, the symbols are those used by Smith and Eilers and not those used in the manual. The model includes the final clarifier. Combining both units in a single model has the advantage of simplifying the iterative calculations and thus the time of execution. The versatility of the activated sludge model, however, is substantially reduced. It is not a practice we recommend.

```
      SUBROUTINE ACSLD1
C
C   SILVESTON MODIFIED VERSION OF SMITH MODEL.
C
C
      DIMENSION NAME(50),NAME2(50),TITLE(24),AEN(2,40),PAPER(2,10)
      DIMENSION SN(75,25),EN(20,20),NPAPER(20)
      DIMENSION NPROCS(14,50),EPS(30),LOOP(10),IFLUN(10)
      DIMENSION STRMI(5,25),STRMO(5,25)
      DIMENSION NAMEN(20,20),NAMESN(25),NAMDEF(15),KEY(20)
      COMMON SN,EN,STRMI,STRMO,AEN,NIN,NOUT,NE
      COMMON NAME,NAME2,TITLE,PAPER,NPAPER,NPROCS,EPS,LOOP,IFLUN,NUMPR
      COMMON KSETS,KRUN,NELMAX,NEMAX,NSLMAX,NSMAX,NOAEN
      COMMON NAMEN,NAMESN,NAMDEF,KEY,NONAME
      DIMENSION S(10),X(10)
      REAL MLSS,MLS
C
C
C  THE MOST IMPORTANT ASPECT OF SIMULATION OF ACTIVATED SLUDGE UNIT IS
C  DETERMINATION OF GROWTH RATE OF CELLS,G*(LB/DAY/LB).THIS SUBROUTINE
C  USES THE MONOD RELATIONSHIP,
C                          G*=KR*S/(KS+S)
C  WHERE KR ISTHE MAXIMUM RATE CONSTANT FOR SYNTHESIS(DAY**-1) AND KS
C  IS THE SATURATION CONSTANT(MG/L OF SUBSTRATE)
C
C  THE DEATH RATE OF CELLS,DE*(LB/DAY/LB) IS CONSTANT AT A VALUE OF KE
C  THE ENDOGENOUS RESPIRATION CONSTANT,FRACTION OF VIABLE CELLS WHICH
C  LYSE PER DAY.
C
C
C**************************************************************************
C  THE EQUIPMENT VECTOR IS AS FOLLOWS,
C     3. VOLUME.                    9. RESPIRATION RATE.
C     4. VRSS.                      10. XRSS
C     5.ACTIVE CELLS.               11. VSS/MLSS RATIO.
C     6. MAX. RATE CONSTANT.        12. VSS
C     7. YIELD COEFF.               13. NTKS(NO. OF AERATION TANKS.)
C     8. SATURATION AMT.            14. CROSS-SECTIONAL AREA(FINAL SETTLERS)
C                                   15. MLSS
C                                   16. TEMPERATURE.
C                                   17. RECYCLE FLOW IN AERATOR.
C**************************************************************************
C
C  SET NO. OF ENTRIES IN EQUIPMENT VECTOR FROM THIS SUBROUTINE
      EN(NE,2)=17.
      KEY(NE)=8
      DATA (NAMEN(8,I),I=1,17)/'NO. ','NTKY','VOL.','VSSS','CELL',
     *'RATE','YLD.','SAT.','RESP','XRSS','VS/M','VSS','NTKS','AREA',
     *'MLSS','TEMP','RCLE'/
C
C
C   Q17 IS SET AT A CONSTANT VALUE OF 7.0 MGD.
C
```

```
      T=EN(NE,16)
      Q17=0.62*STRMI(1,3)
      Q14=STRMI(1,3)
      PC=0.1
      SC=0.277
      MLSS=EN(NE,15)
      VSS=0.6*MLSS
      NTKS=EN(NE,13)
C
C  SS1 IS THE CONCENTRATION OF NON-BIODEGRADABLE VOLATILE SUSPENDED
C  SOLIDS GOING INTO AERATOR.
C
      SS1=STRMI(1,8)*SC
C
C  SET-UP FOR INTERVAL HALVING TECHNIQUE.
C
 10   S(1)=0.5*STRMI(1,7)
      SUP=STRMI(1,7)
      SLOW=0.
      IS=0
 16   CONTINUE
      K=0
 17   CONTINUE
C
C
C  DETERMINATION OF SOLID FRACTION OF BOD COMING INTO AERATOR(SFBOD).
C  EQUATIONS ARE OBTAINED FROM MASS BALANCES.
C
C
      A=STRMI(1,7)*STRMI(1,3)/(Q17*S(1))
      B=EN(NE,4)-1.
      SFBOD=(B-A+SQRT((A-B)**2+4.*A*B*STRMI(1,6)/STRMI(1,7)))/(2.*B)
C
C
C
      Q15=(STRMI(1,3)*(1.-EN(NE,10))-Q17*(EN(NE,4)-1.))/(EN(NE,4)-EN(NE
     X,10))
      IF(Q15.LT.0.05) GO TO 18
      Q14=STRMI(1,3)-Q15
      TEMP1=Q14*EN(NE,10)+Q15*EN(NE,4)
      S17=(1.-SFBOD)*S(1)+S(1)*SFBOD*EN(NE,4)
      BSS=S(1)*SFBOD/0.8
      BNS=SS1*STRMI(1,3)/TEMP1
      X(1)=EN(NE,7)*(STRMI(1,3)*STRMI(1,7)+S17*Q17-S(1)*(Q17+STRMI(1,3))
     *)/TEMP1
      ASS=X(1)
      DSS=0.18*EN(NE,7)*(STRMI(1,7)-S(1))*STRMI(1,3)/TEMP1-0.18*X(1)
      IF(DSS)74,74,75
 74   DSS=0.
 75   VSS=ASS+BNS+DSS+BSS
      SINERT=PC*DSS
      DVSS=(MLSS-VSS)*EN(NE,4)
      IF(DVSS.LT.0.)DVSS=0.
      MLS =VSS+((STRMI(1,4)-STRMI(1,8))*STRMI(1,3)+(SINERT+DVSS)*Q17)/
     *(Q17+STRMI(1,3))
      DMLSS=(MLS-MLSS)/MLS
      IF(ABS(DMLSS).LT.0.01) GO TO 15
      MLSS=MLS
      K=K+1
      GO TO 17
 18   CONTINUE
      Q17=Q17-0.01*Q17
      GO TO 16
 15   CONTINUE
      MLSS=(MLS+MLSS)/2.
C
C  DTAR IS THE DETENTION TIME FOR EACH AERATION TANK.
C
C
      DTAR=EN(NE,3)/(NTKS*(STRMI(1,3)+Q17))
C
C
C  S(I)-CONCENTRATION OF SUBSTRATE OUT OF AERATION TANK.
C  S(K)-CONCENTRATION OF SUBSTRATE INTO AERATION TANK.
C  X(I)-CONCENTRATION OF MICRO-ORGANISMS OUT OF AERATION TANK.
C  X(K)-CONCENTRATION OF MICRO-ORGANISMS INTO AERATION TANK.
C  SIT-VALUE FOR S(1) FROM OVERALL MASS BALANCE.
C  XIT-VALUE FOR X(1) FROM OVERALL MASS BALANCE.
C
C
      DO 11 I=1,NTKS
      K=I+1
      GSTAR=EN(NE,6)*S(I)*X(I)*DTAR/(EN(NE,8)+S(I))
      S(K)=S(I)+GSTAR/EN(NE,7)
```

```
 11   X(K)=X(I)+EN(NE,9)*DTAR*X(I)-GSTAR
      SIT=(STRMI(1,3)*STRMI(1,7)+Q17*S17                )/(STRMI(1,3)+Q17)
      XIT=EN(NE,4)*X(1)*Q17/(Q17+STRMI(1,3))
C
C
C  START OF ITERATION CALCULATIONS.
C
C
      DSI=(S(NTKS+1)-SIT)/SIT
      IF(ABS(DSI)-0.01)29,29,22
 22   IF(IS-15)24,29,29
 24   IF(DSI)25,25,27
 25   SLOW=S(1)
      S(1)=S(1)+0.5*(SUP-SLOW)
      IS=IS+1
      GO TO 16
 27   SUP=S(1)
      S(1)=S(1)-0.5*(SUP-SLOW)
      IS=IS+1
      GO TO 16
 29   DXI=(X(NTKS+1)-XIT)/XIT
      IF(ABS(DXI)-0.1)53,53,10
 53   SFI=S(1)
C
C
C  WHEN ITERATIONS HAVE CONVERGED PROGRAM SKIPS TO HERE.
C
C
C
C  CALCULATIONS FOR OUTPUT QUANTITIES.
C
C
      DBOD=SFI*(1.-SFBOD)
      EFF=EN(NE,10)*1.0
      BOD14=(0.94*ASS+0.8*BSS)*EFF        +S(1)*(1.-SFBOD)
      EN(NE,17)=Q17
      EN(NE,15)=MLSS
      EN(NE,12)=VSS
      STRMO(1,8)=EN(NE,10)*VSS
      STRMO(2,8)=EN(NE,4)*VSS
      STRMO(1,3)=Q14
      EN(NE,5)=X(1)
      STRMO(2,3)=Q15
      STRMO(1,7)=BOD14
      EN(NE,11)=VSS/MLSS
      STRMO(1,5)=DBOD
      STRMO(1,6)=BOD14-DBOD
      STRMO(2,7)=S17
      STRMO(2,5)=DBOD
      STRMO(2,6)=S17-DBOD
      STRMO(1,4)=EN(NE,10)*MLSS
      STRMO(2,4)=EN(NE,4)*MLSS
 200  CONTINUE
      RETURN
      END
```

FIGURE 9-21. SEPSIM MODEL OF AN ACTIVATED SLUDGE AERATOR

10 TRICKLING FILTER MODELS

Use of trickling or biological filters has been limited in Canada even though this method of secondary treatment is widely used in the United States and Europe. The explanation for this, it is claimed, is the sceptical attitude of provincial regulatory agencies toward the process. It is difficult to attain BOD removals greater than 80 to 85 per cent, fly nuisance, ponding problems, and fear of winter freeze-up are cited as reasons for discouraging filter use. The freeze-up problem can be avoided. Biological filters are successfully operating in the Prairies (Regina) and in Northern Ontario during winter. Proper design of the ventilation system and of the distributor alleviates the winter ice formation problem provided recycle is limited. Jank et al. recently demonstrated successful winter operation of a tower filter using the plastic FLOCOR packing on a primary effluent in a Southern Ontario location.[1] Plastic packing also reduces the fly problem, and ponding severity when filters are overloaded. Interest is developing in using filters as a roughing treatment for packing and other food industry wastes before they are discharged to sewers. Trickling filters are, therefore, a biological treatment alternative which must be considered in Canada.

In this chapter, we will examine briefly the function and theory of trickling filters. Our emphasis will be on filters using a plastic packing. We will consider, in particular, models proposed by Kornegay[2, 3, 4] and Roesler and Smith[5] as these have been developed with computer

---

[1] Lancaster, E.A., Silveston, P.L., Drynan, W.R. and Jank, B.E., "Plastic Packed Trickling Filter Under Canadian Climatic Conditions", Pulp and Paper, Dec. 6, 58-61 (1968)

[2] Kornegay, B.H. and Andrews, J.F., "Kinetics of Fixed Film Biological Reactors", J.W.P.C.F. 40, No. 11, R460 (1968)

[3] ibid, "Application of the Continuous Culture Theory to the Trickling Filter Process", Proc. 24th Ind. Waste Conference, Eng. Ext. Series, Purdue Univ., Lafayette, Ind. (1969)

[4] Kornegay, B.H., "Modelling and Simulation of Fixed Film Biological Reactors", 8th Annual Workshop of the Assn. of Envir. Eng. Professors, School of Civil Engineering, Georgia Tech., Atlanta, Georgia (1972)

[5] Roesler, J.F. and Smith, Robert, "A Mathematical Model for a Trickling Filter", Publ. W69-2, F.W.P.C.A., U.S. Dept. of the Interior (February, 1969).

use in mind.

The rotating disc contactor, a process similar to the trickling filter in that the biomass responsible for BOD reduction forms on a solid surface, has been tested in the Northern U.S.A. successfully and must also be considered for Canadian application. We will discuss the process and a model for it briefly.

10.1 Operation

Trickling filters consist of a packing which supports a biomass. Sewage or other dilute waste is distributed continuously over the upper surface of the packing. It trickles and spills through the packing, contacting the biomass, and eventually is collected in a sump under the bed and pumped to a settler. Figure 10-1 shows schematically a conventional filter containing a bed of 2" to 3" coarse rock. The arms shown in the

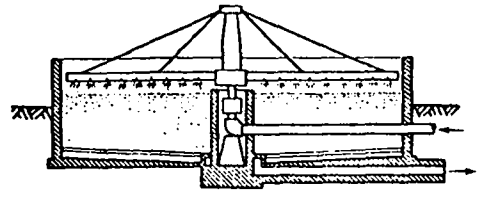


FIGURE 10-1. SCHEMATIC DIAGRAM OF A CONVENTIONAL TRICKLING FILTER WITH ROTATING SPRAY ARMS, ROCK MEDIA, AND TILE UNDERDRAIN*

diagram rotate slowly distributing the sewage. Mechanical draft is not needed to draw air through the bed; natural circulation occurs due to humidification of the air, and usually this is sufficient. Filters are aerobic systems so good liquid-air contact is important for oxygen transfer. Installations using plastic media are similar except that much taller structures are used.

---

*Figure taken from reference (6) with the kind permission of the publisher.

(6) K. Imhoff and G.M. Fair, "Sewage Treatment", 2nd Edition, John Wiley (New York, 1956).

Trickling filters for sewage are designed now for high-rate operation, and recirculation is frequently employed. Recirculation schemes, some of which are patented, are shown in Figure 10-2. The purpose of recirculation is to maintain adequate wetting of the packing, improve waste distribution through the media and to raise the BOD removal. The primary clarifier shown upstream of the filter in Figure 10-2 removes suspended matter which might clog the nozzles of the distributors or contribute to ponding with rock media. Clarification is not necessary for a screened waste when the open structured plastic media are employed.

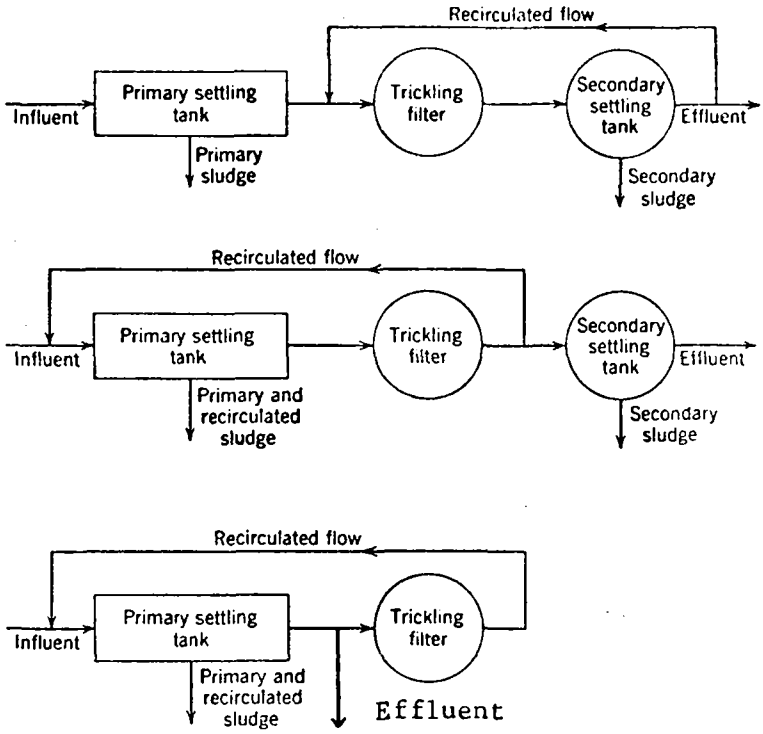


FIGURE 10-2. COMMON METHODS OF RECIRCULATION IN THE OPERATION OF TRICKLING FILTERS*

Figure 10-3 shows FLOCOR, one of the score or so of plastic media which are replacing rock as filter packing. These media are said to provide better liquid distribution, oxygen transfer, and, in some cases, they offer higher specific surface areas. They usually are free from

*Figure taken from reference (6) with the kind permission of the publisher.

ponding, eliminate fly nuisances and can be built to appreciable heights.

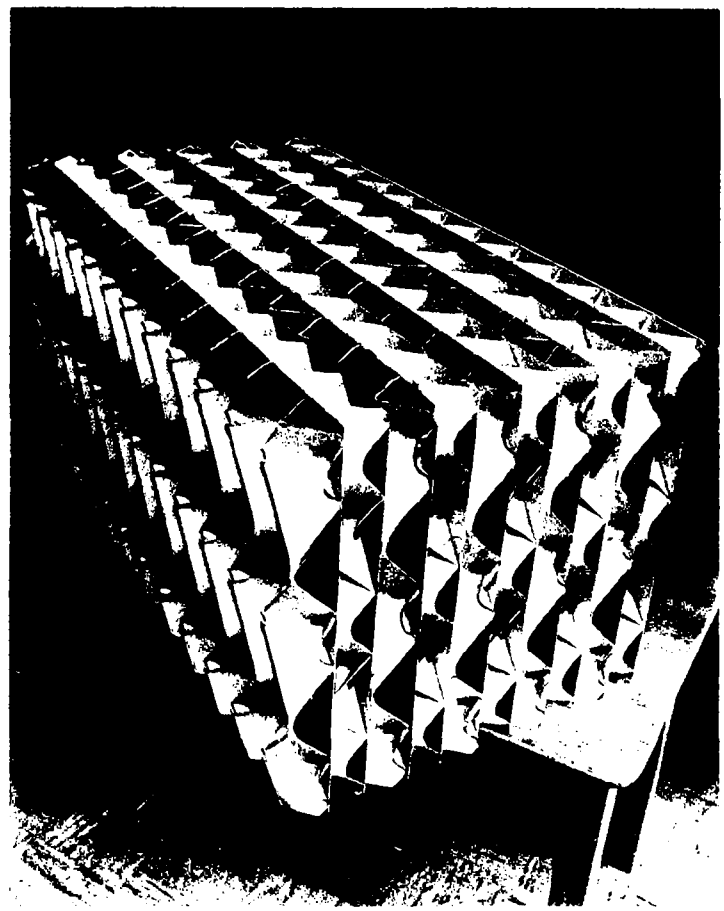


FIGURE 10-3. "FLOCOR" PACKING MODULE*

Figure 10-4 is a photograph of a pilot scale unit operated by the University of Waterloo which had a depth of 18 ft.(1) Rock media beds are rarely deeper than 6 to 8 feet.

---

*Figure taken from reference (7).

(7)Industrial Research Institute, "The Operation and Performance of 'Flocor' Packed Biological Filters Under Canadian Climatic Conditions", Research Report, University of Waterloo, (1969)

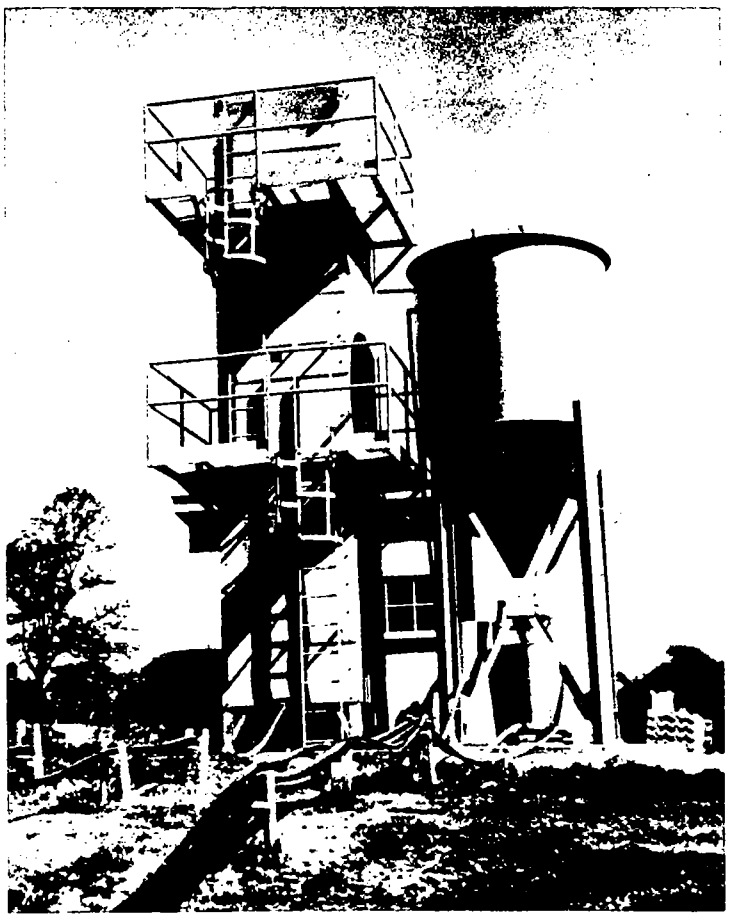


FIGURE 10-4. A PILOT SCALE 'FLOCOR' PACKED TRICKLING FILTER*

10.2 Theory

Five distinct classes of physical phenomena are involved in trickling filter operation:

i) liquid distribution over the filter surface, flow through the complex packing structure, and wetting of the packing surface.

ii) biodegration of organic matter in the slime layer by aerobic and anaerobic bacterial action

iii) sloughing off the slime

iv) oxygen transfer into the liquid phase

v) transfer of organic matter and oxygen through the liquid film

*Figure taken from reference (1) with the kind permission of the magazine "Pulp and Paper".

to the slime layer and hence by diffusion in the layer.

Liquid distribution and wetting (and pooling in rock media) are important because they collectively determine the holdup of liquid on the filter media. The mean contact time depends on holdup. For the liquid:

$$\tau_H = \frac{H\,L}{q} \qquad (10\text{-}1)$$

where H is the holdup in cu. ft. of holdup/cu. ft. of media; L = packing depth (ft.); and q is the waste feed rate in cu. ft./sq. ft. of bed surface. Plastic media provide various lengths of vertical or inclined flat surface. Liquid runs down the surface as a film, collects at the bottom surface, and either flows or drops to the next layer of packing. Film thickness and its contribution to holdup can be crudely estimated using the well-developed theory of laminar flow on plates. Beading of liquid at the bottom edge and holdup due to the slime on the surface would increase this holdup by two to threefold.

Early models[8] for rock media assumed smooth continuous films, but Atkinson et al.[9] demonstrated films on rock were highly irregular and suggested that flow in rock media was primarily by cascades from pool to pool. These pools contained the bulk of the holdup. The pool formation may be due to the slime formation which obstructs some fine passages through the rock media.

In all media, holdup and thus contact time will be some function of the specific surface area (ft^2/cu. ft. of packing).

The complexity of holdup has lead to the practices of empirically correlating holdup or contact time[10]. Roesler and Smith[5] use

---

[8] Howland, W.E., Pohland, F.G. and Bloodgood, D.E., "Kinetics in Trickling Filters" in Eckenfelder and McCabe, "Advances in Biological Waste Treatment", MacMillan Co. (New York, 1963).

[9] Atkinson, B., Swilley, E., Busch, A., and Williams, D., "Kinetics, Mass Transfer and Organism Growth in a Biological Film Reactor", Trans. Inst. of Chem. Engs. 45, T 257 (1967).

[10] Sinkoff, M., Porges, R. and McDermott, J., "Mean Residence Time of Liquid in a Trickling Filter", J. San. Eng. Divl, A.S.C.E. 85, 662 (1959).

$$\tau_H \propto \frac{A_p^m}{q^n} L \qquad (10\text{-}2)$$

in their filter model where A_p is the specific surface area of the packing; L = depth, while q is the hydraulic loading (usually millions of gallons per day per acre of bed surface). The exponents m and n are experimentally determined; m ranges from 0.75 to 1.0[5], while Table 10-1 shows n as a function of A_p for various packing (see p. 10-15).

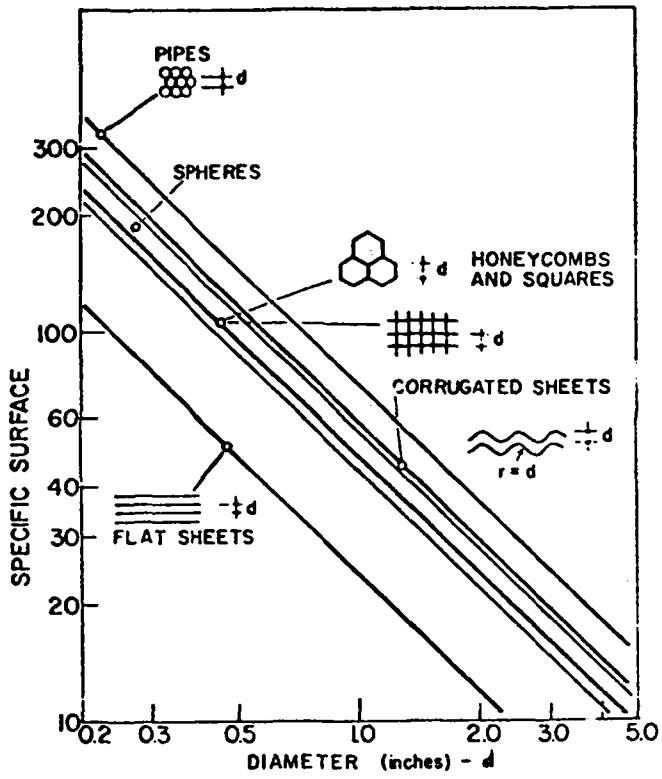


FIGURE 10-5. RELATIONSHIP OF SPECIFIC SURFACE AND DIAMETER FOR VARIOUS MEDIA*

Specific surface areas for various types of plastic media are shown in

*Figure taken from reference (11).

(11) Design Guides for Biological Wastewater Treatment Processes", Water Pollution Control Research Series - 11010 ESQ 08/71, Environmental Protection Agency (Washington, D.C., 1971).

Figure 10-5.

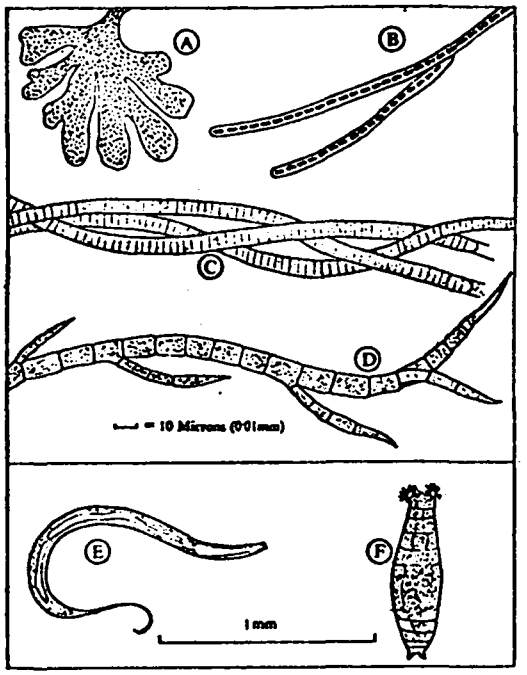
The biomass on a filter is aptly referred to as a slime. Figure 10-6 shows the biomass slime found on a plastic media after several months of continuous operation. The slime, of course, is a community

FIGURE 10-6. APPEARANCE OF THE BACTERIAL SLIME ON THE "FLOCOR" PACKING*

composed of a large number of heterotrophic micro-organisms, of which the most important are bacteria, protozoa, fungi, and worms; each in many genera and species. Bacteria and other micro-organisms secrete enzymes that cause hydrolysis of complex organic compounds into substances that

*Figure taken from reference (7).

can be utilized as food. Species relations are to some extent symbiotic, but competition between species for food, predation and parasitism of one species on another and other interactions are present and indeed essential to the proper function of the slime. Figure 10-7 illustrates a few of the more prominent micro-organisms.



(A) Zooglea ramigera, (B) Sphaerotilus natans, (C) Phormidium sp., (D) Stigeoclonium, (E) a nematode worm, (F) a rotifer.

FIGURE 10-7. MICROORGANISMS IN FILTER SLIME*

The algae and fungi make up most of the attached materials with colonies of bacteria, fungi, algae and individual protozoans developing within or upon the basal mat. The complex is referred to as a zoogleal growth even though it includes filamentous organisms as well as bacterial

*Figure taken from reference (12) with the kind permission of the publisher.

(12) Hawkes, H.A., "The Ecology of Waste Water Treatment", Pergamon Press (New York, 1963)

colonies of "zoogleals". The "zoogleal" bacteria are believed to be primarily responsible for the oxidation of organic compounds. The fungi hold the biomass together through their branch mycelia.

Protozoa form another major group of the slime population. These one-celled animals are primarily i) holozoic feeders which obtain their food by ingesting living organisms as well as small organic particles and ii) saprozoic feeders who can utilize only the material in solution. Worms present in portions of the slime include nematodes, aquatic earthworms, and earthworms. Algae occur in those parts of the bed where sunlight penetrates. Snails and insect larvae complement the grazing fauna on rock media. They are less frequently found on plastic packing.

Although a trickling filter is normally classified as an aerobic device, it is actually a facultative system. The micro-organisms build on the plastic or rock surface and grow with the continued application of fresh wastes. Newly formed organisms at liquid-slime interface obtain most of the organic matter and dissolved oxygen and multiply faster than organisms close to the plastic surface. As the slime builds up, the dissolved oxygen drops near the media surface. Those biomass micro-organisms which are facultative shift from an aerobic to an anaerobic metabolism.

Anaerobic metabolism yields toxic end products which soon causes death of the cells in direct contact with the plastic. This results in weakened surface bonding and flow across the slime causes it eventually to shear off. The free slime is washed from the media and is ultimately removed in a clarifier. New growth starts on the now bare surface and the cycle is repeated.

Early models paid little attention to the biomass, assuming tacitly that it was uniform in age, bacteriological composition, thickness and activity. It is now widely accepted that only the outer surface of the slime is aerobic. In a careful study, Kornegay and Andrews[2] showed that the active portion of the slime film had a thickness "d" of about 70 μ, but the film itself could have thicknesses of about 300 μ ("h" in Figure 10-8). As the film grows, the facultative process sets in leading eventually to the sloughing off the slime. The process then begins afresh. It follows from this viewpoint that the biomass-slime at a point within

the bed should be considered to be a dynamic system exhibiting different characteristics depending upon slime age. Summing over the large number of microscopic dynamic systems gives the impression of steady state.

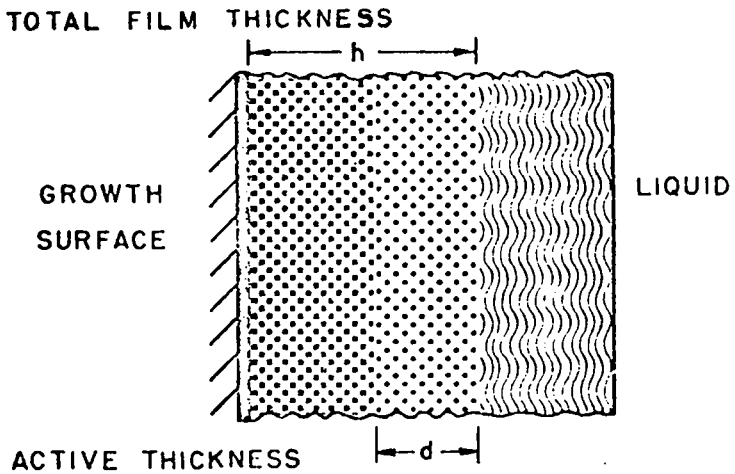


FIGURE 10-8. A SECTION OF SLIME FILM SHOWING SCHEMATICALLY ACTIVE (AEROBIC) AND INACTIVE (PARTIALLY ANAEROBIC) PORTIONS OF FILM*

The dissolved oxygen carried into the filter with the primary effluent is inadequate for the consumption of organic matter by the slime organisms. Thus, oxygen transfer from air through the liquid film into the slime is essential. There should be sufficient circulation of air through the filter that there will be relatively little resistance to O_2 transfer in the gas phase. The main resistance will be in the liquid. Figure 10-9 illustrates schematically the situation[13]. Transport through the liquid is extremely sensitive to the level of turbulence in the liquid. Turbulent mixing will be promoted by downward flow for an uneven, freely moving filamentous slime and through ripple formation. Droplet formation or beading (plastic packing) cuts circulatory mixing so that oxygen transfer is poorer at "beading" points. Transport would be poor in any slowly irrigated pools (rock media) so the slime in such pools could be anaerobic.

*Diagram taken from reference (2) with the kind permission of the Journal.

[13] Notes: "Biological Waste Treatment", Univ. of Waterloo, Waterloo (July, 1967)

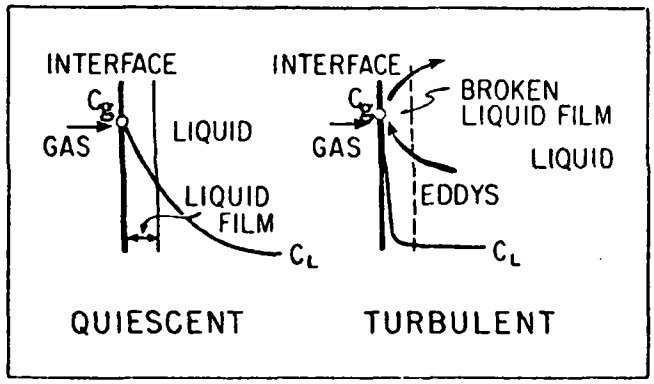


FIGURE 10-9. TRANSPORT OF O_2 INTO LIQUID/SLIME FILMS IN A TRICKLING FILTER*

Measurements of oxygen transport in filters seem to be absent in the Sanitary Engineering literature. By necessity, then, models for BOD removal in filters neglect O_2 transfer.

10.3 General Modelling Considerations

Requirements for a model are essentially those we discussed in Chapter 9. We need quantitative expressions for:

i) reduction of soluble BOD
ii) production of suspended solids
iii) reduction of nutrient levels
iv) temperature change and water loss

Expressions must relate the above changes explicitly to operating parameters such as hydraulic loading and to design parameters such as packing type and characteristic dimension, and packing depth.

10.4 BOD Removal

The simplest filter models assume that the removal of BOD in a filter depends only upon the level of bio-oxidizable matter. The rate of removal is assumed to be a linear function of this level. Thus,

$$\frac{dS}{d\tau} = -kS \qquad (10\text{-}3)$$

where S is the utilizable substrate (or BOD) in mg/l, and k is an experimentally determined rate coefficient. τ is the contact time of liquid in the filter. Assuming time is directly proportional to depth

*Diagram taken from reference (13).

leads on integration of eqn. (10-3) to "Velz's biological law for filter beds"[14], and the basic model proposed by Stack[15]:

$$S_e/S_o = \exp(-k L) \qquad (10\text{-}4)$$

The full models of both Velz and Stack are more complicated than eqn. (10-4). Both authors assume that BOD saturation can occur so that at higher loadings the purification rate is constant. Design equations are derived to predict the BOD leading which will saturate the filter[16]. Operating at this loading provides maximum utilization of the filter; that is, maximum BOD reduction/unit volume. Emphasis now has switched to reducing S_e to low values. This is a different condition than maximum utilization so the approach of Velz and Stack has not been pursued.

Howland et al.[8], Sinkoff et al.[10] and Schulze[17] have employed eqn. (10-3) and attempted to relate τ to specific surface area A_p, media, hydraulic loading (q), and filter depth (L). Schulze[17] proposes,

$$S_e/S_o = \exp(-k' L/q^{0.6}) \qquad (10\text{-}5)$$

In an extension of this treatment, Eckenfelder[18,19] assumes

---

[14] Velz, C.J., "A Basic Law for the Performance of the Trickling Filters", Sewage Works, 20, No. 4, 607 (1948)

[15] Stack, V.T., Jr., "Theoretical Performance of the Trickling Filter Process", Sewage Industrial Wastes, 29, No. 9, 987 (1957)

[16] Behn, V.C., "Trickling Filter Formulations" in Eckenfelder and McCabe, "Advances in Biological Waste Treatment", MacMillan (New York, 1963)

[17] Schulze, K.L., "Elements of a Trickling Filter Theory", in Eckenfelder and McCabe "Advances in Biological Waste Treatment", MacMillan (New York, 1963)

[18] Eckenfelder, W.W., Jr., "Trickling Filter Design and Performance," J. Sanitary Eng. Div., Proc. A.S.C.E., 87, 33 (1961)

[19] Eckenfelder, W.W. and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970)

that the rate is proportional to the biomass (X) present at a point in the filter,

$$\frac{dS}{d\tau} = -k\ X\ S \qquad (10\text{-}6)$$

If the slime depth h is uniform, X will be proportional to the specific surface area of the packing A_p. Using eqn. (10-2), τ can be replaced so that integrating over the depth of the filter,

$$S_e/S_o = \exp\left[-k''\ A_p^{\,m+1} L\ /q^n \right] \qquad (10\text{-}7)$$

k'' is a function of the substrate used, media type, characteristic dimensions and configuration, and oxygen ventilation. Eckenfelder redefines k'' to be a function of A_p as well and proposes

$$S_e/S_o = \exp\left[-k_A\ A_p L/q^n \right] \qquad (10\text{-}8)$$

Roesler and Smith[5] use this model, but with S representing total BOD_5 rather than soluble BOD_5 as Eckenfelder originally proposed. They assume the ratio of soluble to suspended BOD does not change over the filter. All models in this section can be written, similarly, in terms of either soluble BOD (S*) or total BOD(S). The coefficients in the model, of course, will depend on this choice of variable. If S^* is used, it may be assumed that all the suspended BOD contribution in the waste is removed by the filter. The filter effluent, however, has a suspended BOD contribution arising from the slime sloughed off the media.

Rate constants k'', k_A are temperature dependent. Eckenfelder[19] suggests

$$k = k_{20}\ (1.035)^{T-20} \qquad (10\text{-}9)$$

for both k'' and k_A where $T = {}^{o}C$ and k_{20} is the reference value of the constant obtained at $20^{o}C$.

The coefficients in the above equations depend on the units

used. Hydraulic loading (q) in North America is currently reported as million gallons (U.S.)/acre of filter cross-section area/day (mgd/acre = 0.016 gpm/ft^2 = 0.939 m^3/m^2/day). Values for A_p, n and $(k_A)_{20}$ are summarized in Table 10-1. For plastic corrugated packing with A_p = 27 ft^{-1} and plastic rings with A_p = 30 ft^{-1}, values of n = 0.5 and k_A = 0.017 (with q in mgd/acre) were obtained in Texas pilot scale experiments[11]. For rock media, Roesler and Smith[5] suggest n = 0.91 - 6.45/A_p, $(k_A)_{20}$ = 0.0237.

TABLE 10-1. EMPIRICAL VALUES FOR A_p, n, $(k_A)_{20}$ IN EQUATION (10-8)[5]

Media - Size	A_p (ft^{-1})	n	$(k_A)^*_{20}$
Rock 3/4"	50 to 60	0.8 to 0.85	
1"	42	0.78	
1-3/4"	21.6	0.39	0.0209
3"	11.8 to 12.6	0.40 to 0.53	
-	11.6	0.31	0.0223
Gravel	19.7	0.61	0.0233
Surfac (Plastic Media)	25	0.78	0.0260
Dowpac 10 (Plastic Media)	25	0.575	
Polygrid (Plastic Media)	30	0.65	
Mead-Cor (Plastic Media)	30	0.70	
Corrugated Asbestos	25	0.50	
	50	0.75	
	85	0.80	

* $(k_A)_{20}$ values assume substrate is total BOD_5

The Monod equation provides an alternative kinetic model for a trickling filter. We have adapted the treatment of Kornegay and Andrews[2,3,4] in what follows. The rate of change of the biomass at a point in a trickling filter is

$$R_X = \mu X \qquad (10\text{-}10)$$

where the specific growth rate is

$$\mu = \hat{\mu} \left(\frac{S}{k_m + S} \right) \tag{10-11}$$

k_m = saturation constant while $\hat{\mu}$ = maximum specific growth rate. The growth of the biomass is related through a yield coefficient Y to the rate of substrate (BOD_5) consumption, so

$$R_S = - \frac{\mu X}{Y} \tag{10-12}$$

Assuming plug flow through the filter and the continuous film model proposed by Howland et al.[8], a substrate balance on a differential band of depth dz across the filter gives on using eqn. (10-12)

$$Q_o \frac{dS}{dz} = - \frac{\mu X}{Y} A_p \, d \, A_x \tag{10-13}$$

where A_x is the filter cross-sectional area ($q = Q_o/A_x$) and d is the depth of active biomass on the filter (Fig. (10-8)). Substituting in the Monod expression (eqn. (10-11)) and integrating over the filter depth L produces,

$$k_m \ln S_o/S_e + S_o - S_e = \frac{\hat{\mu}}{qY} A_p X \, d \, L \tag{10-14}$$

Use of the continuous film model makes the Kornegay and Andrews model particularly appropriate for the corrugated plastic packing now becoming popular for trickling filters. Jank and Drynan[20] have recently demonstrated the applicability of eqn. (10-14) to film type filters. Equation (10-14) cannot be solved to give an explicit expression for S_e, however, rewriting the equation as

$$S_e = S_o + k_m \ln S_o/S_e - \frac{\hat{\mu}}{qY} A_p \, X \, d \, L \tag{10-15}$$

---

[20]Jank, B.E. and Drynan, W.R., "Substrate Removal Mechanism of Trickling Filters", J. Environ. Eng. Div., Proc. A.S.C.E., 99, No. EE3, 187 (June, 1973)

provides a simple solution by successive substitution. The group $\frac{\hat{\mu}}{Y} X d$ (which is a constant for a given system) and k_m must be evaluated from data.

A group of purely empirical models for rock media have been proposed in the literature. These are summarized in Table 10-2.

TABLE 10-2. EMPIRICAL MODELS FOR BOD REMOVAL FOR ROCK MEDIA BIOLOGICAL FILTERS

Fairall[21]

$$\frac{S_e}{S_o - S_e} = \frac{1}{k} \frac{H_q}{V_{tric}} \qquad (10\text{-}16)$$

where $1 < k\ (day^{-1}) < 10$

"Design Guide for Biological Waste Water Treatment Processes"[11] (based on National Research Council 1946 data on thirty-four U.S. trickling filter plants handling domestic sewage with $BOD_5 < 250$ mg/l.)

$$\frac{S_o - S_e}{S_o} = \frac{1}{1 + 0.0085 \left(\frac{S_o Q}{V_{tric} F}\right)^{\frac{1}{2}}} \qquad (10\text{-}17)$$

where $S_o Q$ = lbs BOD applied/day, V_{tric} = media volume in acre-feet and $F = \frac{1 + r}{(1 + 0.1\ r)^2}$. r is the recirculation so that $F = 1$ for a single pass filter.

Rincke[22]

$$\frac{S_o - S_e}{S_e} = 0.93 - 0.00272 \frac{Q\ S_o}{V_{tric}} \qquad (10\text{-}18)$$

where $Q\ S_o / V_{tric}$ is the volumetric BOD load (lb. BOD applied/1,000 ft^3/day).

---

[21] Fairall, J.M., "Correlation of Trickling Filter Data", J. Sewage and Ind. Wastes, 28, 1069 (1956)

[22] Rincke, G., "Neuere Gesichtspunkte zur Abw asserreinigung mit Tropfkorpern", Das Gas v. Wasserfach, 108, No. 24, 667 (1967)

Since only filters employing plastic packing seem to be of interest in Canada, we recommend eqn. (10-14), the Kornegay and Andrews model, for simulation and design purposes. The Eckenfelder model, eqn. (10-8), has been used for rock media filters and we recommend it for this type of filter and as a possible alternative to eqn. (10-14).

10.5 Suspended Solids Yield

Application of the Monod equation to the BOD removal in a filter requires that at steady state,

$$M_e - M_o = Y (S_o - S_e) \qquad (10\text{-}19)$$

where M is the suspended solids concentration (mg/l).

Data for the biodegradability of the solids produced in a filter are scarce. Bruce and Merkens[23] observe that suspended BOD can be estimated to be 60 to 80 per cent of the effluent suspended solids. Alternatively, it can be assumed that the ratio of biodegradable to total suspended solids does not change over a filter. Roesler and Smith[5] make this assumption but it seems to have little justification.

Equation (10-19) is probably too simple because the filter biomass is capable of trapping solids and feeding on them. Although sludge results from a "sloughing" mechanism, suspended solids coming from a filter will be ultimately determined by the cells produced by the organisms consuming substrate less that cell matter consumed by endogenous respiration. Assuming a continuous film packing,

$$M_e = Y' (S_o - S_e^*) - b \frac{L\, d\, A_p\, X}{q} + (M_{nb})_o \qquad (10\text{-}20)$$

where Y' is a yield constant, the second term containing b accounts for endogenous respiration and $(M_{nb})_o$ is the non-biodegradable suspended solids (mg/l) fed to the filter. X is the concentration of active biomass in the slime film. $b\, d\, X$ will be a constant for any one system.

---

[23] Bruce, A.M. and Merkens, J.C., "Recent Studies of High Rate Biological Filtration", Water Pollution Control (London), 113 (1970)

This equation has been simplified[5] to

$$M_e = Y' (S_o + (M_{nb})_o) - b' \frac{A_p L}{q} \qquad (10\text{-}21)$$

by assuming the biomass is proportional to A_p and that the soluble BOD_5 leaving the filter is essentially zero. The "Design Guide"[11] gives values of 0.5 for both Y' and b' based on Texas data, whereas a plot of data presented by Bruce and Merkens[23] suggests $Y' = b' = 0.37$.

10.6 Nutrient Removal

Roesler and Smith[5] allow for nitrification in their trickling filter model through an expression similar to eqn. (10-8).

$$(N^*_{AM})_e / (N^*_{AM})'_o = \exp\left[- k_N A_p d/q^n \right] \qquad (10\text{-}22)$$

where

$$k_N = (k_N)_{20}\, \theta^{T - 20} \qquad (10\text{-}23)$$

Different authors[5] give $1.071 < \theta < 1.224$ and $0.000212 < (k_N)_{20} < 0.00502$. Roesler and Smith suggest $\theta = 1.141$ and $(k_N)_{20} = 0.00290$. Equation (10-22) should be used only for rock media filters. Nitrification in filters built with plastic media occurs only if S_o is less than 30 mg/l. Roesler and Smith allow for ammoniacal nitrogen production during BOD removal so that $(N^*_{AM})'_o$ should be the sum of the ammonia fed to the filter plus the insoluble organic nitrogen $(N_{ON^*})_o$ converted in BOD reduction, or,

$$(N^*_{AM})'_o = (N^*_{AM})_o + (N_{ON^*})_o \left(\frac{S_o - S_e}{S_e}\right) \qquad (10\text{-}24)$$

Equation (10-24) assumes that the fractional reduction of insoluble organic nitrogen in the filter is the same as the BOD reduction.

Roesler and Smith assume further that phosphorus is not removed in the filter, although insoluble organic phosphorus is solubilized. We

can write,

$$(P_*)_e/(P_*)_o = S_e/S_o \qquad (10\text{-}25)$$

and consequently,

$$(P^*)_e = (P^*)_o + (P_*)_o \left(\frac{S_o - S_e}{S_o}\right) \qquad (10\text{-}26)$$

10.7 Relations for Other Changes

Alkalinity is believed to remain constant over a trickling filter.

Evaporation occurs in filters, but water loss relative to the flow through the filter is negligible. Evaporation, of course, humidifies air next to the water surfaces. Humidification decreases the density and thereby draws air through the filter. Evaporation depends on the relative humidity of the air and the air and water temperatures. The amount is readily predictable from humidity and temperatures if the mass transfer characteristics of the filter are known. In principle, draft through a filter bed can be calculated. The calculation would be useful for predicting O_2 transfer in filters. However, since O_2 transfer is ignored in filter models, draft is not estimated.

Temperature drop of waste flowing through a filter is primarily due to evaporation except at low air temperatures. Humidification theory indicates that the temperature drop relation should have the form,

$$T_e = T_o - a\,(T_o - T_{air}) + b\left[\mathcal{H}_{air} - \mathcal{H}(T_o)\right] \qquad (10\text{-}27)$$

where a and b will be empirically determined coefficients, $\mathcal{H}_{air}$ is the humidity of ambient air, and $\mathcal{H}(T_o)$ that for saturated air at the water temperature.

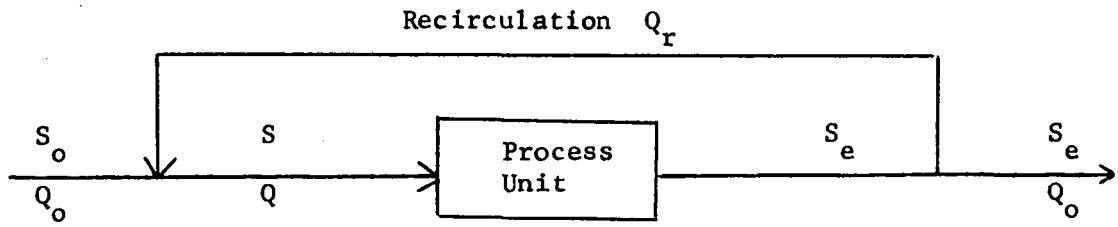
10.8 Recirculation

The normal practice in computer modelling is to include recycle in the network and not in a model for a process unit. Figure 10-2 shows

that recycle around a trickling filter involves either the primary or final clarifier. For these processes, recycle should be treated as part of the network.

It is possible to include recirculation in the process unit model. This could be desirable in computer-aided design if recycle is an operating parameter to be set by an optimization subroutine. It is also desirable if the recycle ratio r is fixed and the recycle occurs around the filter without use of a settler.

All the previous models can be converted to recirculation models. The derivation is straightforward. We will use S(BOD) to illustrate the procedure.



Define the recycle ratio (r) as $r = Q_r/Q_o$. A balance at the first junction gives $Q = Q_o + Q_r$. Replacing Q_r by r, $Q = Q_o (1 + r)$. A similar balance on S gives the feed to the unit as $S = S_e \frac{Q_r}{Q} + S_o \frac{Q_o}{Q}$. Again, replacing Q_r, $S = \frac{1}{1+r} (r S_e + S_o)$.

From the models developed, $S_e/S = f (k_m, \frac{\hat{\mu}X}{Y}, A_p, q, L)$ where S is feed BOD to the filter and q is the actual hydraulic loading on the filter $((1 + r)Q_o)$. Substituting for S through eqn. (10-28) and solving for S_e,

$$S_e/S_o = \frac{f}{(r + 1) - fr} \qquad (10\text{-}29)$$

where f is S_e/S_o for single pass operation but at recycle augmented flow. In eqn. (10-29), f could be given by eqns. (10-4), (10-5) or

(10-8).

10.9 Design Relations

Fractional reduction of BOD over the filter or effluent BOD should be the primary design parameter for trickling filters $(DP)_1$, although BOD loading is often used instead. Loading is defined as lbs. of BOD_5 per day per cubic foot of filter volume ($S\ Q/V_{tric}$). Figure 10-10 plots the relation between loading and fractional reduction in rock media filters allowing for latitude and recirculation. The figure offers an alternate means of sizing filters if the fractional reduction is specified. Loadings for other media can be estimated by

$$(V/V_{rock})_{tric} = \frac{1}{1 + 0.7\left(\frac{A_p - 12}{12}\right)} \qquad (10\text{-}30)$$

The relation comes from "Design Guides for Biological Wastewater Treatment Processes"[11]. V_{rock} is the filter volume using 3" rock estimated from Figure 10-10 or from a BOD loading specification.

Examination of BOD removal models such as eqns. (10-8) or (10-15) show that three parameters A_p, q and L appear. Consequently, at least one more design parameter must be specified in addition to fractional removal or BOD loading.

The specific surface area of the packing (A_p) is not specified through a design parameter, rather it is chosen from economic or performance considerations. There are no specifications which call for a specific surface area. The second design parameter for filters $(DP)_2$ is usually hydraulic loading (q). If not encoded in regulations, hydraulic loading is calculated through a factor from $(q)_{min}$, the minimum flow needed to adequately wet the packing. Thus, $(q)_{min}$ is the effective $(DP)_2$. Conventional rock media (3" with $A_p = 12\ ft^{-1}$) should have a minimum hydraulic loading of 5 gallons (U.S.)/ft^2 hour[11], while studies by Bruce and Merkens[20] indicated that a corrugated plastic media whose A_p was about twice that of rock required a $(q)_{min} = 10.5$ gal/ft^2 hour. This suggests a linear relation for $(q)_{min}$:

$$(q)_{min} = 0.42\ A_p \qquad (10\text{-}31)$$

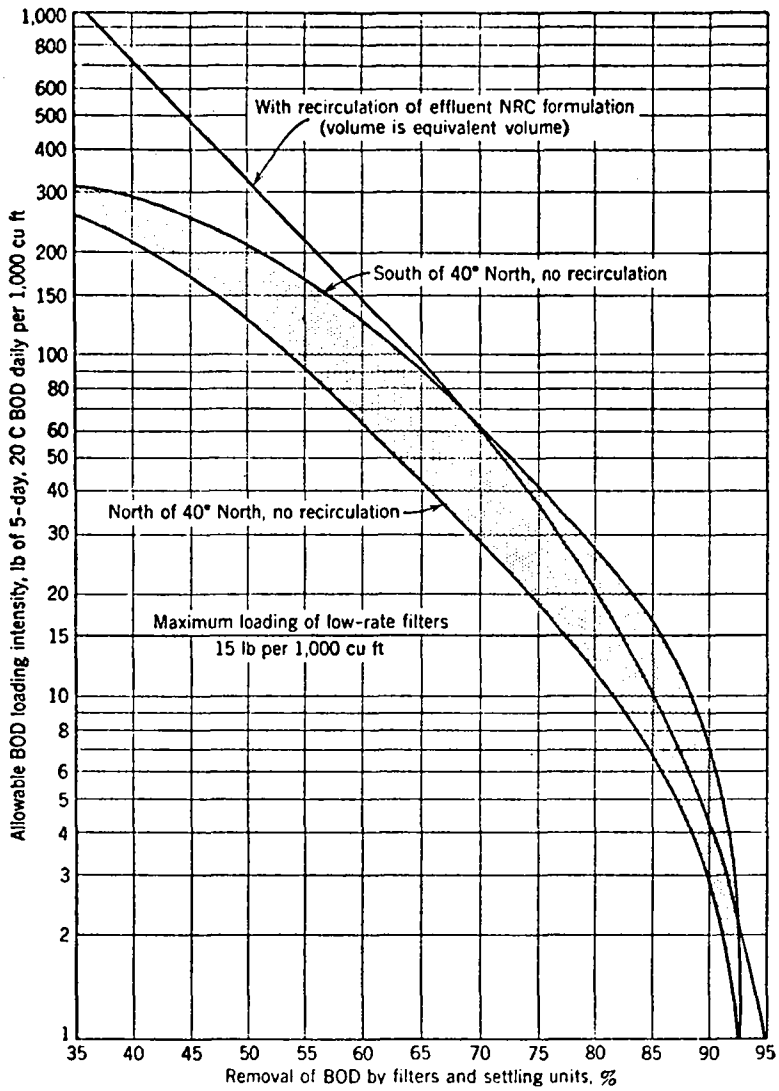


FIGURE 10-10. ALLOWABLE BOD LOADING OF TRICKLING FILTERS FOR GIVEN PERCENTAGE REDUCTIONS OF THE BOD (STANDARDS FOR SEWAGE WORKS, UPPER MISSISSIPPI RIVER BOARD OF PUBLIC HEALTH ENGINEERS AND GREAT LAKES BOARD OF PUBLIC HEALTH ENGINEERS, 1952).*

where A_p is ft^{-1} and H_q has units gallons (U.S.)/ft^2-hour.

Once a media has been chosen, specifications for $(DP)_1$ and $(DP)_2$ can be used with eqn. (10-15), if the media is plastic (and forms a

*Figure taken from reference (6) with the kind permission of the publisher.

continuous film), or eqn. (10-8), if it is rock, to calculate the depth of filter required. Assuming $(DP)_1$ is fractional reduction of BOD (f_s), then eqn. (10-14) can be solved for L:

$$L = \frac{q\,(f_s\,S_o - k_m \ln (1 - f_s))}{\frac{\hat{\mu}\,X_d}{Y}\,A_p} \qquad (10\text{-}32)$$

where the group $(\frac{\hat{\mu}X_d}{Y})$ is a rate term established by pilot scale work or estimated from correlations, A_p is the specific surface for the media chosen and q is either specified or is some multiple of $(q)_{min}$. For a rock media, eqn. (10-8) can be rearranged to give

$$L = \frac{q^n}{k_A A_p} \ln \frac{1}{1 - f_s} \qquad (10\text{-}33)$$

If BOD loading is used as $(DP)_1$, the filter depth required is readily obtained without the use of eqns. (10-8) or (10-15). However, either of these equations or, indeed, any other relation given in section 10-4 must be brought in to calculate the effluent BOD.

With depth and cross section estimated, secondary design parameters such as the maximum depth for a rock media filter and maximum filter diameter or cross section can be introduced to calculate the number of filters in series and in parallel which are required. Plastic media filters can be built fairly tall, while recirculation is often used to achieve high BOD removals in rock filled units. As a consequence, filters are rarely connected in series. We will not consider the design of the waste distributing system above the filter or the design of the collection system underneath the unit.

10.10 Example

Figure 10-11 exhibits a simulation model for a trickling filter prepared as a model for students working on computer simulation of processes. The model assumes a once through rock media filter. Equations (10-8) and (10-9), (10-22 to 10-26) are used, together with the long WAT-

CRAP stream vector (see Chapter 5). Note the wide use of "comment" statements to describe what is happening in the program and that the relations are written in easily interpreted symbols (although the symbols, in general do not conform to the usage in this chapter). COMMON and DIMENSION statements have been left out intentionally.

```
      SUBROUTINE TRFLTR
C
C     THIS IS A TRICKLING FILTER MODEL
C
C
C     THIS SUBROUTINE SIMULATES THE PREFORMANCE OF A ROCK MEDIA
C     BIOLOGICAL FILTER.  THE MODEL IS TAKEN FROM ROESLER & SMITH,
C     'MATHEMATICAL MODEL FOR A TRICKLING FILTER', REPORT OF THE
C     CINCINNATI WATER RESEARCH LABORATORY,F.W.P.C.A., CINCINNATI
C     HOWLAND'S FORMULA IS USED
C
C           BOD(D) = BOD(I)*EXP(-K*AP*D/(HQ**ZN))
C
C     SILVESTON'S MODIFICATION ASSUMES DBOD IS PREFERENTIALLY DESTROYED
C     UP TO A LIMIT DBODMIN.  SUSPENDED MATTER DOES NOT INCREASE IN THE
C     PROCESS.  SUSPENDED ORGANIC NITROGEN IS PARTIALLY AVAILABLE FOR
C     DENITRIFICATION.  DENITRIFICATION CONVERTS AMMONIA TO NITROGEN
C     AND IS GOVERNED BY THE SAME TYPE OF EQUATION AS IS BOD REMOVAL.
C     SUSPENDED ORGANIC PHOSPHOROUS IS PARTIALLY CONVERTED TO A SOLUBLE
C     FORM.  ALKALINITY IS UNCHANGED.WHILE THE TEMPERATURE IS ASSUMMED
C     TO DROP BY 1/2 DEGREE.  IN THE ABOVE FORMULA.
C     ****************************************************************
C     K = K20*1.035**(T-20)
C     K20 IS A CONSTANT **** ROESLER & SMITH RECOMMEND 0.0233
C     AP = SPECIFIC SURFACE AREA OF THE MEDIA **** USE 150 FOR 1/4'' ROCK
C     80 FOR 1/2'' ROCK, 55 FOR 3/4''ROCK, 40 FOR 1''ROCK, 20 FOR 1 3/4''
C     ROCK, AND 12 FOR 3''ROCK
C     D = BED DEPTH IN FEET
C     HQ = HYDRAULIC LOADING IN MGD(U.S.)/ACRE
C     ZN = 0.91 - 6.45/AP    ACCORDING TO ROESLER & SMITH
C     OTHER VARIABLES USED IN THE SUBROUTINE ARE,
C     DBODMIN = MINIMUM DBOD ATTAINABLE **** SILVESTON RECOMMENDS A VALUE
C     OF 10 FOR INPUT BOD IN EXCESS OF 100
C     DELBOD = CHANGE IN TOTAL BOD
C     FRBOD = FRACTIONAL REDUCTION IN TOTAL BOD
C     FRNIT = FRACTIONAL REDUCTION IN NITROGEN
C     DELON = CHANGE IN DISSOLVED NITROGEN
C     KN20 = COEFFICIENT FOR NITROGEN CONVERSION **** ROESLER & SMITH
C     RECOMMEND 0.0029
C     ****************************************************************
C                 SUBROUTINE WRITTEN BY
C                 P.L.SILVESTON AND A.  ROUKENS DE LANGE
C                 DEPT. OF CHEMICAL ENGINEERING
C                 UNIVERSITY OF THE WITWATERSRAND
C                 JOHANNESBURG, SOUTH AFRICA
C                 VERSION 1         MAY, 1969
C                 MODIFIED BY PLS **** FEBRUARY, 1970
C
C     THE SUBROUTINE WAS PREPARED AS A MODEL FOR STUDENT EXERCISES
C     ****************************************************************
C     THE LONG STREAM VECTOR OF WATCRAP-PACER IS EMPLOYED
C
C     1. STREAM NO.                        11. DP - DISSOLVED PHOSPHORGUS
C     2.                                   12. SFM - SUSPENDED FIXED MATTER
C     3. FLOW (MGD)                        13. DFM - DISSOLVED FIXED MATTER
C     4. SNBC - SUSPENDED NONBIO-          14. SBOD - SUSPENDED BIOLOGICAL
C           DEGRADABLE CARBON (MG/L)             OXYGEN DEMAND
C     5. DNBC - DISSOLVED NONBIO-          15. DBOD - DISSOLVED BIOLOGICAL
C           DEGRADABLE CARBON (MG/L)             OXYGEN DEMAND
C     6. SOC - SUSPENDED ORGANIC CARBON    16. TSS - TOTAL SUSPENDED SOLIDS
C     7. DOC - DISSOLVED ORGANIC CARBON    17. TEMPERATURE
C     8. SON - SUSPENDED ORGANIC           18. VSS - VOLATILE SUSPENDED
C           NITROGEN                             SOLIDS
C     9. DN - DISSOLVED NITROGEN           19. ALKALINITY
C     10  SOP - SUSPENDED ORGANIC
C           PHOSPHORUS
C
C     ****************************************************************
```

```
C
C                  FN VECTOR
C
C       1. EQUIPMENT NO.                        8. DBODMIN
C       2. EQUIPMENT FLAG                       9. FREBOD
C       3. AP                                   10. FRENIT
C       4. D
C       5. DIAMETER
C       6. K20
C       7. KN20
C       ************************************************************************
C       DEBUGGING PRINTOUT
        IF (KSETS)90,90,95
   95   PRINT 96, NE
   96   FORMAT(1HO, 10X31HCALCULATION REACHED TREFLTR, NE =,I4/)
   90   CONTINUE
C       PREVENT DIVISION BY ZERO
        IF(STRMI(1,3))1,1,2
    1   STRMI(1,3) = 1.
C       FIND MIXED INPUT CONCENTRATIONS
    2   CONTINUE
        Q = 0.0
        DO 3 I = 1,2
        DO 3 J = 4,19
    3   PAPER(I,J) = 0.0
        DO 55 I = 1,NIN
   55   Q = Q + STRMI(2,3)
        DO 5 J = 4,19
        DO 4 I = 1,NIN
    4   PAPER(1,J) = PAPER(1,J) + STRMI(I,3)*STRMI(I,J)
    5   PAPER(2,J) = PAPER(1,J)/Q
        BODI = PAPER(2,14) + PAPER(2,15)
C       CALCULATION OF FRACTIONAL REDUCTION OF BOD
        A = (3.145*(EN(NE,5)**2.))/(4.*160.*16.5**2.)
C       NOTE THAT Q IS IN MGD(U.S.)
        HO = Q/A
        ZN = 0.91 - 6.45/EN(NE,3)
        ZK = EN(NE,6)*1.035**(PAPER(2,17) - 20.)
        FRBOD = 1. - EXP(-ZK*EN(NE,3)*EN(NE,4)/(HO**ZN))
        DLBOD = BODI*FRBOD
        EN(NE,9) = FRBOD
C       FIND THE CHANGE IN DBOD AND SBOD
        DIFF = PAPER(2,15) - DLBOD
        IF(DIFF-EN(NE,8)) 8,8,6
    8   STRMO(1,15) = EN(NE,8)
        STRMO(1,14)=BODI-EN(NE,8)-DLBOD
        GO TO 7
    6   STRMO(1,15) = PAPER(2,15) - DLBOD
        STRMO(1,14) = PAPER(2,14)
C       FIND NITROGEN REMOVAL
C       ASSUME PART OF THE SUSPENDED NITROGEN IS AVAILABLE FOR REDUCTION
    7   PAPER(3,9)=PAPER(2,9)+PAPER(2,8)*(1.-STRMO(1,14)/PAPER(2,14))
C       CORRECT RATE CONSTSANT FOR TEMPERATURE
        ZKN = EN(NE,7)*1.141**(PAPER(2,17) - 20.)
C       OBTAIN FRACTIONAL REDUCTION IN DISSOLVED NITROGEN
        FRNIT = 1. - EXP(-ZKN*EN(NE,3)*EN(NE,4)/(HO**ZN))
        EN(NE,10) = FRNIT
        DELON = PAPER(3,9)*FRNIT
        STRMO(1,9) = PAPER(3,9) - DELON
        STRMO(1,8) = PAPER(2,8)*STRMO(1,14)/PAPER(2,14)
C       PHOSPHOROUS COMPOUNDS ARE SOLUBILIZED BY THE FILTER
        STRMO(1,10) = PAPER(2,10)*STRMO(1,14)/PAPER(2,14)
        STRMO(1,11) = PAPER(2,11) + PAPER(2,10) - STRMO(1,10)
C       ASSUME FIXED MATTER DOES NOT CHANGE
        STRMO(1,12) = PAPER(2,12)
        STRMO(1,13) = PAPER(2,13)
C       ASSUME NONBIODEGRADABLE CARBON IS UNCHANGED
        STRMO(1,4) = PAPER(2,4)
        STRMO(1,5) = PAPER(2,5)
C       ORGANIC CARBON CHANGES BECAUSE OF THE REDUCTION IN BOD
C       FOLLOWING ROESLER & SMITH ASSUMEBOD = 1.87*CARBON
        STRMO(1,6) = (STRMO(1,14) + 1.87*STRMO(1,4))/1.87
        STRMO(1,7) = (STRMO(1,15) + 1.87*STRMO(1,5))/1.87
C       FLOW RATE DOES NOT CHANGE
        STRMO(1,3) = Q
C       NOW WE FIND THE SUSPENDED SOLIDS TERMS
C       ASSUME SBOD = SUSPENDED SOLIDS
        STRMO(1,18) = STRMO(1,14) + STRMO(1,4) + STRMO(1,8)
        STRMO(1,16) = STRMO(1,18) + STRMO(1,12) + STRMO(1,10)
C       TEMPERATURE DROPS BY 1/2 DEGREES
        STRMO(1,17) = PAPER(2,17) - 0.5
```

```
C     ALKALINITY IS UNCHANGED
      STRMO(1,19) = PAPER(2,19)
C     ************************************************************
      RETURN
      END
```

FIGURE 10-11. EXAMPLE OF A TRICKLING FILTER SIMULATION MODEL

10.11 Rotating Disc Contactor Model

The rotating disc contactor resembles a trickling filter in that the biomass is supported on a surface and the slime is alternately contacted with air and waste. The contactor was developed in Europe, and over 600 installations are operating at this time. It is primarily a secondary treatment system for small to moderate flows. The largest installation handles about 10 MGD. A 400,000 GPD unit is operating in Wisconsin.

"The system (Figure 10-12) consists of a number of large-diameter lightweight plastic discs, which are mounted on a horizontal shaft and placed in a semi-circular shaped tank. The discs are rotated while approximately one-half of their surface area is submerged in the wastewater. Immediately after startup, organisms present naturally in the wastewater begin to adhere to the rotating surfaces and multiply until, in about one week, the entire surface area of the discs is covered with an approximately 1/16 to 1/8 inch thick layer of biomass."[24]

"In rotation, the discs carry a film of wastewater into the air where it trickles down the surface of the discs and absorbs oxygen. Organisms in the biomass then remove both dissolved oxygen and organic materials from this film of wastewater. As the discs continue their rotation through the bulk of the wastewater in the tank, further absorption of dissolved oxygen and organic materials is performed by the biomass. Operating in this manner, the rotating discs serve several functions: provide a medium for the development of a fixed biological growth, contact of the growth with the wastewater, and aeration of the wastewater. Shearing forces exerted on the biomass as it is passed through the wastewater cause excess biomass to slough from the discs into the mixed liquor. This prevents clogging of the disc media and maintains a constant microorganism

[24]Autotrol Corp., "Application of Rotating Disc Process to Municipal Wastewater Treatment", Water Pollution Control Research Series, 17050 DAM 11/71, Environmental Protection Agency (Washington, 1971)

population on the discs. The mixing action of the rotating discs keeps the sloughed solids in suspension until the treated wastewater carries them out of the disc sections for separation and disposal."[24]

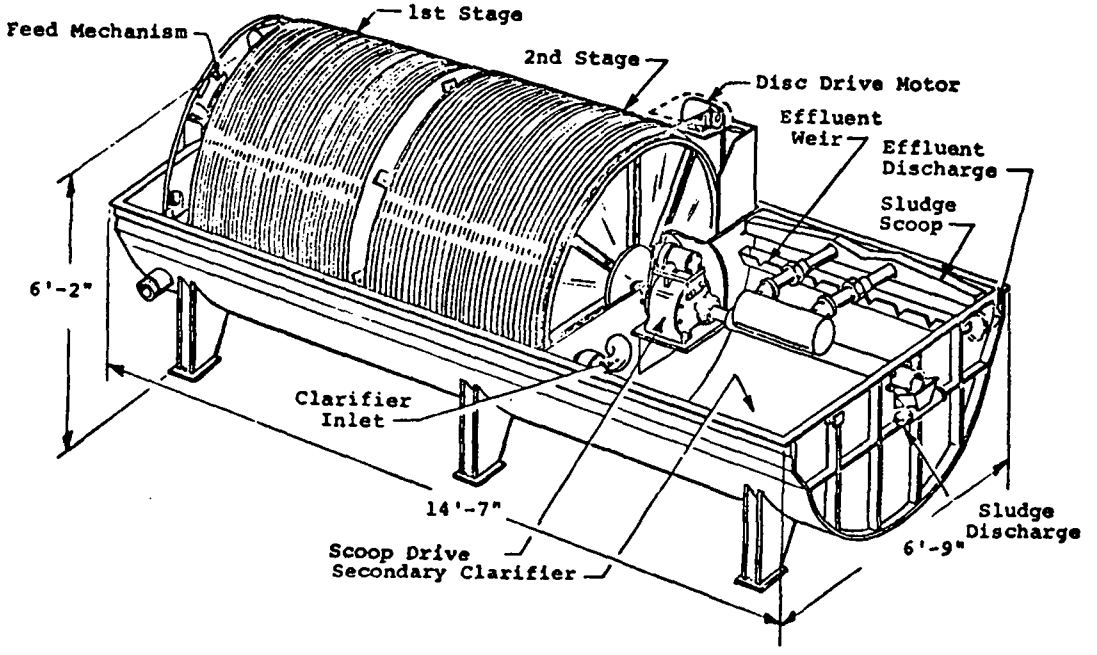


FIGURE 10-12. ROTATING DISC PACKAGE PLANT DETAILS

A simple model for the contactor is readily derived. Assuming that the rotation of the disc stirs the waste held in the tank, the tank contents can be taken to be of uniform composition. If we use Eckenfelder's model for trickling filter kinetics, eqn. (10-6), and neglect any bio oxidation in the bulk liquid, a simple BOD balance on a tank (as shown in Figure 10-12) yields

$$S_e/S_o = \frac{1}{(\frac{kX}{Q} + 1)} \qquad (10\text{-}33)$$

where X is the biomass slime on all the discs in a tank or stage. This biomass will be proportional to the number and area of the discs and presumably its active depth will depend on turbulence in the liquid and shear exerted on the film by rotation of the support surface. The active depth can be expected to be a function of the disc rpm (ω). If we assume an

exponential dependence,

$$X \propto n_{disc}\, d_{disc}^{2}\, \omega_{disc}^{n} \tag{10-34}$$

On substitution,

$$S_e/S_o = \frac{Q}{k'\, n_{disc}\, d_{disc}^{2}\, \omega_{disc}^{n} + Q} \tag{10-35}$$

in each tank. If there are n tanks in series,

$$S_e/S_o = \frac{Q^N}{(k'\, n_{disc}\, d_{disc}^{2}\, \omega_{disc}^{n} + Q)^N} \tag{10-36}$$

Sludge production and nutrient removal can probably be handled by adopting the trickling filter equations presented earlier.

An EPA report[24] presents operating data which could be used to prepare an empirical model or fit eqn. (10-36). Dependence of the performance on the variables n_{disc}, d_{disc}, Q and ω which appear in the model is confirmed in the report.

Kornegay[4] derives a disc contactor model employing the Monod model (eqn. (10-11)) for BOD removal; he allows for BOD reduction by suspended organisms in the tank as well as by the slime on the discs. An implicit equation for S_e is obtained

$$S_e = S_o - \frac{\pi \hat{\mu}\, X_{film}\, d}{2\, Q\, Y}\, n_{disc}\, (\Delta d^2) \left(\frac{S_e}{k_m + S_e}\right) - \frac{\hat{\mu}'\, X_{tank}\, \tau_{tank}}{Y'} \left(\frac{S_e}{k_m' + S_e}\right) \tag{10-37}$$

In this equation, X_{film} and X_{tank} are the biomass concentrations in the slime and suspended in the tank, d is the active film depth and Δd^2 is the difference between the squares of the outer and inner diameters

of the disc. The primes indicate that the biological activity will not be the same in the slime and in the tank.

Kornegay points out the disc contactors are normally operated at throughputs sufficiently high enough to wash out the suspended organisms. Therefore, the third term on the RHS in eqn. (10-37) can be dropped in most cases. The resulting expression differs from eqn. (10-35), then, only in the kinetics assumed.

11 DIGESTER MODELS

Digestion is probably the earliest form of biological treatment practiced intentionally and septic tanks would have to be its most primitive application. Although they are no longer found in sewage works, septic tanks remain a common method of rural waste treatment. The immediate ancestor of the conventional unstirred or low rate digester is perhaps the Travis or Imhoff tank. In the last few decades, the low rate digester has been replaced by the stirred, high rate unit. We will consider primarily the high rate variant in this chapter.

Modelling of digesters has been attempted only in the last decade and the level is still rather primitive. Our treatment is based on the papers of Andrews[1,2,3], McCarty[4] and Pohland[5,6]. We will discuss digester models developed by the Cincinnati Water Research Laboratory[7], Andrews[1,3], McCarty[4] and Eckenfelder and Ford[8]. As in previous chapters we will review the function and operation of digesters and relevant theory before examining models.

---

(1) Andrews, J.F., "Dynamic Model of the Anaerobic Digestion Process", J. Sanitary Eng. Div., Proc. Am. Soc. Civil Eng., 95, SAI, 95 (1969)

(2) Andrews, J.F., "A Mathematical Model for the Continuous Culture of Microorganisms Utilizing Inhibitory Substances", Biotech. and Bioeng., 10, 707 (1968)

(3) Andrews, J.F. and Graef, S.P., "Dynamic Modelling and Simulation of the Anaerobic Digestion Process", Advances in Chemistry Series, 105, 126-162 Am. Chem. Soc. (Washington, D.C. 1971)

(4) McCarty, P.L., "Anaerobic Waste Treatment Fundamentals - Part I to IV in successive issues of Public Works, beginning Sept.: 1964

(5) Pohland, F.G. and Bloodgood, D.E., J.W.P.C.F., 35, 11 (1963)

(6) Pohland, F.A. and Ghosh, S., "Developments in Anaerobic Treatment Processes", in Canale, R.P. (Editor) "Biological Waste Treatment", Interscience Publ. (New York, 1971)

(7) Smith, R., "Preliminary Design and Simulation of Conventional Wastewater Renovation Systems Using the Digital Computer", Water Pollution Control Res. Series, WP-20-9, F.W.P.C.A. (Washington, D.C., 1968)

11.1 Digester Function and Operation

The primary function of sludge digestion is to stabilize and reduce the volume of the solids recovered from primary and secondary clarifiers. Thus, substantial BOD reduction is a major process objective. Digestion also produces sludges which are more easily dewatered than raw primary or secondary sludges. Digestion generates a sludge gas which is used primarily as a fuel to heat the digestion tanks, but which can also serve as a power source for pumping or compressing air for use in activated sludge installations.

Digesters, now, are circular vessels with diameters running anywhere from 10 feet to about 100 ft. Side depth is commonly about 20 ft. Figure 11-1[9] shows cross sections of two types.

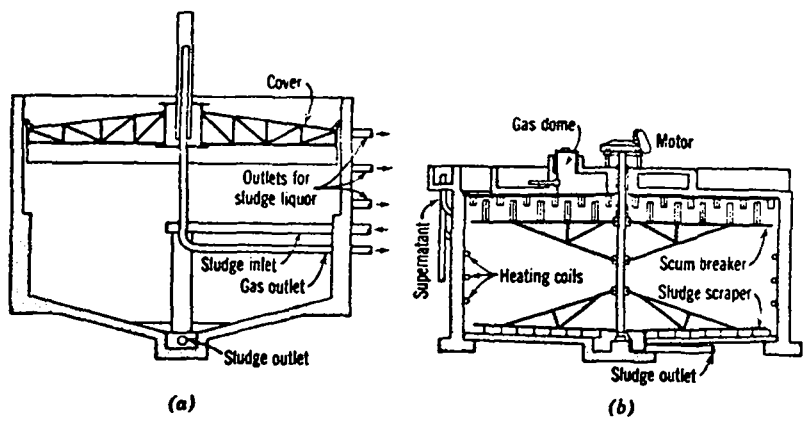


FIGURE 11-1. CIRCULAR SLUDGE DIGESTERS: (a) TANK WITH FLOATING COVER; (b) TANK WITH FIXED COVER, SCUM BREAKER, AND SLUDGE SCRAPER.*

The two drawings show possible arrangements of devices for removing gas

[8] Eckenfelder, W.W. Jr. and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970)

[9] Imhoff, K., and Fair, G.M., "Sewage Treatment" 2nd Edition John Wiley (New York, 1956)

*Figure taken from reference (9) with the kind permission of the publisher.

and digested sludges, and decanting supernatant. The rakes in (b) are moving slowly and do not contribute significantly to mixing. Heating coils (using hot water) are also shown, however, heating of the digester is now more frequently managed by pumping sludge through an external heat exchanger. Pumping for this purpose also provides mixing of the digester contents.

Various types of operation are encountered: i) low rate digestion, formerly referred to as the conventional process, ii) two stage, and iii) high rate digestion. The schematic diagrams in Figure 11-2 and the captions summarize the difference between variants i) and iii).

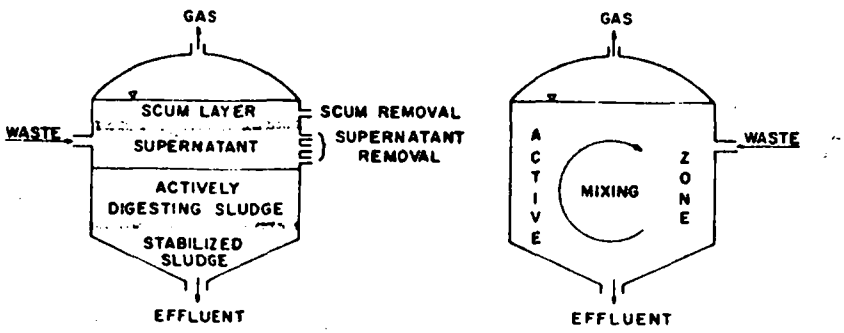


FIGURE 11-2. CONVENTIONAL ANAEROBIC DIGESTION PROCESSES**

		(a) Low Rate Digestion	(b) High Rate Digestion
1)	Temperature	85-95°F	85-95°F
2)	Detention Time	30-60 days	15 days or less
3)	Loading	30-100 lb. VSS/1000 cu. ft./day	100-500 lb. VSS/ 1000 cu. ft./day
4)	Feeding and Withdrawal	Intermittent	Continuous or intermittent
5)	State in Vessel	Stratified	Homogeneous

** Figure taken from reference (6) with the kind permission of the publisher.

In a word, low rate is a semibatch (discontinuous) process while high rate normally is a continuous stirred process. Two stage processes are also used. Figure 11-3 shows two versions of the operation. The first vessel is a high rate unit. The sludge from this unit can go a phase separator, where part of the sludge is recycled to keep the cell concentrations high, while the remainder is wasted. This version is referred to as "anaerobic contact". In the second version, the sludge from the first stage goes to a low rate second stage. The process goes by the name of "staged digestion". Using both together as shown in the figure is unusual.

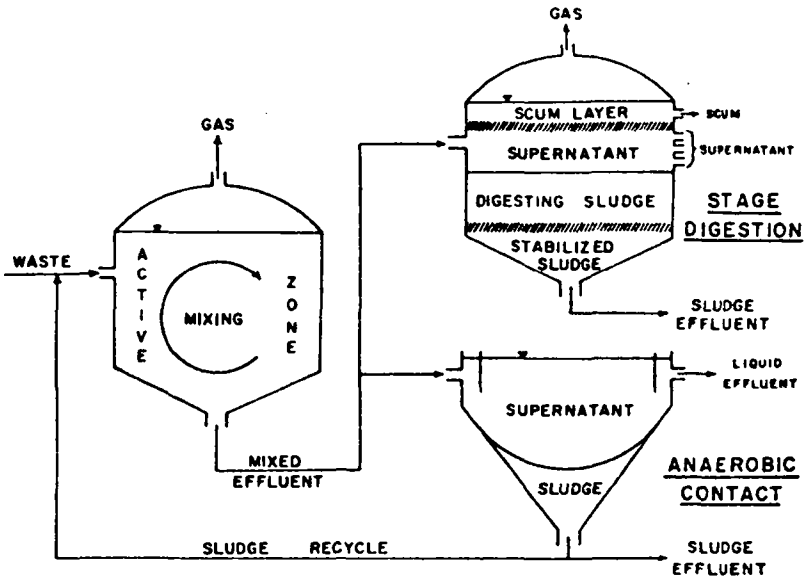


FIGURE 11-3. VERSIONS OF TWO STAGE DIGESTION*

In digestion, raw sludge serves as a metabolic substrate for microorganisms which discharge primarily methane (CH_4) and carbon dioxide (CO_2) as end products. The latter gas remains largely in solution if the pH is 6.8 or above. Some of the substrate is also used for cell synthesis. The net result is a partial destruction of the sludge with the formation on settling of a liquid phase, the supernatant. This supernatant contains cell waste products with BOD's as high as 1,000 to 3,000 mg/l. The re-

*Figure taken from reference (6) with the kind permission of the publisher.

maining solid consists of non-biodegradable matter in the influent, sludge cells and cell debris from the anaerobic process which is non-biodegradable for the most part. The gas yield depends upon the sludge which is being processed but ranges between 12 and 19 $ft^3/lb.$ VSS destroyed. The volatile matter destruction ranges between about 40 and 90%, while BOD_u of the sludge is reduced by between 80 and 90%. These values assume a properly functioning unit and do not differ materially between high and low rate operation.

Destruction of the Zooglea bacteria, the slime formers, in the early stages of digestion causes a partial collapse of the floc structure of the sludge so that on thickening a considerably larger clarified phase is formed than would be the case with an undigested sludge. Floc particles loosen from the sludge structure, entrap gas and form a scum layer. The layer, indicated in Figures 11-2 and 11-3, inhibits circulation. Grease, whose specific gravity is less than water, is released from the sludge during digestion and also concentrates in a scum. When the mixing is low, as it is in low rate digestion where thermal currents and gas generation are the only means of mixing, segregation of phases occurs as suggested in Figure 11-2.

11.2 Theory

Anaerobic digestion of sludge is believed to consist of microbic processes occurring in series as illustrated in Figure 11-4. This is a gross oversimplification since many different microbial species probably participate, and their interactions are not always clearly defined. For example, some nonmethanogenic bacteria may be involved in the conversion of volatile acids to methane and carbon dioxide. The matter is complicated because only a few of the many species taking part in the processes have been identified[10].

The active species in volatile acid formation are believed to be facultative organisms. Research on pure substrates and pure colonies has shown that widely varied organisms are capable of generating volatile

---

[10] Pohland, F.G., "General Review of Literature on Anaerobic Sewage Sludge Digestion", Engineering Extension Series, No. 110 Purdue University (Lafayette, Indiana)

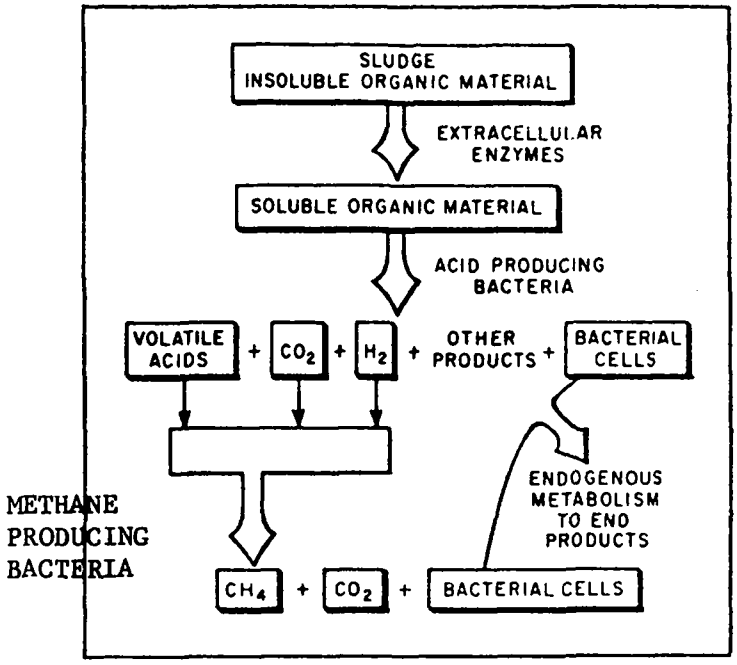


FIGURE 11-4. SEQUENCE OF MICROBIC CONVERSION STEPS IN ANAEROBIC DIGESTION*

organic acids and these species have been implicated in the group of acid producing bacteria in this way. Pohland[10] provides a detailed discussion of this phase of digestion research.

Methane producing bacteria appear to be more limited in species. Eight have been identified[10], but it is not certain that all are present in digesting sludge. The bacteria are strict anaerobes requiring oxidizable and reducing organic matter, CO_2 and the usual nutritive salts. Successive oxidation of higher molecular weight materials through propionic and acetic acid to methane and CO_2 seems to occur. McCarty[4] suggests the proportions of each material formed en route to these end products in Figure 11-5.

It is also possible to examine digestion from the standpoint of an oxidation - reduction sequence. Using the empirical formula for sludge ($C_5H_7O_2N$), the overall reactions for the acid and methane forming steps are

*Figure taken from reference (8) with the kind permission of the publisher.

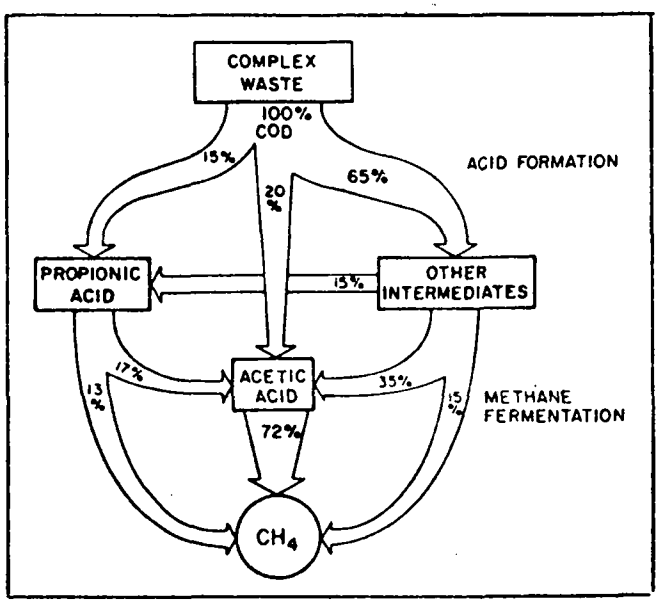


FIGURE 11-5. PATHWAYS IN METHANE FERMENTATION OF SEWAGE SLUDGES. PERCENTAGES REPRESENT CONVERSION OF WASTE COD BY VARIOUS ROUTES*

a) acid fermentation (oxidation step) assuming only acetic acid is formed -

$$6\ C_5H_7O_2N + 28\ H_2O \longrightarrow 10\ CH_3CO_2H + 10\ CO_2 + 6\ NH_3 + 40\ H^+ + 40\ e^-$$

b) methane fermentation (reduction step) -

$$10\ CH_3CO_2H + 40\ H^+ + 40\ e^- \longrightarrow 15\ CH_4 + 5\ CO_2 + 10\ H_2O$$

overall -

$$6\ C_5H_7O_2N + 18\ H_2O \longrightarrow 15\ CH_4 + 15\ CO_2 + 6\ NH_3$$

The pronounced buffering capacity of digested sludge results

*Figure taken from reference (4) with the kind permission of "Public Works".

from the hydrolysis of the digestion products. The hydrolysis reactions are:

$$2\ H_2O + CO_2 \rightleftarrows H_3O^+ + H\ CO_3^-$$

$$H_2O + H\ CO_3^- \rightleftarrows H_3O^+ + CO_3^=$$

$$H_2O + NH_3 \rightleftarrows NH_4^+ + OH^-$$

$$H_2O + CH_3CO_2H \rightleftarrows H_3O^+ + CH_3CO_2^-$$

The most important of these hydrolysis-ionization equilibria is that of CO_2/carbonic acid which buffers in the pH range 6 to 7. Hydrolysis of CO_2 accounts for a significant fraction of the alkalinity encountered in digestion. The oxidation-reduction scheme and the hydrolysis reactions explain low pH observed when digesters are overloaded. The pH will drop sharply for the oxidation reaction, but rises as the volatile acids are consumed by the methane forming bacteria. Under overload, acid forming organisms continue to function, but wash out and inhibition of the methane formers occurs. It was once thought that pH inhibited the latter organisms, but it is now generally agreed that it is a cation toxicity problem. With methane formers out of action, the CO_2 produced is insufficient to buffer the hydrogen ion formed and low pH's are observed.

The kinetics of both high and low rate digestion is dominated by the methane producing bacteria because their specific growth rate is much slower than that exhibited by the acid formers. By splitting digestion into separate "acid" and "methane" forming stages, Ghosh and Pohland[6] found that the maximum specific growth rate of the acid formers is nearly tenfold that of the methane formers in the mesophilic temperature range. The practice is to assume that methane formation is rate limiting so that kinetic modelling, at least until recently, has assumed just a single "reaction" occurs in digestion.

Digestion kinetics are usually modelled by the Monod equation which assumes substrate limited cell growth. Letting X_M be the concen-

tration of methane forming cells and VA the volatile acid concentration, the specific cell growth rate μ_M will be given by

$$\mu_M = \hat{\mu}_M \left(\frac{VA}{(k_m)_M + VA} \right) \qquad (11\text{-}1)$$

An alternative proposed by Andrews[2] uses the Haldane expression:

$$\mu_M = \hat{\mu}_M \left[\frac{VA}{(k_m)_M + VA} + \frac{VA^2}{k_i} \right] \qquad (11\text{-}2)$$

and indicates a decline of the growth rate with increasing volatile acids concentration. The model assumes that acids act as inhibitors to methane formation at higher concentrations. In equations (11-1) and (11-2), $\hat{\mu}_M$ is the maximum specific growth rate in mg. cells/day/mg. VSS (or COD), k_m is a saturation constant in mg./l. and k_i is an ionization constant in the same units.

Mechanical mixing, normally by a pump around technique, prevents segregation, but it is questionable whether the contents are homogeneous. Residence time distribution data which would suggest the state of mixing are not available. In the absence of data, the current practice is to assume digesters are completely backmixed. Continuous feed and continuous sludge and gas withdrawal is also assumed though this is rarely practised.

11.3 General Considerations For Digester Modelling

With stabilization as the primary function of digestion, a digester model should contain expressions for the reduction of the BOD of the sludge. This introduces a problem. BOD of sludges are not normally measured so that little data are at hand to use for modelling and a BOD model would not be useful because of the lack of measurements. As we saw in Chapter 9, cell and sludge concentrations are expressed in terms of volatile suspended solids. This is an acceptable, though hardly ideal measure of organic matter. Consequently, we will express stabilization in terms of VSS. Sometimes COD is used to express sludge concentration. Since

COD, BOD_u and VSS are all assumed to measure the same quantity, any one can be used in a model. The equation will not change if different measures are used; only different sets of coefficients must be employed.

A clarified phase obtained by decanting or in subsequent processing of the digested sludge is normally returned to mix with primary effluent or return sludge. For both simulation and design, the concentration of this "recycle" stream is needed. A digester model must provide, therefore, the BOD, suspended solids and the alkalinity of the supernatant. The amount of supernatant, of course, must be predicted.

Finally, a digester model should contain statements giving the gas production rate and the gas composition.

11.4 Stabilization and Volatile Acids Production Models

In the simplest model, the methane forming bacteria are rate controlling and the digester is assumed to be completely mixed. Writing a balance on the methane forming bacteria cells X_M across the digester at steady states and recognizing that no methane forming bacteria enter,

$$-Q(X_M)_e + R_M V = 0 \qquad (11\text{-}3)$$

The detention time $\tau = V/Q$ and $R_M = \mu_M X_M$ by definition. If the digester is well mixed $X_M = (X_M)_e$. Substitution in eqn. (11-3) yields the well known detention time - specific growth rate relationship

$$\tau = 1/\mu_M \qquad (11\text{-}4)$$

Now introducing the Monod relation, eqn. (11-1),

$$(VA)_e = \frac{(k_m)_M}{\hat{\mu}_M \tau - 1} \qquad (11\text{-}5)$$

Volatile acid concentration (VA) is expressed as mg. of acetic acid/l. or occasionally as COD. Robert Smith in his computer model for a digester[7] uses biodegradable carbon in the sludge in place of VA in eqn. (11-5).

Quoting research by McCarty and his students, Smith gives the following expression for the temperature dependence of the rate and saturation constants in the mesophilic temperature range (20 to 35°C):

$$\hat{\mu}_M = 0.28 \exp\ [-0.036\ (35-T)] \qquad (11\text{-}6)$$

$$(k_m)_M = 700 \exp\ [0.10\ (35-T)] \qquad (11\text{-}7)$$

If the volatile acid concentrations are measured as carbon in mg/l., Smith gives

$$(k_m)'_M = 200 \exp\ [0.12\ (35-T)] \qquad (11\text{-}8)$$

Multiplying eqn. (11-8) by 2.5 gives the constant to be used with VA as mg. of acetic acid/l.

The model proposed by Ghosh and Pohland[6] for a two stage, high rate system reduces to eqn. (11-5) but different maximum specific growth rates and saturation constants are used for each stage.

A model for the volatile acid concentration proposed by Andrews and Graef[3] based on earlier work of Andrews[1] represents the most detailed model proposed to date for digestion. Substituting the Haldane relation, eqn. (11-2), into the methane formers balance (eqn. (11-4)),

$$\frac{\mu_M \tau\ (VA)_e}{(k_m)_M + (VA)_e + \frac{(VA)_e^2}{k_i}} = 1 \qquad (11\text{-}9)$$

This quadratic equation can be solved for $(VA)_e$. Andrews and Graef[3] suggest $\mu_M = 0.40\ day^{-1}$, $(k_m)_M = 0.0333$ moles/l., $k_i = 0.667$ moles/l. assuming VA is measured as acetic acid. A better model for the pH dependence of the rate is obtained according to Andrews and Graef by assuming that the unionized organic acid, HA, is the actual substrate in place of VA. We will drop the effluent subscript, but effluent concen-

trations should be understood in what follows.

The unionized species partially dissociates $HA \rightleftarrows H^+ + A^-$ and gives rise to an equilibrium relation $K_a = \frac{(H^+)\ (A^-)}{HA}$. It can be readily shown that

$$HA = \frac{(H^+)\ (VA)}{K_a} \tag{11-10}$$

where VA is the total acid = $HA + A^-$. K_a is a temperature dependent dissociation constant. Substitution in eqn. (11-9) gives

$$\frac{\mu_M \tau\ (H^+)\ (VA)}{K_a\ (k_m)_M + (H^+)\ (VA) + \frac{(H^+)^2\ (VA)^2}{K_a\ k_i}} = 1 \tag{11-11}$$

H^+ is the antilog of the pH. Thus, eqn. (11-11) gives the residual organic acid as a function of pH. pH can be eliminated from eqn. (11-11) in roughly the same way H^+ was introduced. Details are given in Andrews and Graef, but we can indicate the procedure. The system buffer is the bicarbonate - CO_2 equilibria: $(CO_2)_{aq} + H_2O \rightleftarrows H^+ + HCO_3^-$. The bicarbonate alkalinity varies with pH. Consequently H^+ can be eliminated through the equilibrium expression

$$\frac{(H^+)\ (HCO_3^-)}{(CO_2)_{aq}} = K_1 \tag{11-12}$$

The bicarbonate ion and CO_2 concentrations in the sludge must now be related back to the VA through appropriate material balances. The resulting equation is implicit and rather complicated.

Eckenfelder and Ford[8] derive a stabilization expression by assuming $(k_m)_M \gg (VA)_e$ and allowing for endogenous respiration of the methane forming cells. They express the specific growth rate as,

$$\mu = k(VA) - b \qquad (11\text{-}13)$$

On substitution in eqn. (11-4),

$$(VA)_e = \frac{b\tau + 1}{k\tau} \qquad (11\text{-}14)$$

Eckenfelder and Ford express the substrate VA in COD units and report $k = 5.5 \times 10^{-5}$ day^{-1} and $b = 0.021$ mg/l., but do not indicate the sludge to which the constants apply.

McCarty[4] proposes a model written for the sludge (M) instead of the volatile acids. Sludge concentrations are measured in COD. The effluent COD depends on the influent level:

$$\frac{M_e}{M_o} = (\eta_{dig} - 1.42\ Y_X) \qquad (11\text{-}15)$$

where η_{dig} is the digestion efficiency which, according to McCarty, lies between 0.8 and 0.95. Y_X is a yield coefficient which is

$$Y_X = \frac{\mu_{dig}}{b\tau + 1} \qquad (11\text{-}16)$$

μ_{dig} is a growth rate constant and b can be considered to be an endogenous respiration rate constant.

If ψ_{CH_4} is a gas yield expressed as scf of methane/lb. of COD, the acid level in the discharged sludge must be by difference

$$(VA)_e = (Y_A - \psi_{CH_4}/Y_{CH_4})\ (M_o - M_e) \qquad (11\text{-}17)$$

where Y_A is the yield coefficient for acid COD based on sludge COD and Y_{CH_4} is a yield coefficient for methane in terms of volatile acid COD consumed.

Choice of a "Stabilization" model among those presented depends

on the data available or to be used in the design or simulation study. If volatile acid data is available we recommend using the Monod equation (eqn. (11-5)), where as if COD data is to be used, the McCarty relations just given would be preferable. Equation (11-14) is quite similar to the Monod equation so it is an acceptable alternative. We doubt that data would be available in most applications to permit the use of the approach proposed by Andrews. If the Monod equation is used, it must be assumed that the sludge solids contribute no COD. The COD or BOD of the supernatant, if it is recovered, must then be computed from the VA level through an appropriate factor. The COD of the sludge will depend on the fraction solids achieved on decantation. On the other hand, if the McCarty relation is used, the COD associated with the sludge solids is $M_e - (VA)_e$. A material balance on COD must be used, as just indicated, to calculate sludge COD after decantation.

11.5 Gas Production Models

Sludge gas is mainly methane (60 to 75%) and carbon dioxide (25 to 40%) with just small amounts (<1%) of ammonia, hydrogen sulfide (H_2S), hydrogen (H_2), nitrogen and oxygen present. For modelling purposes, we will ignore the minor components.

Methane is insoluble in the sludge so that all CH_4 generated by the bacteria enters the gas phase and is drawn off in the continuous reactor. The production rate is then

$$q_{CH_4} = Y'_{CH_4} \mu X_M \tag{11-18}$$

where Y'_{CH_4} is the yield coefficient based on the methane forming bacteria. For μ, there is a choice of eqns. (11-1), (11-2) or (11-13). The choice should be consistant with the relation used for stabilization in the previous section. Concentration of the methane forming cells (X_M) is obtained most easily through a yield coefficient:

$$X_M = Y_M (M_o - M_e) \tag{11-19}$$

The sludge concentration is measured in VSS or in some cases in COD units. A conversion factor would be needed to obtain VSS or COD from $(VA)_e$ measurements. Y_M is a yield coefficient for the methanogenic organisms. If COD units are used, Eckenfelder and Ford[8] use $Y_M = 0.136$. Andrews and Graef use $Y_M = 0.02$ but employ mole units. They assume $C_6H_{12}O_6$ as a microorganism formula and give $Y_{CH_4} = Y_{CO_2} = 47$ moles/mole of microorganism.

CO_2 production as a gas is more difficult to formulate because CO_2 is soluble in alkaline solutions through the equilibria: $(CO_2)_{aq} + OH^- \rightleftarrows HCO_3^-$. CO_2 absorption thus converts alkalinity into bicarbonate alkalinity. The specific rate of CO_2 generation is given by eqn. (11-18) with Y'_{CO_2} substituted for Y'_{CH_4}. However, CO_2 leaves the digester as gas, dissolved carbon dioxide $(CO_2)_{aq}$, or as bicarbonate ion HCO_3^-. A CO_2 balance gives therefore

$$q_{CO_2} = Y'_{CO_2} \mu X_M - \frac{C'}{\tau} \left[(CO_2)_{aq} + (HCO_3^-) \right] \qquad (11\text{-}20)$$

Introducing $\dfrac{HCO_3^-}{(CO_2)_{aq} (OH^-)} = K_1/K_W$ and $K_W = (H^+)(OH^-)$ and substituting in eqn. (11-20) gives

$$q_{CO_2} = Y'_{CO_2} \mu X_M - \frac{C' (HCO_3^-)}{\tau} \left[\frac{(H^+)}{K_1} + (1) \right] \qquad (11\text{-}21)$$

This model expresses the CO_2 gas rate as a function of the specific growth rate, cell concentration, pH and bicarbonate alkalinity.

Alternate models for gas production use stoichiometric relations. McCarty[4] uses

$$q'_{CH_4} = 5.62 (\eta_{dig} - 1.42 Y_X) \qquad (11\text{-}22)$$

where q'_{CH_4} is scf/lb. COD consumed. A range for η_{dig} was given following eqn. (11-15). Y_X may be obtained from eqn. (11-16).

Eckenfelder and Ford[8] write

$$q'_{CH_4} = 5.62\ (M_o - M_e)\left[1 - \frac{1.42\ Y'_X}{b\tau + 1}\right] \qquad (11\text{-}23)$$

in which M is expressed as COD and Y'_X is a yield coefficient in terms of COD so q'_{CH_4} is scf/lb. COD consumed. Neither McCarty nor Eckenfelder suggest a relation for CO_2 production.

Smith[7] reasons that methane has a COD while CO_2 has none so that the methane yield must be directly proportional to the COD reduction. He expresses methane production rate as

$$q_{CH_4} = \frac{5.62}{\tau}\ (M_o - M_e) \qquad (11\text{-}24)$$

where M is COD as lb/ft^3 and q_{CH_4} is the CH_4 production rate in scf/day/ft^3 of digester volume. In Smith's model, the gas is 66% methane.

If McCarty's relations are used to express stabilization, we recommend the use of eqn. (11-22) for methane production. Total gas production rate may be calculated by assuming the gas is 65% methane. On the other hand, if the Monod equation was employed to calculate the residual volatile acids, we suggest eqn. (11-24) for the CH_4 rate.

11.6 Models for Other Changes

Digestion has been found to solubilize nitrogen and phosphorus. Smith[7], employing McCarty's investigations, assumes that solubilization is proportional to the COD reduction:

$$(N_{AM})_e = (N_{AM})_o + 0.65\ (N_{ON})_o\ \frac{(M_o - M_e)}{M_o} \qquad (11\text{-}25)$$

In this relation N_{AM} and N_{ON} are ammonia and organically bound nitrogen, both expressed as mg of N/l. The ammonia leaving in the digester gas is allowed for in the 0.65 coefficient. For phosphorus,

$$P_e^* = P_o^* + P_* \frac{(M_o - M_e)}{M_o} \qquad (11\text{-}26)$$

where P^* and P_* are the soluble phosphates and organically bound phosphorus (suspended) both expressed as mg P/1. The effluent COD includes the contribution of the volatile acids, of course.

Alkalinity and particularly bicarbonate alkalinity increase in digestion. Only alkalinity is measured at all routinely for digested sludge. Alkalinity measures carbonate and ammonia in the liquid phase. Smith allows the increase of alkalinity to be proportional to the increase in ammonia. Other contributions, $HCO_3^- \rightleftarrows CO_3^= + H^+$, $HS^- \rightleftarrows S^= + H^+$, etc. are handled by a correction factor so,

$$(A_{Alk})_e = (A_{Alk})_o + \frac{3.57}{f_{Alk}} \left[(N_{AM})_e - (N_{AM})_o\right] \qquad (11\text{-}27)$$

Smith suggests that f_{Alk} varies from 0.6 to 0.8.

Digesters are normally heated. The effluent temperature, then, is the temperature the unit is maintained at.

11.7 Design

Digester design consists essentially of sizing a tank. To this comes the provision of heat exchange surface to provide adequate heating, and the sizing of the pump-around or mixing equipment.

The primary design parameter, $(DP)_1$, will be the specification which provides the digester size. Traditionally, the specification was cubic feet of capacity per capita, if no data on raw sludge characteristics were available. If data are available, $(DP)_1$, is expressed as sludge loading = $M_o Q/V$ with units of lb. of volatile solids/day/cu ft of digester volume. With M_o and Q known, the digester volume falls out. Imhoff and Fair[9] list values ranging from 0.1 to 0.15 lb. VS/day/ft^3 for low rate digesters and from 0.25 to 0.35 for high rate units. These values are at least 50% higher than loadings given by Eckenfelder[11].

If measurements have been made on the sludge, a much more sophisticated treatment can be used. The design parameter can be taken as the fractional reduction of VSS (or COD). If we assume the effluent VSS is

---

[11] Eckenfelder, W.W., Jr. and O'Connor, D.J., "Biological Waste Treatment, Pergammon Press (New York, 1961).

attributable only to the volatile acids, the residual volatile acids $(VA)_e$ can be computed. Equation (11-4) can now be used to find the detention time. Since $\tau = V/Q$, the digester volume may be calculated. Using the Monod equation

$$\tau = \frac{k_{m_M} + (VA)_e}{\hat{\mu}_M (VA)_e} \qquad (11\text{-}28)$$

Of course, eqns. (11-14) or (11-15) and (11-16) could be used in place of the Monod equation and eqn. (11-4). Fractional reduction of VSS is usually specified to be between 0.6 and 0.8.

Smith points out that it is important to consider the washout detention time in digester design. This time, τ_{min}, is calculated from the flow rate Q_{max} at which digestion fails. τ_{min} is given by the reciprocal of the maximum specific growth rate. Smith[7] sugguests a 250% safety factor, so

$$\tau_{min} = \frac{2.5}{\hat{\mu}_x} \qquad (11\text{-}29)$$

Practice is to check that $\tau > \tau_{min}$ where τ is calculated from eqn. (11-28).

Although detention time from eqn. (11-28) gives a digester size, this size is not necessarily the best choice. In some circumstances it may be advantageous to design for the maximum sludge stabilization/ft^3 of volume. Smith[7] gives a relation developed by McCarty for this "optimal" detention time (maximum utilization of digester volume)

$$\tau_{opt} = \frac{1}{\hat{\mu}_M} \left(1 - \frac{k_{m_M}}{(k_{m_M} + M_o)^{\frac{1}{2}}} \right) \qquad (11\text{-}30)$$

Units of M_o are sludge COD or VSS.

A design parameter of considerable importance is the digester temperature. This parameter, $(DP)_2$, is usually chosen to be between 33

and 35°C. Temperature specification determines essentially the heat load and thus the heat transfer requirements.

The heat load of the digester consists of the sensible heat needed to bring the influent sludge to the digester temperature and heat losses through the vessel walls. If q is the load in Btu/hr.:

$$q = q_{sensible} + q_{loss} \tag{11-31}$$

and

$$q_{sensible} = (M + 62.4)\, Q\, (T - T_o) \tag{11-32}$$

in which T_o is the influent and T is the digester temperature. Q is the flow rate in $ft^3/hr.$ and M is the suspended solids as lbs/ft^3. Heat losses are:

$$q_{loss} = UA_{tank}\, (T - T_{amb}) \tag{11-33}$$

where T_{amb} = mean air temperature. A_{tank} is the exposed surface area of the tank and U is an overall heat transfer coefficient defined as

$$\frac{1}{U} = \left(\frac{1}{h_r}\right)_i + \left(\frac{1}{h_r}\right)_o + x/\lambda \tag{11-34}$$

where h_{r_i} and h_{r_o} are suitable heat transfer coefficients and λ is a shell conductivity while x is the shell thickness. A similar term could be added for insulation if used. Equations (11-33) and (11-34) assume negligible heat loss through the underground portion of the digester. For the exposed portion combined radiative and convective heat transfer to the shell and from the shell to the atmosphere is assumed. Values of h's, λ, x and even U are available in various Engineering Handbooks[12]. Imhoff and Fair[9] give values of 0.1 to 0.4 Btu/hr-ft^2 °F for U for ex-

[12] Bolz, R.E. and Tuve, G.L., (Editors), "Handbook of Tables for Applied Engineering Science", Chemical Rubber Co. (Cleveland, 1970)

posed tanks depending on wall thickness and insulation.

Heating can be carried out by circulating low pressure steam or hot water in coils in the digester or alternatively by circulating sludge through a heat exchanger. The area required in either alternative may be computed from the heat load by

$$q = UA\,\Delta T_{lm} \tag{11-35}$$

U, the overall heat transfer coefficient, is given by

$$\frac{1}{U} = \frac{1}{h_i} + \frac{x_p}{\lambda_p} + \frac{A_i}{h_o A_o} + r_{s_i} + r_{s_o} \tag{11-36}$$

where h_o is the heat transfer coefficients outside of the tube carrying either sludge or hot water while h_i is the inside coefficient. λ is the pipe conductivity, x_p is the pipe wall thickness. r_{s_i}, r_{s_o} are scaling coefficients. The inside coefficient h_i depends on flow rate through the exchanger tube or on one side of a plate if this type of exchanger is used. Equations are available for calculating h_i and also for h_o in some circumstances. They can be found in Handbooks along with values for r_{s_i} and r_{s_o}.

In systems where sludge is pumped to an external heat exchanger, an additional design parameter will be the temperature at which the sludge leaves the exchanger. This parameter along with the heat load sets the sludge pumping rate Q_{dig} through

$$Q_{dig} = \frac{q}{(62.4 + M)\,(T_e - T)} \tag{11-37}$$

where T_e is the exit temperature from the exchanger or $(DP)_3$. Further design parameters are the velocities of sludge and hot water through the exchanger. With these specified, the heat transfer coefficients can be obtained and the surface area (size) of the exchanger computed.

Eckenfelder[11] suggests a range of 10 to 39 Btu/h ft^2 ^oF for

U for coils in sludge tanks. Other values are as low as 4.5 Btu/hr ft^2 ^oF. In calculating the energy required for digester heating, burner efficiency of between 60 and 80% must be included. Fuel for these burners is frequently gas produced in digestion.

12 PRELIMINARY TREATMENT, CHLORINATION AND MISCELLANEOUS MODELS

In this short chapter we will deal with chlorination, preliminary treatment devices such as screens and grit chambers, pumps and flow junctions. All of these operations with the possible exception of chlorination and junctions can be neglected in simulation because they cause a negligible change in the conventionally measured properties of waste streams.

12.1 Preliminary Treatment

Preliminary treatment devices serve to remove large objects such as sticks, rags, string or hard material such as sand or gravel which might impede the operation of or even damage downstream mechanical equipment. Other devices, instead of removing the softer material, grind it to a size which avoids problems.

Preliminary treatment devices do not change flows and their effect on sewage composition is negligible. They will not appear in a plant simulation. Thus, only their design concerns us. Many types of devices are available; design consists essentially of selecting the type of device and determining its size. Size determination is probably all that is amenable to computer-aided methods. For preliminary treatment devices, the primary design parameter is the specification which sets area or size.

Bar screens are found in almost all municipal treatment plants. These consist of parallel bars inclined at 30^{o} to 45^{o} to the vertical with bar spacing between 1 and 2 inches. Figure 12-1 shows schematically two typical rack installations.

Design of these racks is based upon a velocity of 2 fps normal to the rack for the design flow. This will be $(DP)_1$ for the device. Thus, the area of rack (A_{Bar}) required is,

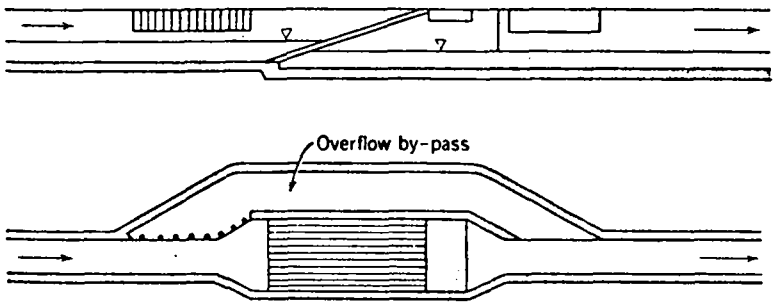
$$A_{Bar} = 0.78 \; Q_o/\cos \phi \qquad (12\text{-}1)$$

if the sewage flow (Q_o) is MGD (U.S.) and ϕ is the angle of inclination. The coefficient is 0.93 if the flow is measured in imperial gallons.

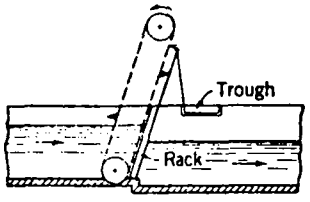
A_{Bar} is in sq. feet. The cross section of the channel in which the screen is located is given by

$$A_{channel} = 4 A_{Bar} \cos \phi \qquad (12\text{-}2)$$

where ϕ is again the inclination from vertical of the rack. The factor 4 is a safety factor.



(a) HAND-CLEANED INCLINED RACK WITH OVERFLOW BY-PASS



(b) MECHANICALLY CLEANED RACK

FIGURE 12-1. TYPICAL BAR SCREEN INSTALLATIONS*

The waste generated by the bar screens (W) is proportional to

*Figures taken from reference (1) with the kind permission of the publisher.

(1) Imhoff, K. and Fair, G.M., "Sewage Treatment", 2nd Edition, John Wiley (New York, 1956)

the flow,

$$W = a\,Q_o \qquad (12\text{-}3)$$

If W is in cubic feet per day and Q_o is mgd, a is estimated to be between 3/4 and 3[1,2].

Fine screens which once followed bar screens have been replaced by comminuters. This device is like a mechanically cleaned screen but it incorporates a cutting mechanism that cuts up the retained material without removing it from the sewage flow. It serves to reduce unsightliness and problems with down stream mechanical equipment. A typical comminuter is a vertically slotted drum screen submerged in the sewage flow and operated so that the drum either revolves against cutting members or the cutting members oscillate against the drum. Figure (12-2) illustrates the device.

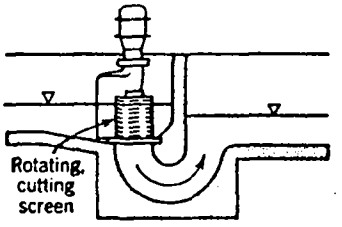


FIGURE 12-2. COMMINUTER*

Comminuters are purchased as packaged units. No relations have been found to indicate how they are sized.

Preaeration or skimming tanks may be used in municipal plants where a mixed industrial and domestic waste is treated. The primary purpose of the unit is to remove excessive grease or oils which have a lower specific gravity than water. These substances float and can be collected and skimmed from the water surface. The unit also removes a portion of

*Figure taken from reference (1) with the kind permission of the publisher.

(2) Anonymous, "Sewage Treatment Plant Design", A.S.C.E. and W.P.C.F. (1959)

the odorous gases such as hydrogen sulphide and it is claimed that preaeration causes some coagulation of colloidal matter which can be subsequently settled out in a clarifier. A schematic diagram of a preaeration tank is shown in Figure (12-3).

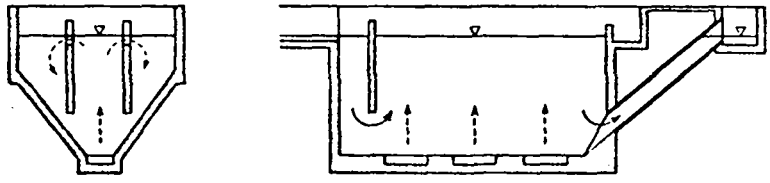


FIGURE 12-3. SCHEMATIC OF A PREAERATION TANK WITH A PLATE DIFFUSER*

Design of a tank is based on the rising velocity of a grease or oil droplet. The tank surface area, A_{skim}, is then

$$A_{skim} = 1110\ Q_o/v_{float} \qquad (12\text{-}4)$$

where A is sq. feet, Q_o is in mgd (U.S.) and v is inches per minute. Stokes' law provides an estimate of the rise velocity,

$$v_{float} = \frac{9.3}{\mu}\ (1 - \rho/\rho_w)\ d_p^2 \qquad (12\text{-}5)$$

where d_p is the drop size in feet and μ, the water viscosity, has the units lbs./ft.-min. and ρ/ρ_w is the specific gravity of the oil or grease. Depth of the tank will range from 5 to 10 feet.

If the droplet size of oil or grease cannot be estimated, an alternate procedure is to use detention time (τ_{skim}) as the design parameter.

$$V_{skim} = 93\ \tau_{skim}\ Q_o \qquad (12\text{-}6)$$

---

* Figure taken from reference (1) with the kind permission of the publisher.

In this relation, Q_o is again MGD (U.S.). For grease removal, $5 \leq \tau_{skim} \leq 15$ minutes; but τ_{skim} will range from 15 to 60 minutes for odor removal, freshening septic sewage and if settling in the clarifier is to be improved. Equations (12-4) and (12-6) will be used to set tank depth in some cases.

Equation (12-3) can be used to predict the scum volume recovered. According to Imhoff and Fair[1] a will be between 0.1 and 6.

Aeration is carried out with between 0.01 and 0.1 scf/gallon of sewage. The specification is a second design parameter. The air requirement is given then by an equation of the form of eqn. (12-3).

Sand, gravel and other firm, dense material are removed in grit chambers. The most common chamber is a simple channel which is slightly larger in cross section than the inlet sewer. Usually these are constructed in pairs for service purposes. The principle is to reduce the velocity sufficiently so that the heavier inorganic solids will be deposited, but that the lighter organic solids will remain in suspension. Channel type chambers are usually designed to provide a controlled velocity close to 1.0 fps. The length and, thus, the retention period is based upon the size of particle to be removed. The rate of flow is maintained at a more or less constant velocity by (1) gates, (2) constant velocity weirs and (3) flumes (see Figure (12-4)).

Other types of grit removal facilities are available which make no attempt to control the velocity. Rather the velocity is kept so slow that all the grit is removed. This also allows some organic material to be removed and this is then separated and returned to the flow either by a hydraulic means or by some other appropriate technique.

The design criteria of 1 fps (or sometimes 0.5 to 1 fps)[2] is based on the scour phenomena. Particles of size and density whose intrinsic scour velocity is equal or less than v_{sc} will be re-suspensed when the flow across a loose bed of granular particles of mixed size reaches this velocity. The scour velocity[1] is given by

$$v_{sc} = b \left(g \left(\rho/\rho_W - 1\right) d_p\right)^{\frac{1}{2}} \qquad (12\text{-}7)$$

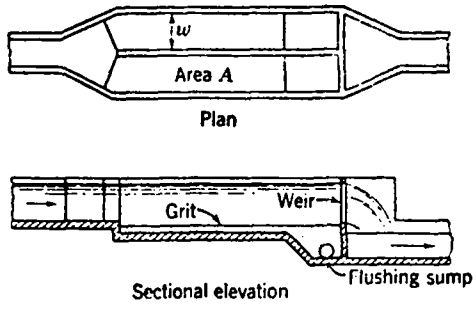


FIGURE 12-4. GRIT CHAMBER WITH A WEIR FLOW CONTROL SYSTEM*

where g is the acceleration of gravity (ft/sec^2), ρ/ρ_w is the specific gravity and d_p the equivalent spherical diameter of the particle. b is a dimensional constant which if d is in millimeters and v_{sc} is inches/min. ranges between 3 and 4.5.

The total cross sectional area of the grit removal channels must be such that the velocity is no more than v_{sc} even at the maximum anticipated flow. Equation (12-4) can be used and becomes

$$A_{grit} = 1.55\ (Q_o)_{max}/v_{sc} \qquad (12\text{-}8)$$

where $(Q_o)_{max}$ is the maximum anticipated flow in mgd and v_{sc} is in ft./sec.

We will not consider the design of weir or gate devices to control flow. The length of the grit channel depends upon sedimentation rather than upon scour. If we let $A_{channel}$ be the surface area, the overflow rate or surface loading as gpd of sewage/sq. ft. is conservatively given as

$$(Q_o)_{max}/A_{channel} = 450\ v_p \qquad (12\text{-}9)$$

where v_p is the settling velocity (inches/min.) of the smallest particle

* Figure taken from reference (1) with the kind permission of the publisher.

to be retained in the grit chamber. Using Stokes' Law, eqn. (12-5), the ratio of surface area to cross sectional area will be

$$\frac{A_{channel}}{A_{grit}} = \frac{18\ b\mu}{\rho_W\ d_p}\ (g\ (f\rho_W - 1)\ d_p)^{-\frac{1}{2}} \qquad (12\text{-}10)$$

If the grit chamber is designed to remove only gravel, Newton's Law must be used instead of Stokes'. The area ratio will be between 1.7 and 2.5. The choice of the critical sand or gravel particle size to be removed is therefore a design parameter. The third design parameter is width or depth. Depth is usually about one foot at the design flow rate[2].

12.2 Pumps

Units in a sewage plant will be arranged, when possible, for gravity flow from the entrance to the plant to the outfall in order to minimize as much as possible the capital cost of pumps and their power requirement. As we have seen in earlier chapters, recycle is a normal component of a treatment plant. If gravity flow exists, then all recycle streams must be pumped.

The character of the stream to be pumped dictates the type of pump to be used. For example, a centrifugal machine will normally be used for raw sewage, filtrates, supernatants, sludges generated in secondary treatment; whereas, a positive displacement pump, such as a screw (Moyno) pump, would be employed for moving primary sludges. Regardless of the type of pump, the pumping unit consists of the pump proper and a driver. The sizing procedure for both these elements is the same.

Selection of a pump depends upon 1) capacity Q, 2) brake horse power (BHP) and 3) head (H). Other factors, such as the fluid, influence primarily the type of machine selected.

The head delivered by a pump H is a sum of 3 separate heads:

$$H = H_{kin} + H_{stat} + H_{suction} \qquad (12\text{-}11)$$

The kinetic head, H_{kin}, refers to downstream side and it encompasses the

energy required to overcome friction in the line plus the kinetic energy associated with the flowing fluid. The static head, H_{stat}, corresponds to the potential energy furnished by the pump, that is, the elevation difference to be overcome. Finally $H_{suction}$ is the head which must be furnished to bring fluid into the pump; it includes static and kinetic contributions.

The static head, $H_{stat} = \Delta h$, the net elevation difference in feet across which the fluid is pumped. H_{kin} is given by the following expression

$$H_{kin} = 310 \frac{f}{d^3} \left(\frac{\rho Q}{d}\right)^2 (L + L_e) \qquad (12\text{-}12)$$

in which Q is gpm (U.S.), d is the pipe diameter in inches, L is the length of piping, L_e is the sum of the equivalent lengths of all fittings and valves in the line. Equivalent lengths are given as tables in Engineering Handbooks[3]. f is a friction factor defined as $H/\frac{u^2 L}{2gd}$. This factor is a function of the Reynolds number $\frac{50.70\rho}{d\mu}$ where μ is in centipoise and d is inches. It is usually given as a plot in Handbooks[3]. The viscosity of sewage and supernatant can be assumed to be the viscosity of water. The suction head, $H_{suction}$, is estimated by summing the net elevation change and H_{kin} calculated through eqn. (12-12) for the suction line of the pump.

The brake horse power of the pump is

$$(BHP)_{pump} = \frac{Q\,H}{3957\,\eta_{pump}} \rho/\rho_W \qquad (12\text{-}13)$$

where H is the head (feet), ρ/ρ_W is the specific gravity, Q is gpm (U.S.), while η_{pump} is the efficiency. For centrifugal machines η_{pump} may vary from 0.2 to 0.8, depending on the machine and its operating conditions. A good mean figure is 0.6. For positive displacement pumps, η_{pump} ranges from 0.55 to 0.75.

---

(3) Perry, J.H. (Editor), "Chemical Engineer's Handbook", 4th Edition, McGraw-Hill (New York, 1968)

Energy losses from the driver to the pump are accounted for by a mechanical efficiency. Thus, the brake horsepower of the driver is

$$(BHP)_{driver} = \frac{(BHP)_{pump}}{\eta_{mech}} \qquad (12\text{-}14)$$

The mechanical efficiency allows for losses in the pump and transmission. It is usually about 0.95. The power required is

$$(W')_{pump} = \frac{(BHP)'_{driver}}{\eta_{driver}} \qquad (12\text{-}15)$$

where the driver efficiency, η_{driver}, is normally between 0.8 and 0.95. The prime indicates the BHP is for the actual flow rate and head, not the design values.

The driver horsepower is the primary criteria for driver selection, whereas the power requirement determines the substation, switch and starting box sizes.

12.3 Headers and Flow Splitting Devices

In some plants, wasted sludge from an activated sludge system is mixed with raw sewage to promote settling in the primary clarifier. Mixing occurs in a "header" or junction device upstream of the clarifier or upstream of a preaeration device if one is used. Filtrate from sludge dewatering and digester supernatant will sometimes be mixed with sewage at the same point. The "header" or junction box is an example of a stream mixing device. Splitting devices also occur. For example, sludge from the secondary clarifiers usually drops into a collecting box or sump. Recycle sludge is drawn off while, in some units, the sludge to be wasted falls over a weir into a second sump from which it is pumped out of the unit.

Modelling of these units is quite simple. The mixing unit involves just an averaging procedure. If Q_i represents the flow rate in mgd of an arbitrary stream entering a mixer and S_i represents a composition in, say, mg./l., then

$$Q = \sum_{i=1}^{n} Q_i \tag{12-16}$$

where Q is the total flow resulting from all n streams and

$$\bar{S} = \frac{1}{Q} \sum_{i=1}^{n} S_i Q_i \tag{12-17}$$

As long as S is measured in the same units for each stream, the conversion units (to give, say, pounds/day) cancel out. $\bar{S}$ is the mean composition, that is, the composition leaving the mixing unit. Figure (12-5) a) shows a schematic of the unit.

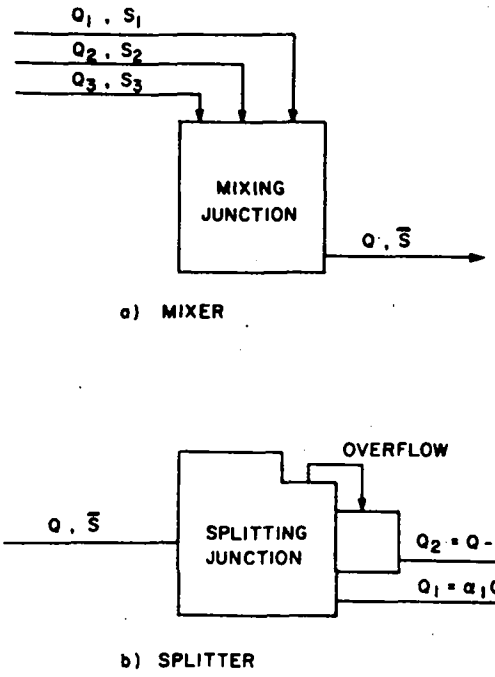


FIGURE 12-5. SCHEMATIC DIAGRAMS OF STREAM JUNCTIONS

The splitter can be modelled in two ways depending upon its operation. If all streams are pumped from a sump, we can let f_j = the fraction of the total flow pumped out of the splitter in the jth stream.

Then

$$Q_j = f_j Q \tag{12-18}$$

and

$$S_j = \bar{S} \tag{12-19}$$

since composition does not change in splitting. In the second mode of operation, all but one stream are pumped. The remaining stream is generated by an overflow (see Figure (12-5)). The splitting of final clarifier underflow to generate a waste sludge, which we mentioned two paragraphs before, is an example of this type of device. For all streams, other than the overflow, eqn. (12-18) applies. The overflow stream, Q_0, is then

$$Q_0 = Q\left(1 - \sum_{j=1}^{n-1} f_j\right) \tag{12-20}$$

Figure 12-6 shows mixing junction simulation model used in the earliest simulation studies undertaken at the University of Waterloo.

```
      SUBROUTINE MIXER3
C
C                     MIXER SUBROUTINE
C
C     THIS SUBROUTINE ACCEPTS NIN INPUT STREAMS, SUMS THEM, AND
C     DISTRIBUTES THE OUTPUT, USING FACTORS IN EN MATRIX, TO
C     NOUT OUTPUT STREAMS
C
C     A FORM OF THIS SUBROUTINE WAS ORIGINALLY SUPPLIED WITH THE
C     PACER EXECUTIVE IN 1967. IT WAS MODIFIED FOR THE UNIVERSITY
C     OF WATERLOO WATCRAP PROJECT BY R.N.ZWICKER IN FEBRUARY, 1968
C     MOST RECENT UPDATE BY P.L.SILVESTON IN 1973
C
C     STREAM VECTOR  SN
C          1. STREAM NO.
C          2.
C          3. ALL ADDITIONAL COMPONENTS HAVE UNITS OF
C        . CONCENTRATION OR ARE INTENSIVE PROPERTIES
C
C     EQUIPMENT PARAMETERS VECTOR EN
C          1. EQUIPMENT NO.
C          2.
C          3. FRACTION OF TOTAL INPUT IN FIRST OUTPUT STREAM
C          4. AS 3. UP TO LIMIT OF FIVE OUTPUT STREAMS
C
C     DEBUG PRINTING
      IF(ASETS)10,10,200
```

```
 200  PRINT 30,NE
 30   FORMAT(26HSEPSIM HAS GOTTEN THIS FAR,I4)
 10   CONTINUE
C
C     OVERFLOW PROTECTION
      IF (STRMI(1,3))40,40,50
   40 STRMI(1,3) = 1.0
   50 CONTINUE
C
C     SUM ALL FLOWS IN.
C     PAPER MATRIX IS USED FOR TEMPORARY STORAGE
      PAPER(1,1)=0.0
      DO 1 I=1,NIN
 1    PAPER(1,1)=PAPER(1,1)+STRMI(I,3)
C     CALCULATE OUTFLOWS.
      DO 2 K=1,NOUT
      L=K+2
 2    STRMO(K,3)=EN(NE,L)*PAPER(1,1)
      DO 3 J=4,NSLMAX
      K=J-2
      PAPER(1,K)=0.0
      DO 4 I=1,NIN
 4    PAPER(1,K)=PAPER(1,K)+STRMI(I,J)*STRMI(I,3)
 3    CONTINUE
      DO 6 I=4,NSLMAX
      DO 5 J=1,NOUT
      K=I-2
C     WEIGHTED MEAN CONCENTRATION.
 5    STRMO(J,I)=PAPER(1,K)/PAPER(1,1)
 6    CONTINUE
      RETURN
      END
```

FIGURE 12-6. EXAMPLE OF A JUNCTION MODEL SUBROUTINE

The junction model can be written into the models for other process units so that the models are capable of handling more than one influent or capable of generating multiple effluent streams.

Size of a header of a junction box is determined by the design flow and a specified detention time t_{Box} so

$$V_{junction} = 0.134\ Q\ t_{Box} \qquad (12\text{-}21)$$

where V is cu. ft., t_{Box} is in minutes and Q is the design flow in gpm (U.S.)

12.4 Chlorination

Chlorination is normally the last unit in a waste treatment plant before the effluent is discharged into receiving waters. It is a disinfection process, probably the cheapest available, intended to destroy

or inactivate pathogenic (disease producing) organisms such as certain bacteria or viruses. Other less routine uses of chlorination are for odor control in preliminary or primary treatment. Chlorine halts anaerobic decomposition of wastes and oxidizes hydrogen sulfide. It is also used to sweeten digester supernatants and to correct bulking in activated sludge systems and ponding in trickling filters.

Chlorine is added either directly as a gas or a small portion of the effluent is saturated with the gas and then mixed with the remainder of the stream. On contact with an aqueous media, the following rapid, reversible reactions occur

$$Cl_{2(g)} \rightleftarrows (Cl_2)_{aq.}$$

$$(Cl_2)_{aq} + 2H_2O \rightleftarrows H_3O^+ + Cl^- + HOCl \text{ (Hypochlorous acid)}$$

$$HOCl + H_2O \rightleftarrows H_3O^+ + OCl^- \text{ (Hypochlorite ion)}$$

The disproportionation reaction of chlorine has an equilibrium constant

$$K_{Cl_2} = \frac{(H_3O^+)\ (Cl^-)\ (HOCl)}{(Cl_2)_{aq}} = 3 \times 10^4$$

at 15°C so the reaction goes virtually to completion at $pH > 3$ provided Cl^- concentrations are not excessive. On the other hand the dissociation of hypochlorous acid has an equilibrium constant,

$$K_{HOCl} = \frac{(H_3O^+)\ (OCl^-)}{HOCl} = 2.5 \times 10^{-8}$$

at 20°C. Hypochlorous acid, aqueous chlorine (if present) and the hypochlorite ion constitute "free available chlorine". The acid, however, is the effective disinfectant so pH's below 7 must be maintained.

Ammonia and certain organic substances, such as phenols, react

with chlorine. The predominate ammonia reaction is

$$NH_3 + HOCl \rightleftarrows NH_2Cl + H_2O$$

At high Cl_2 concentrations and with long holding times, NH_2Cl is oxidized to N_2O by chlorine,

$$NH_2Cl + NHCl_2 + HOCl \rightleftarrows N_2O + 4HCl$$

Both NH_2Cl and $NHCl_2$ are called chloramines. They exert a slow disinfecting action and represent forms of "combined chlorine". It is assumed they function as disinfectants through the reverse reaction to give hypochlorous acid.

Break point chlorination is practised in most sewage plants, that is, sufficient chlorine is added to satisfy the chlorine demand of inorganic reducing agents (such as Fe^{2+}), organic compounds and destroy the chloramines (at least partially) by oxidation. This results in a residual chlorine content (free available chlorine) in the effluent leaving the plant. Usually the standard is a 0.5 mg/l. Cl_2 residual after a detention time of 15 minutes.

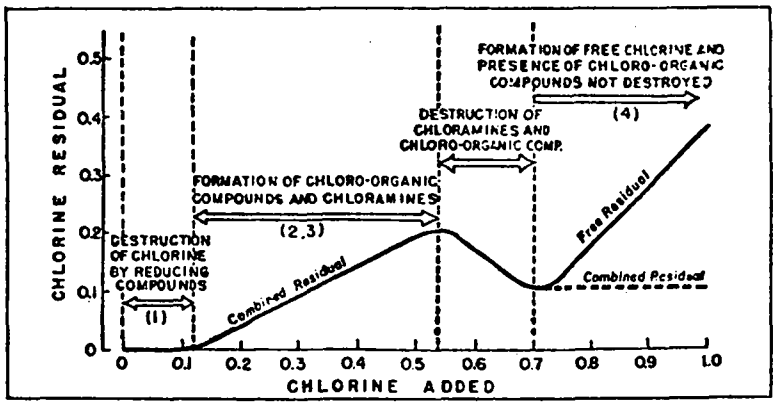


FIGURE 12-7. SCHEMATIC OF BREAK POINT CHLORINATION*

*Figure taken from reference (4) with the kind permission of the publisher.

Details of the disinfection mechanism are not known. It is believed that chlorine destroys cell protein and inactivates critical enzyme systems. The process is not instantaneous. Indeed, it is described in terms of Chick's Law[4]

$$X_e = X_o e^{-kt} \tag{12-22}$$

In the relation, X is a count of cells, k is a specific rate constant which depends on the concentration of the disinfectant, pH and temperature and t is contact time. Consequently, a chlorination tank is necessary to provide a sufficient detention time at the residual Cl_2 level for some specified destruction level. E. Coli are frequently used as a test bacteria. A 15 minute detention time at a Cl_2 residual between 0.2 and 1.0 mg/l. destroys 99.9% of the cells[1].

With this background, we can now proceed to simulation and design models for chlorinators. BOD reduction in raw sewage through chlorination of between 10 and 35% have been reported[1]. On the other hand stoichiometry suggests a reduction of 2 mg/l. of BOD per mg/l. of Cl_2 added up to the break point. Susag[5] has recently modified this rule to

$$\Delta S = 2.08\ \Delta Cl_2 - 0.21\ (\Delta Cl_2)^2 \tag{12-23}$$

where ΔS is reduction in BOD in mg/l. while $\Delta Cl_2 = Cl_2^{\,o} - (Cl_2)_{resid.}$ in mg/l. and represents the Cl_2 consumed. $Cl_2^{\,o}$ is the concentration of Cl_2 which would have been obtained if all Cl_2 dissolves, but none is reduced. This concentration is

$$Cl_2^{\,o} = \frac{0.12\ W_{Cl_2}}{Q_e} \tag{12-24}$$

---

[4] Weber, W.J., Jr., "Physicochemical Processes for Water Quality Control", Wiley-Interscience (New York, 1972)

[5] Susag, R.H., Sew. and Ind. Wastes 40, 434 (1968)

where Q_e is the outfall flow rate in MGD and W_{Cl_2} is the chlorine dosage in lbs./day. Cl_2^o is usually of the order of 2 to 3 mg/l., thus BOD reduction ranges from 3 to 4 mg/l.

Protons (H_3O^+) produced by disproportionation of chlorine cause a loss in alkalinity. From the definition of alkalinity, assuming all the Cl_2 disproportionates,

$$\Delta A_{Alk} = 1.4\ (Cl_2^o) \tag{12-25}$$

Dissolved solids increase through the addition of chlorine. The increase is given by eqn. (12-24). No other changes, however, are believed to occur.

As for design, the objective of chlorination is disinfection. For this purpose, a dose must be specified which is sufficient to generate a residual Cl_2 level of the order of 0.5 mg/l. This residual level may be viewed as the primary design parameter of a chlorinater. It determines the BOD and alkalinity reduction in the unit. An equally important design parameter is the detention time (τ_{Chlor}). The size of the chlorination tank can be estimated from

$$V_{Chlor.} = 0.134\ Q\ \tau_{Chlor.} \tag{12-26}$$

The units are the same as those in eqn. (12-21).

The application rate - which dictates the size of the chlorination equipment, building size, inventory of chlorine required - depends on the dosage as well as the flow. Dosage is obtained by rearranging eqn. (12-24). Cl_2^o, the maximum free chlorine, can be eliminated through ΔS and ΔCl_2 by eqn. (12-23).

13 SLUDGE TREATMENT PROCESSES

Our objective in this chapter is to examine models for the major sludge treatment processes: elutriation, vacuum filtration, centrifugation, sludge drying and incineration.

Sludge treatment is frequently troublesome and it is costly. Burd[1] estimates that if digestion is included sludge treatment and disposal accounts for 25 to 50% of the capital cost of a waste treatment plant and similar percentages of the annual operating cost. In Ontario, provincial policy is to encourage land spreading of sludges whenever possible. Land spreading normally will require digestion but it by passes the sludge treatment processes to be discussed in this chapter. We have added this chapter inspite of this policy because large metropolitan areas do not use spreading and because a stiffening of the spreading restrictions with respect to heavy metals salts in the sludge may force municipal sewage plants treating mixed domestic and industrial wastes in smaller urban areas to use land fill instead of spreading and to thereby use sludge treatment processes.

The alternatives in sludge treatment and the interrelationships of the individual treatment steps are indicated in Figure 13-1. Five stages are discernible in the figure. In the first, raw sludge undergoes volume reduction (thickening, digestion) and possibly biological treatment (digestion). An alternative at this stage is aerobic digestion. This process has not been widely used in Canada and for this reason,it will not be considered in this chapter, even though it is receiving a good deal of attention now. The next stage is sludge conditioning. Conditioning, when it is used at all, is usually done by washing the sludge with treatment plant effluent. Alternatives are heat treatment by either the Farrer or Wet Air Oxidation Processes[2]. These alter-

---

[1] Burd, R.S., "A Study of Sludge Handling and Disposal", Publication WP-20-4, Water Pollution Control Research Series, F.W.P.C.A.-U.S.D.I., U.S. Gov't. Printing Office (Washington, D.C.,1968)

[2] Balakrishnan, S., Williamson, D.E. and Okey, R.W., "State of the Art Review on Sludge Incineration Practice", Water Pollution Control Research Series" 17070 DIV 04/70, F.W.Q.A.-U.S.D.I., U.S. Gov't Printing Office (Washington, D.C.,1970)

natives are seldom used and will not be discussed further. Sludge dewatering is the third stage. The competing processes for this stage are drying beds, vacuum filtration, and centrifuging. Mechanical dewatering by plug presses and filter presses is rarely used in North America. The dewatered cake from this stage can be disposed of directly in sanitary land fill facilities, but in some situations, the sludge will go on to a fourth stage - oxidation and decomposition (incineration). The final stage is ultimate disposal.

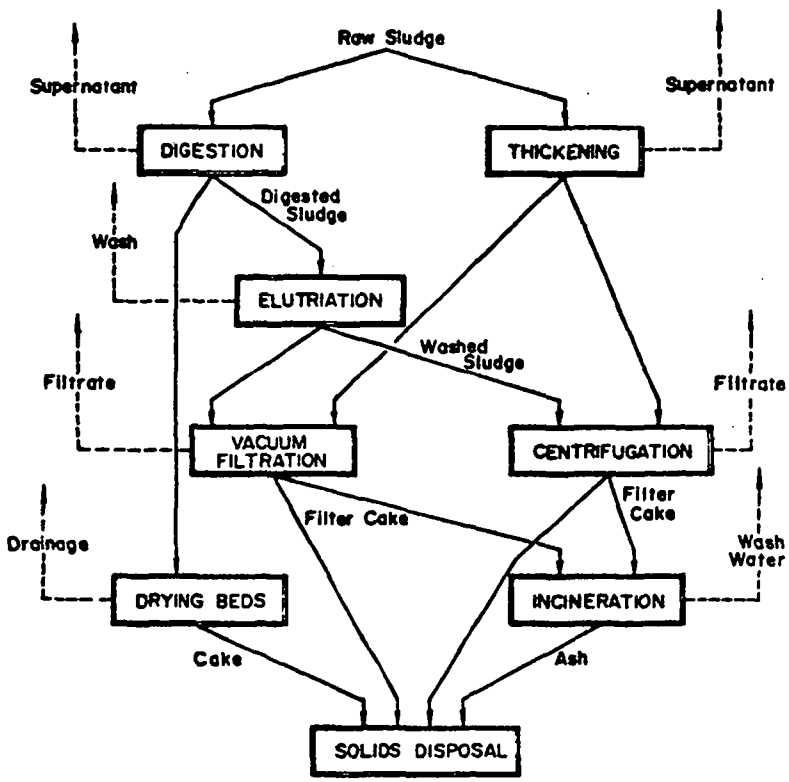


FIGURE 13-1. SCHEMATIC DIAGRAM OF SLUDGE PROCESSING IN MUNICIPAL WASTE TREATMENT PLANTS

The sludge treatment processes can be considered, as a first approximation, independently from the rest of the treatment plant once sludge flows and compositions are established. The recycle link with the remainder of the treatment plant is weak. Flows, such as filtrate from filtration and centrifuging (Figure 13-1), which return to the treatment plant are quite small when compared to the sewage flow even

though these streams have high BOD and suspended solids levels. Thus, these recycle streams have only a small influence on fluid side performance of a waste treatment plant.

From the standpoint of simulation, it is only the composition of these recycle streams and the gross amount of sludge or ash sent to ultimate disposal which are of interest. Since these recycle streams affect the waste levels in the treatment plant outfall only slightly, sophisticated modelling is hardly warranted. On the other hand, sludge treatment processes are costly so that modelling for design purposes is worthwhile. Our emphasis will be on design in this chapter.

13.1 Elutriation

Elutriation is employed primarily for digested sludge. It is simply a "washing" operation whose object is to remove dissolved matter, mainly inorganic salts, from the sludge. Removing these salts reduce the requirement for sludge conditioning chemicals in the subsequent dewatering stage. Figure 13-2 taken from Genter's 1956 article[3] illustrates the dramatic reduction in chemical requirement which can be achieved.

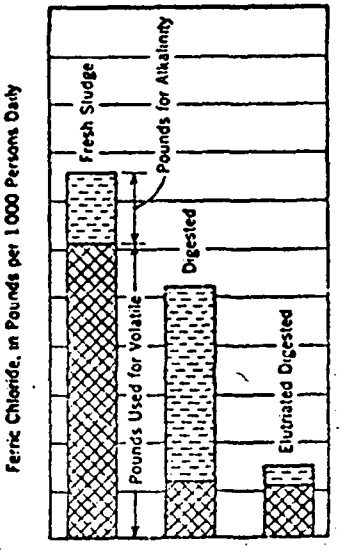


FIGURE 13-2. REDUCTION IN CHEMICALS DEMAND FOR VACUUM FILTRATION THROUGH ELUTRIATION*

*Figure taken from reference (3) with the kind permission of the Journal.

(3) Genter, A.L. "Conditioning and Vacuum Filtration of Sludge", Sewage and Industrial Wastes, 28, No.7,829 (1956)

The figure suggests that chemicals demand depends on the sludge alkalinity and volatile suspended solids. We will use this information in section 13-2 when we discuss vacuum filtration. Volatile suspended solids are not decreased in elutriation as Figure 13-2 indicates, but alkalinity is sharply reduced. The alkalinity of digested sludge is due to the formation of carbon dioxide in the methanation stage of digestion (see Chapter 11) which dissolves in the sludge to form bicarbonates. The most important of these is ammonium bicarbonate. Bicarbonates are soluble and thus are removed by washing.

Elutriation equipment is simple. Sludge and wash water are mixed either in the line feeding an elutriation basin or in a separate mixing chamber ahead of the basin. When used, this chamber will be stirred (Figure 13-3). The basin itself is simply a clarifier or thickener (see Chapter 8). Sludge separates from the wash water in this basin and is recovered as the underflow. The wash water overflows the weirs and is returned either to the primary clarifier or to the aerator of the treatment plant. A serious problem is suspended solids swept out of the sludge by the wash water. Suspended solids concentrations can reach 4,000 mg/l.

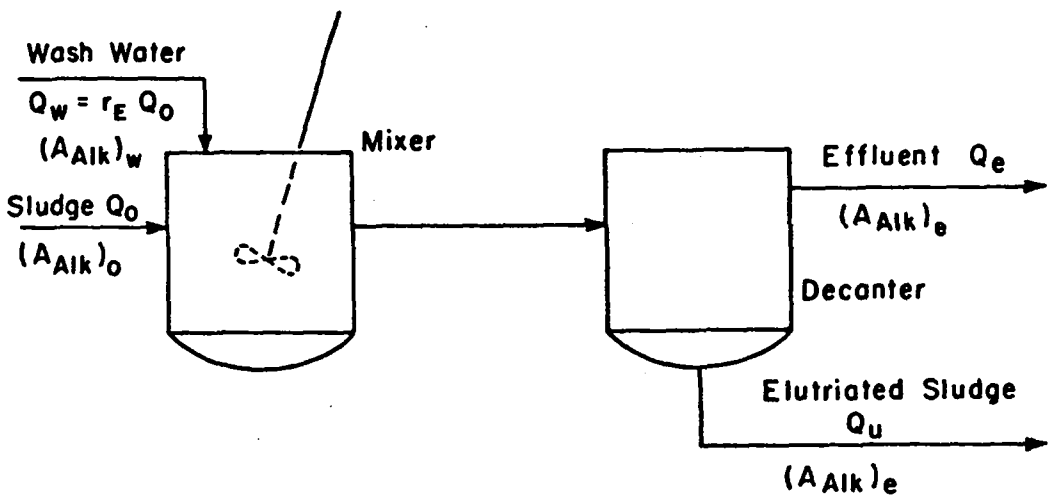


FIGURE 13-3. SCHEMATIC DIAGRAM OF AN ELUTRIATOR

Both single stage and two stage counter current units are in use. The ratio of wash water to sludge (r_E) usually ranges from 2:1 to 3:1.

Since the reduction of alkalinity in the sludge and the loss of suspended solids to the wash water are of primary interest in elutriation, models for the process must account for alkalinity change and for suspended solids in the wash. An elutriator model should also cover any thickening of the sludge, although this is a secondary consideration.

An elutriator model was developed in section 7.3 (Chapter 7) to illustrate simple, deterministic, lumped parameter models. A material balance on alkalinity was used along with the assumption that on entering the settler (after mixing) the alkalinity is the same in the sludge and in the wash water. The relation obtained for sludge alkalinity $(A_{Alk})_u$ was

$$(A_{Alk})_u = \frac{(A_{Alk})_o + r_E\ (A_{Alk})_w}{1 + r_E} \qquad (13\text{-}1)$$

where the subscripts u, o, w represent underflow (sludge) inlet and wash water. Alkalinity of the overflow $(A_{Alk})_e$ was assumed to be the same as $(A_{Alk})_u$. r_E is the volumetric ratio of wash water to sludge. Relations identical to eqn. (13-1) are given by Genter[3], Smith[4] and Imhoff and Fair[5]. Genter has also derived a relation for a two stage (two mixing and two settling tanks) countercurrent washing system[3]:

$$(A_{Alk})_u = \frac{(A_{Alk})_o + (A_{Alk})_w\ (r_E)\ (r_E + 1)}{r_E^{\,2} + r_E + 1} \qquad (13\text{-}2)$$

---

[4] Smith, R., "Preliminary Design and Simulation of Conventional Wastewater Renovation Systems Using the Digital Computer", Publication WP-20-9, Water Pollution Control Research Series, F.W.P.C.A.-U.S.D.I., U.S. Gov't Printing Office (Washington D.C., 1968).

[5] Imhoff, K. and Fair, G.M., "Sewage Treatment", 2nd Ed., John Wiley & Sons (New York, 1956).

The relation assumes no change in sludge concentration. Alkalinity in the wash water leaving the unit (A_{Alk_e}) is

$$(A_{Alk})_e = \frac{1}{r_E} \left((A_{Alk})_o + r_E (A_{Alk})_w - (A_{Alk})_u\right) \qquad (13\text{-}3)$$

No theory or correlation of plant data has been found which predicts the level of suspended solids in the wash water after mixing or after settling. In principle, clarifier and thickening models should provide this information, but information on settling of elutriated sludges seems to be absent from the Sanitary Engineering literature so that constants in these models cannot be evaluated. However, crude models for sludge treatment processes are probably acceptable for the reasons we have indicated earlier. Consequently empirically determined factors may be used to predict the suspended solids in the overflow from the settling stage. If y_E is the ratio of sludge concentration as mg/l. before and elutriation and f_E is the fraction of the sludge solids lost to the wash water (see section 7.3),

$$M_e = \frac{y_E f_E M_o}{y_E(1 + r_E) + f_E - 1} \qquad (13\text{-}4)$$

$$Q_u = \frac{1 - f_E}{y_E} \qquad (13\text{-}5)$$

$$Q_e = Q_o \left(1 + r_E - \frac{(1 - f_E)}{y_E}\right) \qquad (13\text{-}6)$$

f_E is normally less than 0.1, but values as high as 0.3 have been reported[1]. The amount of thickening accomplished is small so that usually $y_E < 1.1$. If f_E is greater than 0.1 and $y_E = 1.1$, the change in sludge volume is significant and eqns. (13-2) and (13-3) must be re-derived to allow for the change.

When a mixing chamber is used, sizing of the chamber is based upon detention time. Burd[1] cites a detention time of 30 seconds if the agitation is vigorous.

The settling basin should be designed as a clarifier would be since the primary concern is reducing the sludge solids which leave with wash. Ideally, the design would be carried out using settling data obtained with elutriated sludges to evaluate an overflow rate corresponding to a reasonable loss of solids. However, in many cases the design is based on a specified overflow rate or a solids loading. Burd cites an overflow rate of 200 gpd/ft^2, but indicates that rates up to 400 gpd/ft^2 are used. The solids loading according to McLaren[6] should be 8 to 10 lbs of dry solids/ft^2/day, but loadings in the range of 10 to 15 lbs are used.

Sludge concentrations are considered in the settler design as well. The discussion in section 8.7 applies. Equation (8-36) can be used to check the solids loading used to design the settler or calculated from the design if the overflow rate is used as the design parameter. The equation contains blanket height and holdup time in the sludge blanket (τ_{bl}). Blanket depths run to a maximum of three feet, while sludge holdup is about 24 hours according to Burd's survey.

As for clarifiers, a weir loading is often specified as $(DP)_2$. For elutriators, this loading is about 5,000 gallons (U.S.)/ft/day.

13.2 Vacuum Filtration

For some time now vacuum filters have replaced drying beds as the most popular dewatering process in Canada. These units are intended not only to dewater sludge, but also to keep the solids in the filtrate as low as feasible.

13.2.1 Operation and Theory.

Filtration is carried out by forcing sludge through a porous film which "traps" the solids but allows the liquid to flow through. After the initial contact with the filter media, the trapped solids build up on the media and form a "cake". The cake actually accomplishes most of the enmeshing and trapping of solids. The filter media's is main purpose, then, is to initiate and support the cake.

---

[6] McLaren, J.W., "Evaluation of Sludge Treatment and Disposal", Canadian Municipal Utilities, 23, 51 (May, 1961)

A wide variety of filtration equipment is available, but the only type of unit which is used extensively in North America for sludges is the rotating drum vacuum filter. Figure 13-3 shows the schematic of an installation, while the drum itself is illustrated by Figure 13-4. Filtration occurs when the drum, whose surface is perforated and covered by

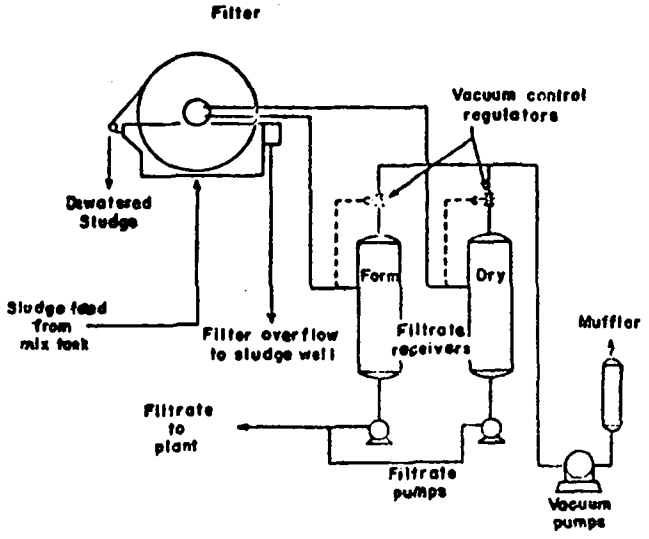


FIGURE 13-4. VACUUM FILTER INSTALLATION (SLUDGE CONDITIONING TANK AND SLUDGE PUMPS NOT SHOWN)*

---

*Figure taken from reference (7) with the kind permission of the Journal.

(7) Schempman, B.A., and Cornell, C.F., "Fundamental Operating Variables in Sewage Sludge Filtration", Sewage and Industrial Wastes 28 No. 12, 1443 (1956)

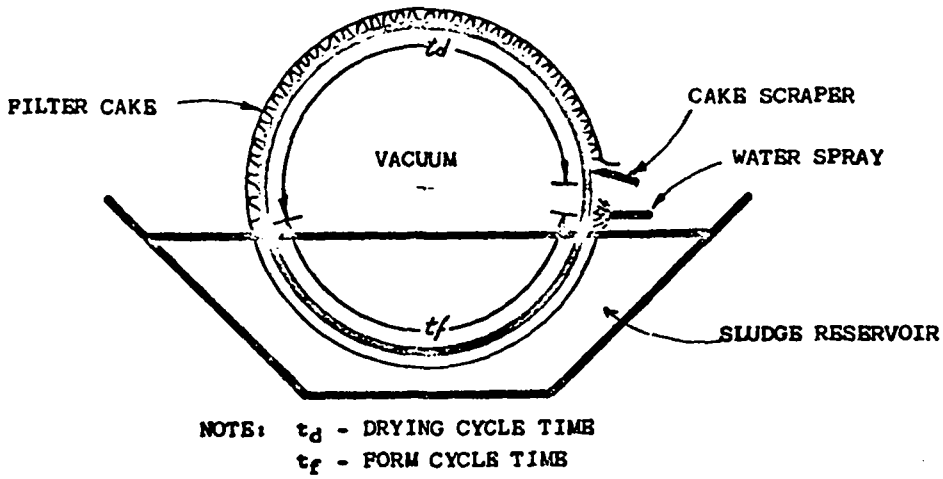


FIGURE 13-5. SCHEMATIC OF FILTER DRUM OPERATION (t_f = time for cake formation, t_d = time for cake drying)*

a septum, revolves through a "pan" holding the sludge. Movement of the filter is usually sufficient to prevent settling of the sludge, but additional agitation is sometimes used. Vacuum maintained in side the drum draws sludge to the septum surface. Solids are trapped, but filtrate drains from the sludge through the septum. Thus, as the drum revolves a sludge mat builds up. The mat thickness depends on the sludge, of course, but also on the contact time t_f. This time depends, in turn, on the rpm of the drum and its submergence in the pan. The rpm ranges from 0.1 to 1, while 20 to 40% of the drum cross section is submerged. The drum is divided internally into drainage compartments which are connected to a rotary valve and hence to the vacuum source and filtrate disengaging system (Figure 13-4). The rotary valve makes it possible to control the vacuum applied for different portions of the filtration cycle. Maximum vacuum drawn depends on the sludge, but it is usually in the range of 10 to 26 inches of mercury.

---

*Figure taken from reference (2).

As the drum rotates, the mat is lifted out of contact with the sludge. Vacuum continues to be drawn inside the drum compartment, thereby dewatering or "drying" the sludge cake. The drying time is slightly less than the difference between the cycle and mat forming times. At the end of the cycle, before the drum revolves through the sludge pan, the dewatered cake is lifted from the drum by closely spaced strings or a knife edge and the cake falls onto a conveyor. The filter septum is usually washed with a water spray before it is re-immersed in the sludge pan.

The quantity of solids which can be filtered per unit time and unit area, and the dryness of the cake formed depend upon sludge and operating variables. The sludge variables include: solids concentration, sludge age, temperature, viscosity, compressibility of the sludge, chemical composition, and the other sludge characteristics such as volatiles content, bound water, and particle size and shape. The operating variables are: applied vacuum, drum submergence, drum speed, degree of agitation in sludge pan, filter septum and the conditioning of sludge. Burd[1] discusses the effect of these variables on filter performance quantitatively.

The thickness of the mat formed on the filter must be a function of the drainage of liquid through the mat, the solids clogged septum and the mechanical system holding the septum in place. Of these flow resistances in series only the first, flow through the forming mat, is usually considered. Filtration theory is founded upon treating this "drainage" as flow through a bed of densely packed solids caused by a pressure difference across the solids. Figure 13-6 shows the mat forming system in a form amenable to mathematical treatment.

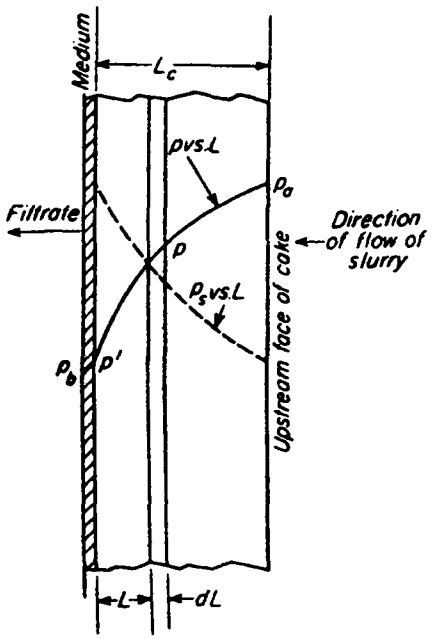


FIGURE 13-6. SECTION THROUGH FILTER SEPTUM AND CAKE SHOWING VARIATION OF FLUID PRESSURE (p) AND COMPRESSIVE STRESS (p_s) WITH CAKE DEPTH*

The change in pressure with depth in the mat or cake is given by[8]

$$\frac{dp}{dL} = \frac{k\,\mu\,(1-\varepsilon)^2\,(A_p/V_p)^2}{g_c\,\varepsilon^3}\,q_{filt} \qquad (13\text{-}7)$$

where μ is filtrate viscosity, A_p/V_p is surface to volume ratio of the solids, and ε is cake porosity. q_{filt} is the specific flow rate of filtrate through the filter surface. It has the units of velocity. Noting that depth can be replaced by the mat formed so that if w is the mass of solids deposited per unit area of the filter,

$$\frac{dp}{dw} = \frac{k\,\mu\,(A_p/V_p)^2\,(1-\varepsilon)}{g_c\,\rho_*\,\varepsilon^3}\,q_{filt} \qquad (13\text{-}8)$$

*Figure taken from reference (8) with the kind permission of the publisher.

(8) McCabe, W.L., and Smith, J.C., "Unit Operations of Chemical Engineering", 2nd Edition, McGraw-Hill (New York, 1967)

where ρ_* is the density of the sludge cake. Since most of the variables in eqn. (13-8) are difficult to measure, they are replaced by a specific cake resistance (α) which is the pressure drop required to give a unit of flow velocity per unit viscosity for a cake containing a unit mass per unit surface of the filter. The specific resistance is normally measured by a filter leaf or Buchner funnel test[1,9]. Equation (13-8) in terms of the specific resistance becomes

$$\frac{dp}{dw} = \frac{\alpha \mu}{g_c} q_{filt} \qquad (13\text{-}9)$$

With sewage sludges, α is a function of the cake thickness or the pressure difference applied to the cake. The reason for this behaviour is that the solids, particularly the organic matter (cell debris), in the sludge deform when compressed. Figure 13-6 shows the compressive stress increases as the septum surface is approached. Deformation increases with this stress leading to a blinding of the filter septum and reduction of cake porosity. Volatile solids content of the sludge correlates closely with compressibility. This is illustrated by the general rule that primary sludge is more easily filtered than biological sludge, while raw sludge filters better than digested sludge. Fine matter in sludge hinders filtration and some researchers claim that the benefit of elutriation comes partially from stripping out some of the fine matter in the sludge. The effect of compression is usually expressed through the specific resistance as

$$\alpha = \alpha_o (\Delta p)^s \qquad (13\text{-}10)$$

where Δp is the pressure difference used in the measurement.

Chemical conditioning is one means of countering the problem caused by sludge compressibility. Conditioning enhances sludge dewatering and increases filter loading rates. It is economically attractive for most sludges. The action of the chemical flocculants is believed to be solids agglomeration. The higher rigidity of the agglomerate increases the granular character of the solids thereby resisting better the compressive stresses in the cake.

---

(9) Eckenfelder, W.W., and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970)

In Canada the popular chemical conditioning agents are ferric chloride, lime and cationic polyelectolytes. Often combinations of ferric salts and lime are used to reduce chemical conditioning costs. The dual use of anionic and cationic polymers has been very successful because of the two basic phenomena thought to be involved with flocculation-charge neutralization and particle bridging (or agglomeration). The first function is performed by the cationic materials; the second by the anionic materials. Ferric salts are also used together with the polymeric agents.

13.2.2 Modelling.

Recalling that the objectives of filtration are sludge dewatering and retention of solids in the sludge, the primary variables to be modelled must be sludge moisture and the level of suspended solids in the filtrate. Since the filtrate is returned to the fluid side of the treatment plant, BOD and nutrient levels should be modelled, although, as we have pointed out earlier in this chapter, the filtrate flow is small so that an approximate composition is all that is needed.

For design, the area of filter needed to handle the sludge load is of primary interest. This can be calculated from either the solids loading or the filtrate loading[1]. The designer also needs to know the quantities of chemical conditioning agents required.

Unfortunately, the vacuum filter theory we considered in the previous section is useful only for predicting the load. To maintain continuity we will consider, therefore, design models first.

Equation (13-9) applies only to the mat forming portion of the filter cycle. During this portion a mat is built up on the septum surface under constant pressure. The buildup is proportional to the filtrate collected. Letting $q_{filt} = d\,(V_{filt})/A_{filt}\,d\,t_f$ and assuming that α is defined in terms of eqn. (13-10) so that eqn. (13-9) can be integrated to give a relation between Δp applied and the mat laid down at any time during the forming cycle, the rate at which filtrate is collected is given by

$$\frac{d\,V_{filt}}{dt_f} = \frac{g_c\,A_{filt}^2\,\Delta p}{\mu\,(\alpha_o\,\Delta p^s\,M_o V_{filt} + \alpha'_m\,A_{filt})} \qquad (13\text{-}11)$$

where α'_m is the filter medium specific resistance. This can be added to α because the resistances are in series and are thus additive. In eqn. (13-11), we have substituted $w = V_{filt}\,M_o/A_{filt}$. The steps involved in obtaining eqn. (13-11) are given in many textbooks[8]. Equation (13-11) is also used by Eckenfelder and Ford[9] to obtain a loading relation. Integrating eqn. (13-11) over the mat forming period gives an expression of the form,

$$t_f = \frac{A\,V_{filt}^2}{2} + B\,V_{filt} \qquad (13\text{-}12)$$

V_{filt} is the filtrate collected in each cycle so that Q_{filt}, the filtrate recovered per unit time is V_{filt}/t_c. t_c is the cycle time. Cycle time and forming time are related through the submergence of the drum (f_{sub})

$$f_{sub} = t_f/t_c \qquad (13\text{-}13)$$

In the filtration of sewage sludges the $B\,V_{filt}$ is usually negligible; eqn. (13-12) becomes

$$\bar{q}_{filt} = \left(\frac{2\,(\Delta p)^{1-s}\,g_c\,f_{sub}}{\alpha_o\,\mu\,M_o\,t_c}\right) \qquad (13\text{-}14)$$

In the equation $\bar{q}_{filt}$ is the liquid loading in gallons of filtrate per day per unit area of the filter; Δp is the vacuum applied. Consistent units must be used in eqn. (13-14). Eckenfelder and Ford give an empirical form of eqn. (13-14) as a dimensional equation for the solids loading in lbs/ft^2/h:

$$M_o\,\bar{q}_{filt} = 35700\,\left(\frac{10\,\Delta p^{1-s}}{\alpha_o\,\mu}\right)\,\frac{(M_o/10^6)^m}{t_f^n} \qquad (13\text{-}15)$$

The units in eqn. (13-14) are psi for Δp, sec/gm for α_o, gm/cm - sec for μ, mg/l. for M_o and minutes for t_f. The exponents m, n, s, must be determined experimentally from leaf filter or Buchner funnel tests[9].

If the amount of liquid in the sludge at the end of the mat forming portion of the cycle was known, eqn. (13-12) with t_c substituted for t_f would give an estimate of the dewatering of the sludge during the "drying" portion of the cycle. Unfortunately, an analytical approach to calculating the cake moisture level does not seem to have been pursued. Cake moistures are estimated now through correlations. Smith[4] has fitted a graphical correlation based on plant data proposed by McCarty[1] between cake moisture as a weight fraction (Ψ_{moist}) and the solids concentration in the sludge feed to give

$$\Psi_{moist} = 0.88 \ (M_o/10^4)^{-0.123} \qquad (13\text{-}16)$$

Burd reports suspended solids in the filtrate range enormously from as low as 100 to as high as 20,000 mg/l. Sludges from activated sludge units, particularly after digestion, contain relatively large amounts of fine solids and show high solids levels in the filtrate. In the absence of further data, we are reduced to using a retention factor for a solids concentration model. Let the retention factor (Ψ_{filt}) be the fraction of solids in the filter feed retained in the cake, the solids concentration in the filtrate is then

$$M_e = (1 - \Psi_{filt}) \ M_o \frac{Q_o}{Q_e} \qquad (13\text{-}17)$$

If we assume that all classes of solids (BOD, nutrients) are retained in the same fraction as the total solids, and that the composition of the liquid portion of the sludge is not changed, eqns. (13-16) and (13-17) provide the basis for simulation of a vacuum filter. The rate of sludge production per day is given by

$$W_{fit} = \frac{8.34 \ M_o Q_o}{(1 - 10^{-6} \ M_o)} \left(\frac{\Psi_{filt}}{1 - \Psi_{moist}} \right) \qquad (13\text{-}18)$$

if Q is MGD(U.S.) and M_o is the total solids concentration in the sludge in mg/l. The filtrate flow rate will be approximately

$$Q_e = Q_o \frac{(10^6 (1 - \psi_{moist}) - \psi_{moist} M_o)}{(10^6 (1 - \psi_{moist}) - \psi_{moist} M_e)} \qquad (13\text{-}19)$$

As a first approximation, M_e can be set to zero in eqn. (13-19). The filtrate flow obtained can be used to calculate M_e through eqn. (13-17) and this value may be substituted into eqn. (13-19) to refine the estimate of Q_e.

Conditioning chemicals required will depend on the dosage rate. Usually this rate will be determined from pilot or bench scale filtration tests. Dosages as weights percent of dry sludge are usually expressed as

$$w = a \left(\frac{A_{Alk}}{M_o}\right) + b \left(\frac{M_b}{M_i}\right) \qquad (13\text{-}20)$$

where M_b is the volatile suspended solids concentration in the sludge and M_i is the inert matter in the sludge. If ferric chloride is used as the conditioning agent alone, Smith[4] and Imhoff and Fair[5] quoting Genter[10] give $a = 108$ and $b = 2$. If ferric chloride and lime are used together, the ferric chloride dosage is reduced by a factor of 3. This results probably by using lime to meet the alkalinity demand of the sludge. Data quoted by Burd suggest that the polymer dosage is about 5 to 10% of the ferric chloride dose.

13.2.3 Design

The primary design parameter $(DP)_1$ for a vacuum filter installation is conventionally the solids loading. Burd suggests a design loading of 3.5 lbs/ft^2/h but mentions this is conservative and that a rule of thumb is to use the % solids in the feed sludge for $(DP)_1$. This rule would give loadings between 2 and 10 lbs/ft^2/h. The low values represent filtration of fresh and digested activated sludge; the high values are typical for raw primary sludge.

---

(10) Genter, A.L., "Computing Coagulent Requirements in Sludge Conditioning", Trans. Am. Soc. Civil Engrs., 71, 307 (1945)

A preferred design procedure would utilize either eqns.(13-14) or (13-15) together with bench scale filtration data. When this procedure is premissible under design codes, the design parameters become drum submergence, cycle time and vacuum. Ranges normally encountered for these parameters were listed at the beginning of this section.

Secondary design parameters are detention times in sludge conditioning tanks, agitation in sludge pans, and holdup in chemicals mixing facilities. Once drum area is chosen, the design of the rest of the filter installation is fixed as these are designed as functions of total filter area.

Burd summerizes performance information gathered from many sources in Table 13-1. This table serves as a design guide. The table shows that activated sludges are much more difficult to filter than are primary sludges. Trickling filter sludges (which are not shown in the table) behave much like primary sludges.

TABLE 13-1. VACUUM FILTER PERFORMANCE[1]

Type of Sludge	Conditioning Chemical Dosage (Wt. %)			Solids Loading	Cake Moisture
	Ferric Chloride	Lime	Polymer	(lbs/ft^2/h)	(wt. %)
Raw Primary	2	9	-	7	69
	-	-	0.2 to 1.2	6 to 20	63 to 72
Digested Primary	4	12	-	7	73
	-	-	0.2 to 1.5	4 to 15	66 to 74
Elutriated Digested Primary	3.5	-	-	7.5	69
Raw Primary + Activated Sludge	2.5	10	-	4.5	78
Digested Primary + Activated Sludge	5.5	19	-	4	78
	-	-	0.5 to 2.0	4 to 8	68 to 76
Elutriated Digested Primary + Activated Sludge	8.5	-	-	4	79

13.3 Centrifugation

It is widely claimed that centrifuges will eventually replace vacuum filters as the preferred means of sludge dewatering. A number of units have been installed in Ontario in the last few years. The advantages of centrifuges over vacuum filter are said to be lower capital cost, simplicity of operation, lack of odor problems associated with vacuum filters and the ability to dewater difficult sludges without an inordinate use of chemicals.

From a modelling standpoint, centrifugation is difficult to handle. Theory and relationships have been developed for basket type centrifuges, but these have poor solids retention and are not widely used. Most installations employ horizontal, cylindrical-conical, solid bowl machines. A quantitative theory, suitable for building models, does not seem to have been developed for this type of machine. Consequently, we will offer a crude model based on the interpretation of performance data.

13.3.1 Operation.

The principle of all types of centrifuges is that forces arising from density difference in a dispersed system, which cause higher density matter to settle under gravity, can be enormously increased by subjecting the system to high angular velocities. The force in this case is centrifugal rather than gravitational. Applied to a sewage sludge, the angular velocity causes the denser suspended matter to collect at the bowl wall, furthest removed from the centrifuge axis, while the less dense clarified liquor is held at the surface of the solids closer to the axis. Various types of machines use different techniques to separate solids and liquids. All machines share a common feature; the drainage of liquid from the solids before these are discharged.

Figure 13-7 shows a schematic diagram of a horizontal, cylindrical-conical solid bowl machine produced by the Sharples company. The operation is more easily followed in Figure 13-8 which shows also some of the terminology used. In this type of machine sludge is fed through a stationary feed tube placed along the centerline of the bowl through the

hub of the screw conveyor. The screw conveyor is mounted inside the rotating conical bowl. It rotates at a slightly lower speed than the bowl. Sludge leaves the end of the feed tube, passes through the ports in the conveyor shaft, and is distributed to the periphery of the bowl. Solids settle through the liquid pool, are compacted by centrifugal force against the walls of the bowl, and are conveyed by the screw conveyor to the drying or beach area of the bowl. The beach area is an inclined section of

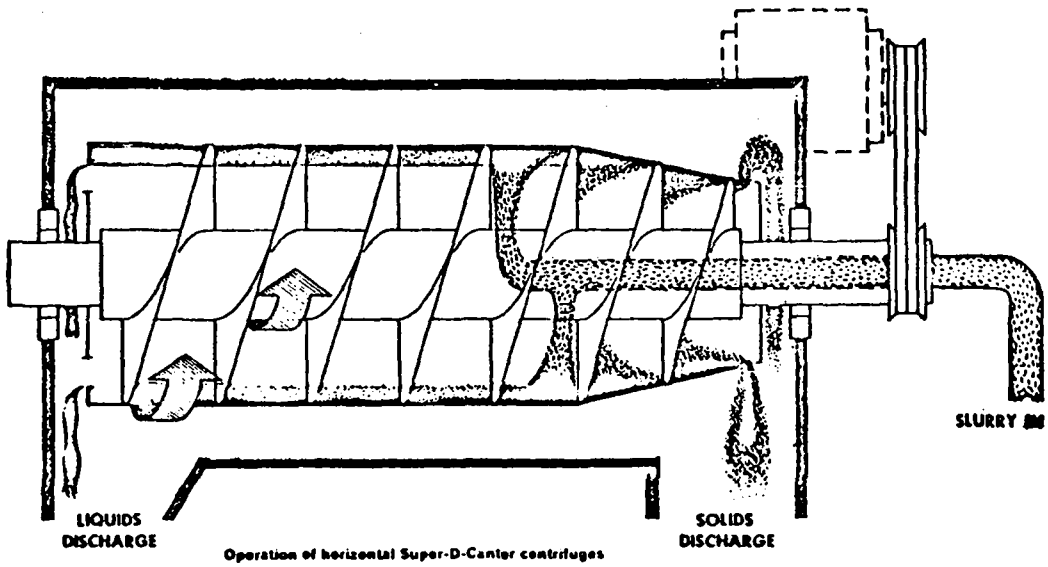


FIGURE 13-7. DIAGRAM OF THE SHARPLES SUPER-D-CANTER CENTRIFUGE INDICATING MEANS OF LIQUID SOLIDS SEPARATION*

*Figure taken from reference (1).

the bowl where dewatering occurs before the solids are discharged. Centrate is discharged continously over adjustable weirs and the opposite end of the bowl. The setting of the weirs control the pool volume.

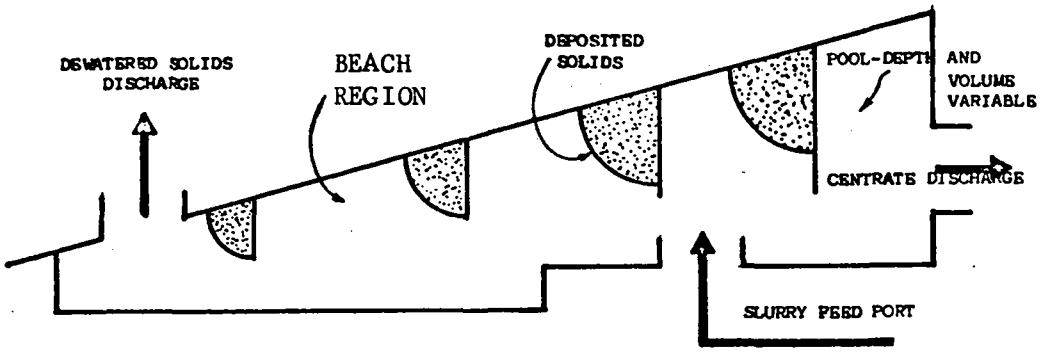


FIGURE 13-8. SCHEMATIC OF A CONTINUOUS FEED HORIZONTAL, CONICAL, SOLID BOWL CENTRIFUGE*

The performance of a centrifuge depends, of course, on sludge characteristics and chemical conditioning. It also depends upon the speed of rotation, sludge throughput, and the pool depth as well as the specific design of the unit. The main problem of centrifugation is poor recovery of solids. This recovery can be as low as 50% and centrates containing solids levels from 10,000 to 40,000 mg/l. are common. Polymeric flocculents in the range of 0.5% by weight are added to reduce solids loss. Although expensive, the increase in retention achieved is remarkable.

13.3.2 Modelling.

Modelling requirements for centrifugation are essentially the same as those for vacuum filtration as might be expected. Cake moisture and solids levels in the centrate are of primary interest. Since machines are purchased as units, design consists of selecting the type and size of machine required. Selection is based on bench scale tests which indicate capacity.

---

*Figure taken from reference (2).

Using graphical summaries of performance data obtained with raw and biological sludges, the fractional recovery of solids (Ψ_{cent}) in a horizontal, cylindrical-conical solid bowl machine is given by

$$\Psi_{cent} = a + b \frac{\omega^n}{Q} h_{pool}^m \qquad (13\text{-}21)$$

Without polymer $a \tilde{=} 0.7$, $n \tilde{=} \frac{1}{2}$ and $m \tilde{=} 0.9$. The constant b is much less than one. Adding polymeric flocculents raises a to about 0.8 and increases b. The fraction moisture as weight percent (ψ_{moist}) is given by

$$1 - \psi_{moist} = a' + b' \frac{Q^p \omega^n}{h} \qquad (13\text{-}22)$$

where $a' \tilde{=} 0.2$ and the exponent p on the feed rate is less than one.

13.4 Drying Beds

Once the predominant method of sludge dewatering in Canada, drying beds are losing favor because of the switch to the disposal of liquid sludges on the land. In large urban treatment plants, beds have been replaced by mechanical dewatering devices because of odor problems, the demand for land for plant expansion, and the cost associated with lifting the sludge for ultimate disposal. Enough units still operate in Canada to justify considering models for the operation.

Modelling of drying beds is confounded by the lack of performance data suitable for correlation or analysis. We must be satisfied, therefore, with very crude models for this process unit.

Drying beds are usually constructed of 4 to 9 inches of sand (0.3 to 1.2 mm.) supported by 8 to 18 inches of graded gravel or crushed stone (1/8 to 1 inch). Width of the beds varies depending on the method used for lifting the sludge, while their lengths are seldom much over 50 feet. Drainage from the beds is collected by tile underdrains spaced 8 to 20 feet apart with a slope somewhat greater than 1%.

Sludge is pumped onto the beds, usually at one end to an average depth of from 6 to 12 inches and allowed to stand until it can be readily lifted. The time required depends on both sludge type and characteristics, and on climatic conditions. Loading depth and chemical conditioning is also important. MacLaren[6] reports a digested sludge can be dewatered to 55% moisture by weight in about 6 weeks under Canadian conditions. Sludge cake, however, can be lifted from a bed at higher moisture contents than this. Front end loaders are now being widely used for cake lifting.

Drying beds are limited effectively to digested sludges because of the odor, insect nuisance and the poor drying characteristics of raw sludge.

Dewatering of sludges on drying beds occurs by drainage of water from the sludge through the sand bed into the drainage collectors and evaporation of water from the surface of the sludge. Drainage is substantially complete in from 1 to 3 days and leaves a cake containing 75 to 85% moisture. The latter is consistant with an estimate that 60% of the water in a sludge is "free" and therefore drainable, while 35% is capillary or occluded water[1]. Only 5% is chemically bound.

Drying of the sludge follows and it is a considerably slower process. Two to five weeks are normally required depending on climate. Drying rates in summer can be 3 fold winter rates. Initially drying is controlled by evaporation of water from the surface of the sludge. The rate depends on temperature, air humidity, wind and is relatively constant. As drying continues further, transport of water through the sludge to the air surfaces controls the drying rate which falls with time until an equilibrium level is reached. Figure 13-9 illustrates the drying behaviour. The equilibrium level will depend on the balance of evaporation and rainfall. Sludge beds in Canada now are not usually covered so precipitation must be considered. Cracks open up in the sludge cake surface during the constant rate drying period. These cracks accelerate evaporation and enhance drainage of rainfall.

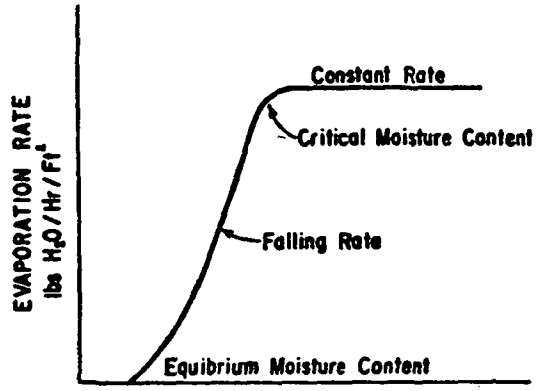


FIGURE 13-9. PHASES OF SLUDGE DRYING

Drainage collected from drying beds is relatively free from suspended solids and is often diluted by rain water.

Modelling of drying beds must be concerned with cake moisture on lifting, drainage recovered and the concentration of BOD and nutrients dissolved in the drainage.

If ϕ_{rain} is the ratio of the mean inches of rain fall collected annually to the inches/sq. foot of undiluted drainage, the drainage flow is

$$Q_e = Q_o (1 + \phi_{rain}) \left(1 - \frac{10^{-6} M_o Q_o \psi_{moist}}{1 - \psi_{moist}}\right) \qquad (13\text{-}23)$$

The cake moisture in the relation must be specified. The BOD concentration in the drainage will be

$$S_e^* = \frac{1}{1 + \phi_{rain}} S_o^* \qquad (13\text{-}24)$$

and all other soluble species will follow this equation. Suspended solids concentrations can be assumed to be negligible. The weight of sludge produced (W_{dry}) is given by eqn. (13-18) if ψ_{filt} is replaced by one. Eqn. (13-20) models the conditioning chemical demand. Alum and polymeric flocculating agents are widely used. As a guide, about 1 lb. of alum is recommended for each 100 gallons (U.S.) of sludge, polymer requirement is about 1/3 of this amount. Conditioning chemicals cut the drying time by about one half if used in sufficient quantities.

The design parameter for drying beds is sq. feet of bed per capita or sludge loading as lbs. of dry solid/sq. feet of bed/year. Eckenfelder and O'Connor give the following values for sludge loading[1]:

	Loading lbs. dry solids/sq. ft./yr.
Digested Primary Sludge	28
Digested Primary + Activated Sludge	15
Digested Primary + Trickling Filter Sludge	22

13.5 Incineration

Although incineration of municipal sludge is used in only a few places in Canada, it could become much more wide spread if restrictions on land spreading increase sufficiently to discourage the spreading alternative. For our discussion, we will make extensive use of Report 17070 EBP 07/71 of the U.S. Environmental Protection Agency which deals with computerized design of the multiple hearth type of incinerator[11]

13.5.1 Operation and Theory of Incinerators.

The primary objective of incineration is volume reduction. A secondary one is sterilization of the waste solids.

Most incinerators are of the multiple hearth type shown in Figure 13-10. The unit consists of a number of circular hearths stacked one above the other in a refractory lined, cylindrical shell. Arms, known as rabble arms, are attached to a rotating central shaft and serve to distribute the sludge across each hearth and to move it to the next hearth below. The sludge is swept alternatively inwardly on one hearth and outwardly on the next.

Air for combustion is mainly recycled cooling air, but some air can be drawn through ports at the bottom of the furnace. The cooling air, is supplied by a blower and passes up through the hollow central shaft where it cools the moving equipment and is preheated at the same time.

---

[11] Unterberg W., Sherwood, R.J. and Schneider, G.R., "Computerized Design and Cost Estimation for Multiple-Hearth Sludge Incinerators", Report 17070 EBP 07/71, Water Pollution Control Research Series, U.S. Environmental Protection Agency, U.S. Government Printing Office (Washington, D.C.,1971)

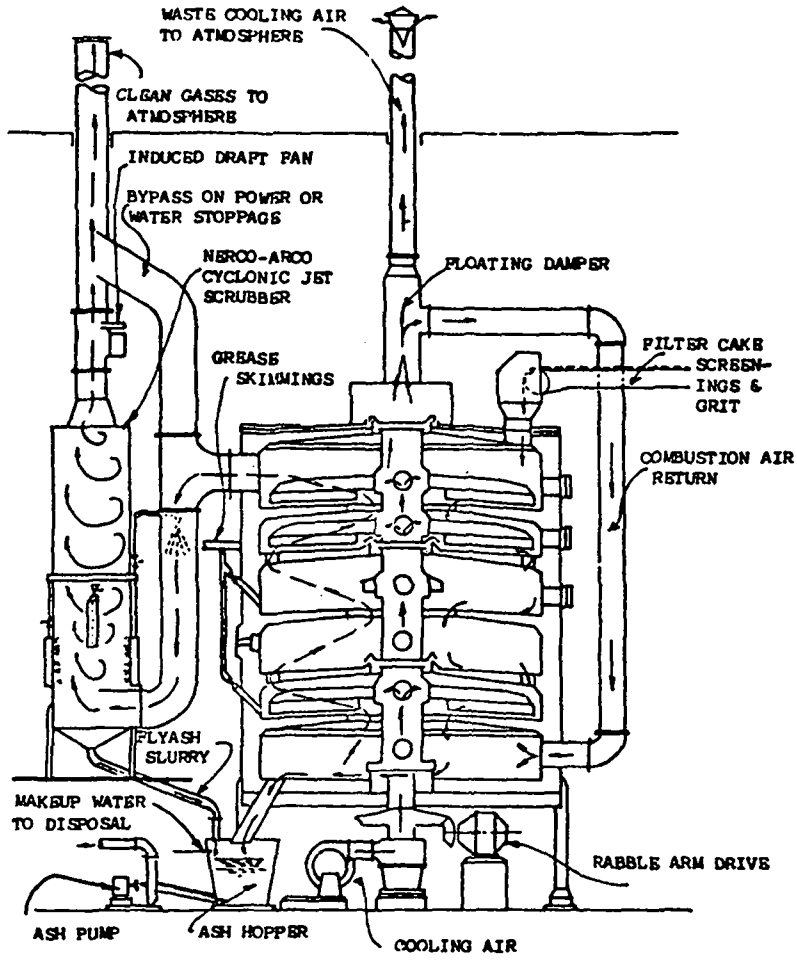


FIGURE 13-10. SCHEMATIC DIAGRAM OF A MULTIPLE HEARTH INCINERATOR SHOWING OPERATION*

About 300 lbs. of air are used for 100 lbs. of wet sludge, this includes excess air.

The incinerator proper operates in roughly three zones. The upper hearths preheat and dry the sludge which enters on the average with about 75% moisture by weight. The gases cool to about 500°F and sludges reach about 50% moisture. The middle hearth serve as a combustion zone. Sludge with less than 50% moisture ignites. Temperatures will reach about 1400 to 1600°F in this zone. The final zone consisting of the bottom hearths cools the ash and preheats the air.

Combustion, on the average, generates about 390 lbs. of flue gas

*Figure taken from reference (2).

per 100 lbs. of wet sludge along with 10 lbs. of ash. The off gases in some designs will pass into an economizer (air preheater) before going to a wet scrubber. The scrubber knocks out fly ash and reduces odors. In Figure 13-10, the scrubber wash is mixed with the ash. The slurried ash is then settled and the wet ash goes to land fill. The decant liquor is recycled back to the liquid side of the treatment plant.

In the last few years a fluidized bed incinerator has been developed and a number of installations of this type of device have been made in the United States. In the device, the multiple hearths are replaced by a bed of sand supported on a distributing plate. Air passing through the plate suspends the sand particles and keeps them violently agitated giving the bed a "fluid" character (hence the name fluidized bed). This type of incinerator is illustrated in Figure 13-11.

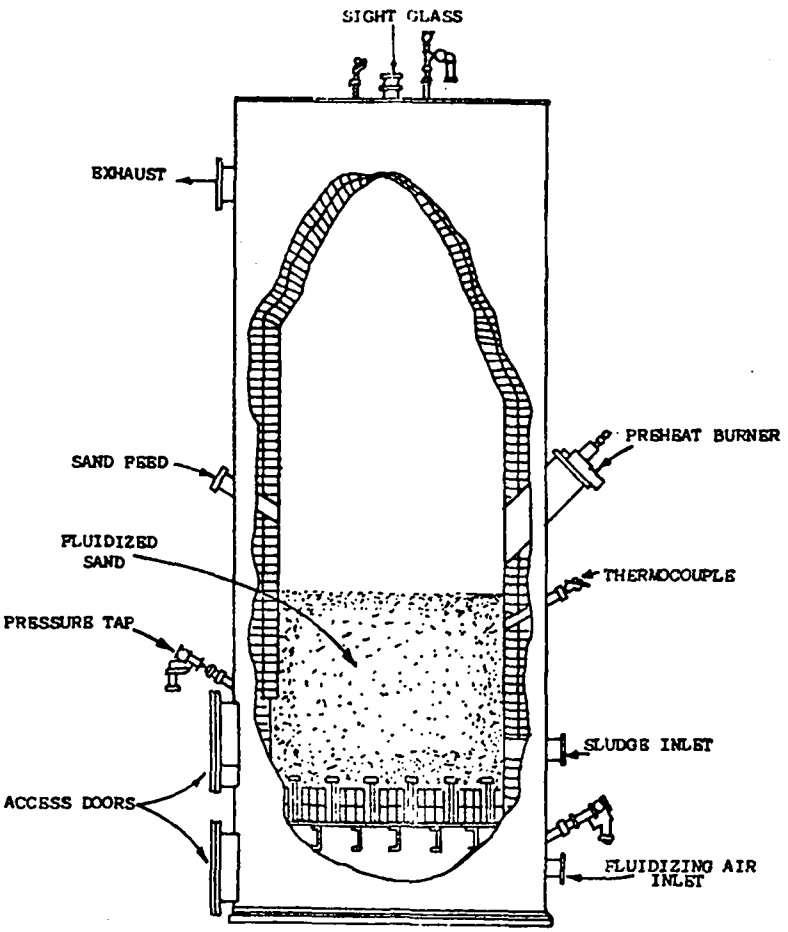


FIGURE 13-11. SCHEMATIC DIAGRAM OF A FLUIDIZED BED INCINERATOR*

*Figure taken from reference (2)

As shown in the figure, sludge is injected directly into the sand bed. The ash formed is blown over and taken out of the off gas by cyclones and scrubbing.

Heat recovery in the incinerator is poorer than that achieved in multiple hearth units so that either auxiliary fuel or dryer feed sludge is required.

From a modelling stand point, the two types of incinerators are sufficiently alike so that models developed for multiple hearth incinerators will be applicable to the fluidized bed device for the most part.

13.5.2 Modelling.

A waste treatment system is virtually independent of the incinerator because the scrubber wash water returned to the plant from the unit is a very small stream when compared with the sewage flow, if, indeed, any is returned. Simulation, therefore, is not an important application of modelling. Most incinerator modelling is centered on design.

Design models should give the amount of ash produced, the flow of off gas leaving the unit, the amount of air required as well as the diameter of the hearth. Once the size is specified, the internal design of the incinerator is effectively determined since the units are standardized. The temperatures of flue gas, off gas leaving the scrubber and the ash temperature are design parameters. In simulation, on the other hand, these temperatures are usually calculated along with the ash produced and the off gas flows. The amount of scrubber wash water recovered and the BOD and nutrients level in the wash water are also desirable.

Since design is a more important application than simulation for incinerator models, we will develop the relations assuming a design situation. The relations, however, will be useful for both design and simulation.

Let W be the weight of sludge to be fed to an incinerator per unit of time (lbs/hr.), the weight of air (W_{air}) can be obtained by a material balance assuming complete combustion of all the volatile matter in the sludge:

$$W_{air} = 4.3\ (1 + \Psi_{xair})\ W\ \Psi_{VS}\ (2.66\ f_C + 8 f_H + f_{Su} - f_{O_2}) \qquad (13\text{-}25)$$

In the above equation ψ_{xair} is the excess air (as a fraction of the stoichiometric air) required, while ψ_{VS} is the weight fraction of volatile matter in the sludge on a dry basis and f_C, f_H, f_{Su}, f_{O_2} are weight fractions of the carbon, hydrogen, sulfur and oxygen in the sludge, again on a dry basis. Combustion results in a flue gas; the weight of the major components of this gas will be:

$$W_{CO_2} = W\,(3.67\,\psi_{VS}\,f_C + 0.44\,\phi_{decomp}\,\psi_{CaCO_3}) \qquad (13\text{-}26)$$

$$W_{H_2O} = W\,(\psi_{moist} + 9\,\psi_{VS}\,f_H + .254\,\phi'_{decomp}\,\psi_{Fe(OH)_3} + 0.346\,\phi''_{decomp}\,\psi_{Al(OH)_3}) \qquad (13\text{-}27)$$

$$W_{O_2} = \frac{0.233\,\psi_{xair}}{1 + \psi_{xair}}\,W_{air} \qquad (13\text{-}28)$$

$$W_{SO_2} = 2\,\psi_{VS}\,f_{Su}\,W \qquad (13\text{-}29)$$

In these equations, ϕ_{decomp} represents the fractional decomposition of the various chemical agents, while Ψ is their weight fraction in the dry sludge. Unterberg et al.[11] suggest some average values for the various parameters used in the above equations: $\Psi_{VS} = 0.75$, $\Psi_{moist} = 0.75$, Ψ_{xair} ranges from 0.5 to 1.5 with a mean value of 0.75. Elemental weight fractions depend on the sludge, but again average values are $f_C = 0.55$, $f_H = 0.06$, $f_{O_2} = 0.35$, $f_N = 0.03$ and $f_{Su} = 0.01$.

The heat supplied (q_{sup}) by the combustion of the sludge is

$$q_{sup} = \Delta H_c\,\psi_{VS}\,W + f_{cair}\,W_{air}\int_{T_o}^{T_{cair}} (c_p)_{air}\,dT + (1 - f_{cair})\,W_{air}\int_{T_o}^{T_{amb}} (c_p)_{air}\,dT \qquad (13\text{-}30)$$

where ΔH_c is the heat of combustion of the sludge, f_{cair} is the fraction of the cooling air sent through the center shaft of the incinerator which is cycled back for combustion, and T_{cair} is the temperature at which the cooling air emerges from the shaft (see Figure 13-10). The heat required (q_{req}) is given by

$$
\begin{aligned}
q_{req} &= (1 - \psi_{VS})\, W\, c_{ash}\, (T_{ash} - T_o) \\
&+ W\, \psi_{moist} \left[c_W\, (212 - T_o) + 970 + \int_{212}^{T_{fg}} c_{p_W}\, dT \right] \\
&+ 0.076\, Q_{cair} \int_{T_o}^{T_{cair}} (c_p)_{air}\, dT \\
&+ W \left[761\, \phi_{decomp}\, \psi_{CaCO_3} + 225\, \phi'_{decomp}\, \psi_{Fe(OH)_3} \right. \\
&\left. + 381\, \phi''_{decomp}\, \psi_{Al(OH)_3} \right] + h_r\, A_{xsurf}\, (T_{xsurf} - T_{amb}) \\
&+ \Sigma\, W_i \int_{T_o}^{T_{fg}} (c_p)_i\, dT + 1048\, W_{H_2O}
\end{aligned}
\qquad (13\text{-}31)
$$

In this long equation, c_{ash} and c_W are the specific heats of the ash and water, while Q_{cair} is the volume of cooling air fed to the center shaft. T_{fg} is the flue gas temperature leaving the top hearth; T_{xsurf}, T_{ash}, T_{amb} and T_o are the temperatures of the external surface of the incinerator, ash leaving the bottom hearth, ambiant surroundings and the feed sludge respectively.

The heat of combustion of the sludge is given by[11]

$$\Delta H_c = 100\, a - \frac{1 - \psi_{moist}}{\psi_{VS}}\, ab \qquad (13\text{-}32)$$

where $a = 131$ and $b = 10$ for raw or digested primary sludge and $a = 107$ and $b = 5$ for raw activated sludge. Q_{cair} is about 36 SCFM/

ton of wet sludge per day, while f_{cair} is normally about 0.7.

The exit temperature of the cooling air T_{cair}, T_{ash} and T_{fg} are design parameters. T_{cair} is usually in the range of 215 to 375°F with an average value of 325°F. T_{ash} ranges from 150° to 850°F depending somewhat on f_{cair}. A standard choice is 400°F. The flue gas temperature can be as low as 500°F or reach 1100°F. Often a value of 800°F will be chosen. Other design parameters are ψ_{xair} and f_{cair}.

If $q_{sup} = q_{req}$, all the design parameters have been chosen correctly. However, if $q_{sup} > q_{req}$ the parameters are inconsistant. Usually a higher ψ_{xair} will be chosen because this insures more complete combustion. On the other hand, if $q_{sup} < q_{req}$, auxiliary fuel must be burnt to reach the design level of T_{fg}.

The fuel requirements are easiest to calculate by determining specific rates, that is weight per weight (lb. per lb.) of fuel.

$$w'_{air} = 4.3\,(2.66\,f'_C + 8\,f'_H + f_{Su} - f_{O_2}) \qquad (13\text{-}33)$$

$$w'_{CO_2} = 3.67\,f_C \qquad (13\text{-}34)$$

$$w'_{H_2O} = 9\,f_H \qquad (13\text{-}35)$$

$$w'_N = f_N + 0.767\,w'_{air} \qquad (13\text{-}36)$$

$$w'_{SO_2} = 2\,f_{Su} \qquad (13\text{-}37)$$

The fuel required (W_{fuel}) is based on the net heat available from the fuel

$$W_{fuel} = \frac{\Delta H_{fuel} - (\Sigma\, w'_i \int_{T_o}^{T_{fg}} (c_p)_i\, dT + 1048\, w'_{H_2O})}{\Delta H_{fuel}} \qquad (13\text{-}38)$$

Then, the auxiliary air required (excess is not usually used) is

$$W_{air}' = w_{air}' \; W_{fuel} \tag{13-39}$$

For each of the components in the flue gas, the total weight produced is

$$W_i' = W_i + w_i' \; W_{fuel} \tag{13-40}$$

where i is CO_2, H_2O, O_2, N_2 and SO_2 successively. The volumetric flow rate is

$$Q_i' = 10.73 \; W_i' \; \frac{(T_{fg} + 460)}{(MW)_i \; p_{atm}} \tag{13-41}$$

where p_{atm} is the atmospheric pressure at the location.

Different fuels can be used. Unterberg[11] gives the following values:

	Fuel Oil	Natural Gas	Digester Gas
ΔH_{fuel} (Btu/lb)	19,000	21,000	12,000
f_C	0.86	0.67	0.50
f_H	0.11	0.22	0.12
f_{O_2}	--	0.01	0.38
f_N	--	0.10	--
f_{Su}	0.03	--	--

Design of the scrubber depends on the operation. If odor removal is not a problem, the scrubber may operate with just enough water make up to allow for saturation of the scrubber off gas. Otherwise, additional water will be added as a direct function of the sludge feed rate to the incinerator. The off gas flow rate leaving the scrubber will be

$$Q_e' = (\Sigma \; W_i' - W_{H_2O}') \; v_{sat} \tag{13-42}$$

where v_{sat} is the specific volume of humid air at 100% humidity

$$v_{sat} = 10.73 \; \left(1 + \frac{p_w}{p_{atm} - p_w}\right) \; \frac{\left(\frac{T_e + 460}{\Sigma \; Q_i' \; (MW)_i}\right)}{\Sigma \; Q_i' - Q'_{H_2O}} \tag{13-43}$$

where T_e is the exit temperature from the scrubber. This is a design parameter and it is usually set at about 175°F. The water fed to the scrubber will be given by

$$\dot{W}_{scrub} = \gamma W + 18 \left(\frac{p_W}{p_{atm} - p_W}\right) \frac{(\Sigma W_i' - W_{H_2O}')}{\Sigma Q_i (MW)_i} \Big/ \Sigma Q_i' - Q_{H_2O}' \qquad (13\text{-}44)$$

The volumetric flow (gals/hr) Q_{scrub} will be

$$Q_{scrub} = 0.12 \; W_{scrub} \qquad (13\text{-}45)$$

Only the fraction $\gamma W/W_{scrub}$ will be recovered and returned to the treatment plant. No information seems to be available on how the BOD and suspended solids level in this return stream depend on incinerator and scrubber operation.

The hearth area required in an incinerator has been developed from a correlation of hearth loading. The correlation indicates the loading is about 2 lbs. of dry solid/hr./sq. feet of hearth area. The actual size depends on the operating factor for the incinerator. Unterberg et al.[11] discuss this question and further details of incinerator design.

LIST OF REFERENCES

Chapter 1

Nil

Chapter 2

1. Lynn, W.R., J.A. Logan and A. Charnes, J.W.P.C.F., 34, 565 (1962).

2. Galler, W.S., and H.B. Gotaas, J. San. Eng. Div., A.S.C.E., 92 (SA1), 163 (1966).

3. McBeath, B.C., and R. Eliassen, J. San. Eng. Div., A.S.C.E., 92 (SA2), 147 (1966).

4. Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control, 69, No. 6, pp. 686-693.

5. Smith, R., "Preliminary Design and Simulation of Conventional Waste Water Renovation Systems Using the Digital Computer", Water Pollution Control Research Series Publication, WP-20-9, Ohio Basin Region, F.W.P.C.A., Cincinnati, Ohio, May 1968.

6. Smith, R., Eilers, R.G. and Hall, E.E., "Executive Digital Computer Program for Preliminary Design of Waste Water Treatment Systems", Water Pollution Control Research Series Publication, WP-20-14, F.W.P.C.A., Ohio Basin Region, Cincinnati, Ohio, August 1968.

7. Chen, G.K., Fan, L.T. and Erickson, L.E., "Computer Software for Waste Water Treatment Plant Design", J.W.P.C.F., 44, 746-762 (1972).

8. Silveston, P.L., "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research, 6,1101 (1972)

9. Hoffman, T.W., Woods, D.R., Murphy, K.L. and Norman, J.D., "The Strategy and an Example of Simulation as Applied to a Petroleum Refinery Waste Treatment Process", J.W.P.C.F., in print (1973).

10. Naito, M., T. Takamatsu and L.T. Fan, Water Research, 3, 433 (1969).

11. Matsumoto, J., and M. Onuma, J. Jap. Sew. Works Assn., 5, (46), 37 (1968).

12. Evenson, D.E., G.T. Orlob, and J.R. Monser, Ind. Water Engrg., 6 (2), 16 (1969a).

13. Armstrong, G.M. and Olson, L.R., "Improving a Chemical Plant via Process Simulation", Chemical Engineering, September 3, 1962, pp. 135-142.

14. Shah, M.J. and Stillman, R.E., "Computer Control and Optimization of a Large Methanol Plant", Ind. Eng. Chem. 62, No. 12, 59.(1970).

Chapter 2

15. Klumpar, I.V., "Process Predesign by Computer", Chem. Eng., Sept. 22, 1969, pp. 114-122.

16. Cullen, P.D., "The Turbo-Expander Process A Critical Analysis", Engineering Report, Dept. of Chem. Eng., Univ. of Waterloo, Waterloo, Ontario (1972).

17. Wilhelm, D.J., "Scale-Up, A Status Report", Chemical Age of India, 21, No. 2, 162 (1970).

18. Fan, L.T., Chan, G.K.C. and Erickson, L.E., J.W.P.C.F. 44, No. 5, 746 (1972)

Chapter 3

1. Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control, 69, No. 6, 686 (1970)

2. Shannon, P.T. et al., "Computer Simulation of a Sulfuric Acid Plant", Chem. Eg., Progress 62, June, 49, (1966).

3. Smith, R., "Preliminary Design and Simulation of Conventional Waste Water Renovation Systems Using the Digital Computer", Water Pollution Control Research Series, WP-20-9, F.W.P.C.A., U.S.D.I. (Washington, 1968).

4. Fan, L.T., Erickson, L.E. and Chen, G.K.C., "Computer Optimization of Biological Waste Water Treatment Processes", in WATER - 1971, Chem. Eng. Progress Symp. Series, (1973).

5. Singh, D.P., "Steady State Simulation of the Kitchener Waste Water Treatment Plant", M.A.Sc. Thesis, Dept. of Chem. Eng., Univ. of Waterloo (1970).

6. Silveston, P.L., "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research, 6, 1101 (1972)

7. Silveston, P.L., "Computer Simulation of Waste Treatment Plants", ACS/CIC Symposium, "Pollution Problems of Our Environment", Joint ACS/CIC Conference, Toronto, May 1970.

8. Silveston, P.L., "Computer Simulation of Waste Water Treatment Plants", Proc. 1st PACHEC Meeting, Kyoto, Japan (1972).

9. Peeling, D.A., "Simulation of Waste Treatment Plants Using SEPSIM", Engineering Report, Dept. of Chem. Eng., University of Waterloo (1972).

10. Hoffman, T.W., Woods, D.R., Murphy, K.L. and Norman, J.D., "The Strategy and an Example of Simulation as Applied to a Petroleum Refinery Waste Treatment Process", J.W.P.C.F., in print (1973).

Chapter 3

11. Curry, E.V., "Computer Simulation of a Biological Waste Treatment Facility", Engineering Report, Dept. of Chem. Eng., University of Waterloo (1971).

12. Tan, P.G.C., M. Eng. Thesis, Dept. of Chemical Engineering, McMaster University, Hamilton, Ontario (1972).

13. Smith, R., Eilers, R.G., Hall, E.D., "Executive Digital Computer Program for Preliminary Design of Waste Water Treatment Systems", Water Pollution Control Series WP-20-14, F.W.P.C.A., U.S.D.I. (Washington, D.C., 1968).

14. Goering, S.W., "A Computer Model of the Sewage Treatment Process of Boulder, Colorado", M.Sc. Thesis, Dept. of Chemical Eng., University of Colorado (1972).

15. Chen, G.K., Fan L.T., and Erickson, L.E., "Computer Software for Waste Water Treatment Plant Design", J.W.P.C.F., 44, 746 (1972)

16. Fan, L.T., Mishra, P.N., Chen, G.K.C., Erickson, L.E., "Application of Systems Analysis Techniques in Biological Waste Treatment", 4th Int. Fermentation Symp., Kyoto Japan (1972).

Chapter 4

1. C. M. Crowe et al., "Chemical Plant Simulation", Prentice-Hall (Englewood Cliffs, N.J., 1971).

2. D.M. Himmelblau & K.B. Bischoff, "Process Analysis and Simulation", Wiley (New York, 1968).

3. P.L. Silveston, "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", J. Water Pollution Control (London) 69, No. 6, 686 (1970).

4. Rudd, D.F. and Watson, C.C., "Strategy of Process Engineering", John Wiley (New York, 1968).

5. Norman, R.L., "A Matrix Method for Location of Cycles in a Directed Graph", A.I.Ch.E.J., 11, 450 (1965).

6. Himmelblau, D.M., "Decomposition of Large Scale Systems I", Chemical Eng. Sci., 21, 425 (1966).

7. Lee, W. and Rudd, D.F., A.I.Ch.E.J., 12, 1184 (1966).

8. Christensen, J.H. and Rudd, D.F., A.I.Ch.E.J., 14, (1968).

9. Sargent, R.W.H. and Westerberg, A.W., "Speed-up in Engineering Design", Trans. Inst. Chem. Engs. 42, 190 (1964).

Chapter 5

1. Smith, R., "Preliminary Design and Simulation of Conventional Waste Treatment Systems Using the Digital Computer", Water Pollution Control Research Series, WP-20-9, F.W.P.C.A./U.S.D.I. (Washington, 1968).

2. Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control 69, 686 (1970).

3. Smith, R., Eilers, R.G., Hall, E.D., "Executive Digital Computer Program for Preliminary Design of Waste Water Treatment Systems", Water Pollution Control Research Series, WP-20-14, F.W.P.C.A./U.S.D.I. (Washington, 1968).

4. Hoffman, T.W., Woods, D.R., Murphy, K.L., Norman, J.D., "The Strategy and an Example of Simulation as Applied to a Petroleum Refinery Waste Treatment Process", J.W.P.C.F., in print (1973).

5. Peeling, D.A., Engineering Report, Dept. of Chemical Engineering, University of Waterloo (1972).

6. Silveston, P.L., "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research 6, 1101 (1972).

7. Silveston, P.L., "Computer Simulation of Waste Water Treatment Plants", Proc. 1st Pacific Chem. Eng. Congress, Part III, (Kyoto, Japan, 1972).

8. Fan, L.T., Erickson, L.E. and Chen, G.K.C., Paper, National A.I.Ch.E. Meeting, Cincinnati, Ohio (May, 1971).

9. Curry, E.V., "Computer Simulation of a Biological Waste Treatment Facility", Eng. Report, Dept. of Chem. Eng., Univ. of Waterloo (1971).

10. Singh, D.P., "Steady State Simulation of the Kitchener Waste Treatment Plant by Digital Computer", M.A.Sc. Thesis, Dept. of Chem. Eng., University of Waterloo (1971).

11. "Standard Methods for the Examination of Water and Waste Water", 12th Edition, Am. Public Health Service, Inc. (New York, 1965).

12. Eckenfelder, W.W., Jr. and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970).

13. "Biological Waste Treatment", Notes for a Technical Seminar, University of Waterloo, Waterloo, Ontario (1967).

14. "Design Guides for Biological Waste Water Treatment Processes", Water Pollution Control Research Series, 11010 ESQ, E.P.A. (Washington, D.C., 1971).

Chapter 6

1. H. Mosler, M.S. Thesis in Chemical Engineering, Purdue University, Lafayette, Indiana (1963).

2. Silveston, P.L., "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research, 6, 1101 (1972).

3. Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control 69, 686 (1970).

4. Hoffman, T.W., Woods, D.R., Murphy, K.L. and Norman, J.D., "The Strategy and an Example of Simulation as Applied to a Petroleum Refinery Waste Treatment Process", J.W.P.C.F., in print (1973)

5. Smith, R., Eilers, R.G., Hall, E.D., "Executive Digital Computer Program for Preliminary Design of Waste Water Treatment Systems", Water Pollution Control Series WP-20-14, F.W.P.C.A., U.S.D.I. (Washington, D.C. , 1968).

Chapter 7

1. Himmelblau, D.M. and Bischoff, K.B., "Process Analysis and Simulation", John Wiley (New York, 1968).

2. Himmelblau, D.M.,"Process Analysis by Statistical Methods", John Wiley (New York, 1970).

3. Smith, C.L., Pike, R.W. and Murrill, P.W., "Formulation and Optimization of Mathematical Models", International Textbook Co. (Scranton, Pennsylvania, 1970)

4. H. M. Hulburt and S. Katz, Chem. Eng. Sci., 19, 555 (1964).

5. A. D. Randolph, Can. J. of Chem. Eng., 42, 280 (1964).

6. Manual of Engineering Practice - No. 36, "Sewage Treatment Plant Design", A.S.C.E. (New York, 1959).

7. Smith, R. "Preliminary Design and Simulation of Conventional Waste Water Renovation Systems Using the Digital Computer", Water Pollution Control Research Series, WP-20-9, F.W.P.C.A. - U.S.D.I. (Washington, 1968).

8. Crowe, C.M., Hamielec, A.E., Hoffman, T.W., Johnson, A.I., Shannon, P.T. and Woods, D.R., "Chemical Plant Simulation", Prentice-Hall (Englewood Cliffs, New Jersey, 1971).

9. Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control 69, No. 6, 686 (1970).

Chapter 8

1. Weber, W.J., Jr., "Physicochemical Processes for Water Quality Control", Wiley-Interscience (New York, 1972).

2. "Design Guides for Biological Waste Water Treatment Processes", Water Pollution Control Research Series, No. 11010 ESQ, U.S. Environ. Protect. Agency (Washington, D.C., 1971).

3. Eckenfelder, W.W., Jr., and O'Connor, D.J., "Biological Waste Treatment", Pergamon Press (London, 1961).

4. Silveston, P.L., "Design of Settling Basins with Allowance for Residence Time Distributions", Can. J. Chem. Eng., 47, 521 (1969).

5. Camp, T.R., "Sedimentation and the Design of Settling Tanks", Trans. Am. Soc. of Civil Eng., III, 895 (1946).

6. Eckenfelder, W.W., Jr. and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970).

7. Takamatsu T., and Naito, M., "Effect of Flow Conditions on the Efficiency of a Sedimentation Vessel", Water Research, 1, 433-450 (1967).

8. Rebhun, M. and Argaman, Y., "Evaluation of Hydraulic Efficiency of Sedimentation Basins", J. Sanitary Eng. Div., Proc. A.S.C.E., SA5, 37 (1965).

9. Thomas, H.A., Jr., and Archibald, R.S., "Longitudinal Mixing Measured by Radioactive Tracers", Trans. Am. Soc. of Civil Eng. 117, 839 (1952).

10. Wills, R.F. and Davis C., "Flow Patterns in a Rectangular Sewage Sedimentation Tank", Adv. in Water Pollution Research, Volume 2, Pergamon Press (London, 1964).

11. Thirumurthi, D., "A Break-through in the Tracer Studies of Sedimentation Tanks", J.W.P.C.F., 41, No. 11, R405 (1969).

12. Villemonte, J.R., Rohlich, G.A., and Wallace, A.T., "Hydraulics and Removal Efficiencies in Sedimentation Basins", Adv. in Water Pollution Research 2, 381, Pergamon Press (London, 1967).

13. Wallace, A.T., "Design and Analysis of Sedimentation Basins", Water and Sewage Works, 114, R-219 (1967).

14. Singh, D.P., "Steady State Simulation of the Kitchener Waste Treatment Plant", M.A.Sc. Thesis, Dept. of Chem. Eng., University of Waterloo (Waterloo, Ontario, 1970).

Chapter 8

16. Stepko, W.E., "Comparison of Mathematical Models of a Continuous Sedimentation Basin", M.A.Sc. Thesis, Dept. of Chem. Eng., Univ. of Waterloo (Waterloo, 1970).

17. Sakata, N. and Silveston, P.L., "Exponential Approximation for Settling Rate", Unpublished Manuscript (1973).

18. Fitz, L.W., "The Use of Tracers in Sedimentation Basins", M. Eng. Thesis, McMaster University, Hamilton, Ontario (1969).

19. Smith, R., "Preliminary Design and Simulation of Conventional Waste Water Renovation Systems Using the Digital Computer", Water Pollution Control Research Series WP-20-9 F.W.P.C.A./U.S.D.I. (Washington, 1968).

20. Silveston, P.L. "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research, 6, 1101 (1972)

21. Goering, S.W., "A Computer Model of the Sewage Treatment Process of Boulder Colorado", M.Sc. Thesis, Dept. of Chem. Eng., Univ. of Colorado (1972).

22. Voshel, D. and Sak, J.G., "Effect of Primary Effluent Suspended Solids d BOD on Activated Sludge Production", J.W.P.C.F. 40, Part 1, 203 (1968).

23. Chen, G.K., Fan, L.T. and Erickson, L.E., "Computer Software for Wastewater Treatment Plant Design", J.W.P.C.F. 44, 747 (1972).

24. Tracy, K.D. and Keinath, T.M., "Dynamic Model for Thickening of Activated Sludge", Paper, 74th National Meeting, A.I.Ch.E., New Orleans (March, 1973).

25. Scott, K.J., "Mathematical Models of Mechanism of Thickening", Ind. and Eng. Chemistry Fund, 5, 109 (1966).

26. Dick, R.I. and Ewing, B.B., "Evaluation of Activated Sludge Thickening Theories", J. Sanitary Eng. Div., Proc. A.S.C.E. 93, SA4, 9 (1967).

27. Edde, H.J. and Eckenfelder, W.W., Jr., "Theoretical Concepts of Gravity Sludge Thickening and Methods of Scale-up from Laboratory Units to Prototype Design", Tech. Rep't. EHE-02-6701, CRWR-15, Center for Research in Water Resources, Univ. of Texas (1967).

28. Eckenfelder, W.W. Jr., and Mancini, J.L., "Thickening of Industrial Sludges", Proc. 5th Texas Industrial Water and Waste Conf. (1965).

Chapter 8

29. Roberts, E.J., "Thickening - Art or Science", Mining Eng., 1, 61 (1949).

30. Smith, R. and Eilers, R.G., "A Generalized Computer Model for Steady State Performance of the Activated Sludge Process", FWQA Report No. TWRC-15, Cincinnati Water Research Laboratory, Cincinnati, Ohio (1969).

31. Planz, P., "The Sedimentation of Activated Sludge in Final Settling Tanks", J. Int. Assocn. of Water Pollution Research, 2, No. 1, 80 (1968).

32. Fan, L.T., Chen, G.K.C., Erickson, L.E. and Naito, M., "Effects of Axial Dispersion on the Optimal Design of the Activated Sludge Process", Water Research 4, 271 (1970).

33. Naito, M., Takamatsu, T. and Fan L.T., "Optimization of the Activated Sludge Process-Optimum Volume Ratio of Aeration and Sedimentation Vessels", Water Research 3, 433 (1969).

34. Rex Chainbelt Inc., "A Mathematical Model of a Final Clarifier", Water Pollution Control Research Series No. 17090 FJW, E.P.A. (Washington, D.C., 1972).

Chapter 9

1. Eckenfelder, W.W., Jr. and O'Connor, D.J., "Biological Waste Treatment", Pergamon Press (New York, 1961).

2. Eckenfelder, W.W., Jr. and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970).

3. "Biological Waste Treatment", Notes for a course at the University of Waterloo (July, 1967).

4. Eckenfelder, W.W., Jr. and McCabe, Joseph (Editors), "Advances in Biological Waste Treatment", MacMillan Co. (New York, 1963).

5. "Water Pollution Research", Dept. Scient. and Indust. Research, H.M. Stationary Office (London, 1967), also 1968.

6. "Design Guides for Biological Wastewater Treatment", Water Pollution Control Research Series, 11010 ESQ, 08/71, U.S. Environmental Protection Agency (Washington, D.C., 1971).

7. Eckenfelder, W.W., Jr., "Biological Treatment of Waste Water", Adv. in Hydroscience, Vol. 3, Academic Press (New York, 1966)

8. Himmelblau, D.M. and Bischoff, K.B., "Process Analysis and Simulation", John Wiley (New York, 1968).

Chapter 9

9. Silveston, P.L., "Use of Residence Time Distributions for Design of Aerobic Waste Treatment Units", Proc. 1st Annual Symp. Water Pollution Res., (Univ. of Waterloo, 1966).

10. Murphy, K.L., "Significance of Flow Patterns and Mixing in Biological Waste Treatment in Canale, R.P. (Editor), "Biological Waste Treatment", Interscience Publ. (New York, 1971).

11. Monod, J., "The Growth of Bacterial Cultures", Ann. Rev. of Microbiology, 3, 371 (1949).

12. Smith, Robert, and Eilers, R.G., "A Generalized Computer Model for the Steady State Performance of the Activated Sludge Process", Division of Research, Report, F.W.P.C.A., U.S. Dept. of the Interior (October, 1969).

13. Fan, L.T., Chen, G.K.C., Erickson, L.E. and Naito, M., "Effects of Axial Dispersion on the Optimal Design of the Activated Sludge Process", Water Research, 4, 271 (1970)

14. Chiu, S.Y., Erickson, L.E., Fan, L.T., and Kao, I.C., "Kinetic Model Identification in Mixed Populations Using Continuous Culture Data", Biotech. and Bioeng., 14, 207 (1972)

15. Naito, M., Takamatsu, T. and Fan, L.T., "Optimization of the Activated Sludge Process - Optimum Volume Ratio of Aeration and Sedimentation Vessels", Water Research, 3, 433 (1969)

16. Downing, A.L., Painter, H.A. and Knowles, B.A., "Nitrification in the Activated Sludge Process", J. of Inst. of Sewage Purification, Part 2, 130 (1964)

17. Kalinske, A.A., "Power Consumption for Oxygenation and Mixing", in Eckenfelder and McCabe (Editors), "Advances in Biological Waste Treatment", Macmillan (New York, 1963).

18. Silveston, P.L., "Simulation of the Mean Performance of Municipal Waste Treatment Plants", Water Research 6, 1101 (1972)

Chapter 10

1. Lancaster, E.A., Silveston, P.L., Drynan, W.R. and Jank, B.E., "Plastic Packed Trickling Filter Under Canadian Climatic Conditions", Pulp and Paper, Dec. 6, 58 (1968).

2. Kornegay, B.H. and Andrews, J.F., "Kinetics of Fixed Film Biological Reactors", J.W.P.C.F. 40, No. 11, R460 (1968).

3. ibid, "Application of the Continuous Culture Theory to the Trickling Filter Process", Proc. 24th Ind. Waste Conference, Eng. Ext. Series, Purdue Univ., Lafayette, Ind. (1969).

Chapter 10

4. Kornegay, B.H., "Modelling and Simulation of Fixed Film Biological Reactors", 8th Annual Workshop of the Assn. of Envir. Eng. Professors, School of Civil Engineering, Georgia Tech., Atlanta, Georgia (1972).

5. Roesler, J.F. and Smith, Robert, "A Mathematical Model for a Trickling Filter", Publ. W69-2, F.W.P.C.A., U.S. Dept. of the Interior (February, 1969).

6. K. Imhoff and G.M. Fair, "Sewage Treatment", 2nd Edition, John Wiley (New York, 1956).

7. Industrial Research Institute, "The Operation and Performance of 'Flocor' Packed Biological Filters Under Canadian Climatic Conditions" Research Report, University of Waterloo, (1969).

8. Howland, W.E., Pohland, F.G. and Bloodgood, D.E., "Kinetics in Trickling Filters" in Eckenfelder and McCabe, "Advances in Biological Waste Treatment", MacMillan Co. (New York, 1963).

9. Atkinson, B., Swilley, E., Busch, A., and Williams, D., "Kinetics, Mass Transfer and Organism Growth in a Biological Film Reactor", Trans. Inst. of Chem. Engs. 45, T 257 (1967).

10. Sinkoff, M., Porges, R. and McDermott, J., "Mean Residence Time of Liquid in a Trickling Filter", J. San. Eng. Divl, A.S.C.E. 85, 662 (1959).

11. Design Guides for Biological Wastewater Treatment Processes", Water Pollution Control Research Series - 11010 ESQ 08/71, Environmental Protection Agency (Washington, D.C., 1971).

12. Hawkes, H.A., "The Ecology of Waste Water Treatment", Pergamon Press (New York, 1963).

13. "Biological Waste Treatment", Notes for a Technical Seminar, University of Waterloo, Waterloo, Ontario (1967).

14. Velz, C.J., "A Basic Law for the Performance of the Trickling Filters", Sewage Works, 20, No. 4, 607 (1948).

15. Stack, V.T., Jr., "Theoretical Performance of the Trickling Filter Process", Sewage Industrial Wastes, 29, No. 9, 987 (1957).

16. Behn, V.C., "Trickling Filter Formulations" in Eckenfelder and McCabe, "Advances in Biological Waste Treatment", MacMillan (New York, 1963).

17. Schulze, K.L., "Elements of a Trickling Filter Theory", in Eckenfelder and McCabe "Advances in Biological Waste Treatment", MacMillan (New York, 1963).

Chapter 10

18. Eckenfelder, W.W., Jr., "Trickling Filter Design and Performance", J. Sanitary Eng. Div., Proc. A.S.C.E., 87, 33 (1961).

19. Eckenfelder, W.W. and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970).

20. Jank, B.E. and Drynan, W.R., "Substrate Removal Mechanism of Trickling Filters", J. Environ. Eng. Div., Proc. A.S.C.E., 99, No. EE3, 187 (June, 1973).

21. Fairall, J.M., "Correlation of Trickling Filter Data", J. Sewage and Ind. Wastes, 28, 1069 (1956).

22. Rincke, G., "Neuere Gesichtspunkte zur Abw asserreinigung mit Tropfkorpern", Das Gas v. Wasserfach, 108, No. 24, 667 (1967).

23. Bruce, A.M. and Merkens, J.C., "Recent Studies of High Rate Biological Filtration", Water Pollution Control (London), 113 (1970).

24. Autotrol Corp., "Application of Rotating Disc Process to Municipal Wastewater Treatment", Water Pollution Control Research Series, 17050 DAM 11/71, Environmental Protection Agency (Washington, 1971).

Chapter 11

1. Andrews, J.F., "Dynamic Model of the Anaerobic Digestion Process", J. Sanitary Eng. Div., Proc. Am. Soc. Civil Eng., 95, SAI, 95 (1969).

2. Andrews, J.F., "A Mathematical Model for the Continuous Culture of Microorganisms Utilizing Inhibitory Substances", Biotech. and Bioeng., 10, 707 (1968).

3. Andrews, J.F. and Graef, S.P., "Dynamic Modelling and Simulation of the Anaerobic Digestion Process", Advances in Chemistry Series, 105, 126 Am. Chem. Soc. (Washington, D.C. 1971).

4. McCarty, P.L., "Anaerobic Waste Treatment Fundamentals - Part I to IV in successive issues of Public Works, beginning Sept.: 1964.

5. Pohland, F.G. and Bloodgood, D.E., J.W.P.C.F., 35, 11 (1963).

6. Pohland, F.A. and Ghosh, S., "Developments in Anaerobic Treatment Processes", in Canale, R.P. (Editor) "Biological Waste Treatment", Interscience Publ. (New York, 1971).

7. Smith, R., "Preliminary Design and Simulation of Conventional Wastewater Renovation Systems Using the Digital Computer", Water Pollution Control Res. Series, WP-20-9, F.W.P.C.A. (Washington, D.C., 1968).

Chapter 11

8. Eckenfelder, W.W. Jr. and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970).

9. Imhoff, K., and Fair, G.M., "Sewage Treatment" 2nd Edition, John Wiley (New York, 1956).

10. Pohland, F.G., "General Review of Literature on Anaerobic Sewage Sludge Digestion", Engineering Extension Series, No. 110 Purdue University (Lafayette, Indiana).

11. Eckenfelder, W.W., Jr. and O'Connor, D.J., "Biological Waste Treatment, Pergamon Press (New York, 1961).

12. Bolz, R.E. and Tuve, G.L., (Editors), "Handbook of Tables for Applied Engineering Science", Chemical Rubber Co. (Cleveland, 1970).

Chapter 12

1. Imhoff, K. and Fair, G.M., "Sewage Treatment", 2nd Edition, John Wiley (New York, 1956).

2. Anonymous, "Sewage Treatment Plant Design", A.S.C.E. and W.P.C.F. (1959).

3. Perry, J.H. (Editor), "Chemical Engineer's Handbook", 4th Edition, McGraw-Hill (New York, 1968).

4. Weber, W.J., Jr., "Physicochemical Processes for Water Quality Control", Wiley-Interscience (New York, 1972).

5. Susag, R.H., Sew. and Ind. Wastes 40, 434 (1968).

Chapter 13

1. Burd, R.S., "A Study of Sludge Handling and Disposal", Publication WP-20-4, Water Pollution Control Research Series, F.W.P.C.A.-U.S.D.I., U.S. Gov't Printing Office (Washington, D.C.,1968)

2. Balakrishnan, S., Williamson, D.E. and Okey, R.W., "State of the Art Review on Sludge Incineration Practice", Water Pollution Control Research Series" 17070 DIV 04/70, F.W.Q.A.- U.S.D.I., U.S. Gov't Printing Office (Washington, D.C.,1970)

3. Genter, A.L. "Conditioning and Vacuum Filtration of Sludge", Sewage and Industrial Wastes, 28, No.7,829 (1956)

4. Smith, R., "Preliminary Design and Simulation of Conventional Wastewater Renovation Systems Using the Digital Computer", Publication WP-20-9, Water Pollution Control Research Series, F.W.P.C.A.-U.S.D.I., U.S. Gov't Printing Office (Washington, D.C.,1968)

Chapter 13

5. Imhoff, K. and Fair, G.M., "Sewage Treatment", 2nd Ed. John Wiley & Sons (New York, 1956)

6. McLaren, J.W., "Evaluation of Sludge Treatment and Disposal", Canadian Municipal Utilities, 23, 51 (May, 1961)

7. Schempman, B.A., and Cornell, C.F., "Fundamental Operating Variables in Sewage Sludge Filtration", Sewage and Industrial Wastes 28 No. 12, 1443 (1956)

8. McCabe, W.L., and Smith, J.C., "Unit Operations of Chemical Engineering", 2nd Edition, McGraw-Hill (New York, 1967)

9. Eckenfelder, W.W., and Ford, D.L., "Water Pollution Control", Pemberton Press (Austin, Texas, 1970)

10. Genter, A.L., "Computing Coagulent Requirements in Sludge Conditioning", Trans. Am. Soc. Civil Engrs., 71, 307 (1945)

11. Unterberg W., Sherwood, R.J. and Schneider, G.R., "Computerized Design and Cost Estimation for Multiple-Hearth Sludge Incinerators", Report 17070 EBP 07/71, Water Pollution Control Research Series, U.S. Environmental Protection Agency, U.S. Government Printing Office (Washington, D.C.,1971)

Appendix A

1. Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control 69, No.6, 686 (1970).

Appendix B

Nil

ACKNOWLEDGEMENT

Preparation of an acknowledgements always comes near the end of a writing job so it affords the double pleasure of knowing that the job will soon be over and of expressing thanks to those who either made the job possible or assisted in its execution.

Our thanks go first of all to the contract officer for the project, Mr. Alex Redekopp, Chief, Training and Technology Transfer Division, Water Pollution Control Directorate, Environmental Protection Service of Environment Canada for his patience and many not-so-subtle prods to greater activity. Mr. Redekopp also handled the tedious arrangements for the Workshop which these Notes, of course, were prepared for. It's a pleasure to acknowledge the help of Mr. Redekopp's editorial staff in Ottawa - Mr. Boris Woloschuk and Vicky Jones - for their assistance in those most difficult of all subjects: writing style, English grammar and spelling.

The modelling chapters were materially aided by discussions with the writers colleagues at the University of Waterloo: Professors Scharer, Drynan and Farquhar. Competent and most helpful reviews of the text and models were undertaken by Professor W.R. Drynan (Chapter 11 - Digestion), Dr. Bruce Jank of C.C.I.W. (Chapter 10 - Trickling Filters), and Mr. K.C. Lin and Professor G.W. Heinke of the University of Toronto (Chapter 9 - Activated Sludge Units). Robert Smith, Chief, Treatment Optimization Research Program at the National Environmental Research Center in Cincinnati, Ohio reviewed the complete text and the workshop plan.

The writer of these Notes was first introduced to the subject of simulation and computer-aided design through a workshop held in Dartmouth College in 1967 and conducted by Professors Crowe and Hoffman of McMaster University, Dean Johnson of the University of Western Ontario, and Professor Shannon of Dartmouth. The approach adopted in Chapters 3 to 6 of these Notes and, indeed, some of the material can certainly be traced to this early workshop. The writer has also used material, particularly in Chapters 4 & 5, from a book "Chemical Plant Simulation", Prentice Hall (1971),written by the organizers of the same Dartmouth Workshop. This book is an excellent introduction to the general topic

of process simulation. The writer's understanding of computer-aided methods has been further enriched by teaching experience at the University of Waterloo and projects held both at the University of the Witwatersrand and at the National Institute for Water Research in South Africa.

Past and present colleagues at B & P Silveston, Engineers - Messrs. Ken Birkett, Phil Wood, and Jim Allan - all assisted with phases of the project. The skill and persistance of our secretary, Ms. Bonnie Armour, in preparing the many revisions the Notes underwent must be mentioned and in this way most inadequately acknowledged. She was ably assisted in this task by Ms. Gaye Henry and Judy Tam.

APPENDIX A

USER'S MANUAL FOR SEPSIM

A USER'S MANUAL FOR SEPSIM

A.1 Introduction

The purpose of this manual is to assist you in applying SEPSIM to your process system. Following this brief introduction to process applications of executive computer programs, we will deal with the operation of the Executive, discuss steps involved in formulating your process system for SEPSIM and finally we will examine data preparation for the program.

Information on the effect of equipment or feed stream changes on process performance is useful for many engineering purposes. This type of information is the result of simulation. Simulation presumes a process arrangement, equipment sizes, operating conditions, and feed stream flows and compositions. It provides the flows and compositions of product streams or indeed any stream in the process. Design, on the other hand, seeks the type, operation and size of equipment to achieve a specified product when the feed streams are known. Design and simulation are related in many ways. Both can make use of the same models. Both are amenable to handling by computer. Design may be handled by successive simulation in which equipment type and size are varied until the overall performance is achieved. Usually, however, design is carried out by selecting criteria for each unit of the process and sizing the unit directly from these criteria, using simulation to check on the results.

A process consists of units and a network which represents the arrangement and interconnection of the individual units. Units operate to change the compositions, conditions and flow in the network streams. They may be considered as information modifiers acting on the information content of the streams. The information content in this terminology, is the composition of a stream, its temperature and pressure and its flow. Process simulation or computer-aided design, therefore, must provide a means of encoding for the computer the information content, the modifying action of individual process units, and the network.

The "modifying action" of process units is encoded by computer models for different types of units. A model for a unit is a mathematical statement of the properties of unit output streams in terms of the properties of unit input streams, expressed in language which can be processed by a computer. We will refer to such models as process model subroutines.

"Simulation", as it concerns us here, denotes a special way to find the properties of the streams in the process when the process units are operating at steady-state, for given process unit parameters and constant inputs to the system. Therefore the mathematical models for the process units need not be valid for dynamic, but only for steady state, operation. Starting with initial estimates for the properties of the streams, provided by the user, a simulation program repeatedly modifies this information by applying the mathematical process models to it, in the order determined by the process network information provided by the user, until the stream properties no longer vary outside of tolerances provided by the user. This is analogous to solving a large set of simultaneous equations by iteration. Usually the solution converges easily, but in some cases the user must try different initial estimates and process model calculation sequences to obtain convergence within the desired tolerance.

As the properties of the streams change from their initial estimates to their final steady-state values, they appear to describe some dynamic behaviour; but of course this is <u>not</u> a valid interpretation unless the mathematical models are valid for dynamic processes and some method is incorporated for measuring the passage of time. The simulation of dynamic behaviour is outside the scope of this manual.

The best sequence for the process models to be applied to the process stream information is usually similar to the path of material as it flows through the process network. Where a feedback loop occurs, calculations should proceed around the loop repeatedly until it attains steady state. Where nested loops occur, the inner ones should be brought to steady state before the outer ones. Where parallel paths occur, calculations should alternate between one path and the other, this being a compromise between the actual flow and the sequential nature of computation. When the end of the process is reached, calculations should start again at the beginning of the first feedback loop in order to converge further upon the steady-state stream properties: thus we think of an imaginary feedback loop going from the process' end to its beginning. So long as this outside loop is used, satisfactory convergence is often obtained even if the process models are applied in any arbitrary sequence.

The process network is therefore encoded in the simulation for two pusposes: to relate the inputs and outputs of different units, and

to determine the sequence in which the process models are applied to the stream information.

Two quite different ways can be used to encode the process network. The first of these is to use directed GØ TØ statements which would link the models together so as to actually reproduce the network in the logic of the computer program. A separate program would have to be written for each process. Developing a design or simulation program for a complex network would be a time consuming and costly exercise. Thus, this first approach is not widely used.

The second way of handling the network is to encode it in a matrix which can be read in to simulation or design programs as data. This approach is basically modular and leads to an executive program which reads in the network and other information needed in the job, orders calculations, calls in subroutines to perform the computations, and prints out the results. The matrix used to encode the network is commonly called, appropriately, the process matrix.

SEPSIM is an executive program of the character just described. It reads in parameters of the models used; compositions, conditions and flows of input streams, convergence tolerances for iterative calculations, and a process matrix of course. SEPSIM performs no network analysis nor does it attempt to optimize the calculation sequence. These functions, often found in executive programs, were omitted to keep the program a reasonable size and to leave this instructive task to students. SEPSIM, after all, was originally developed as an educational tool.

Of course, SEPSIM is but one of a number of executives available. All have the same objective of simplifying the engineer's effort in simulation or in design by reducing the programming required and by organizing the computation algorithms. SEPSIM differs from other executives because of its simple way of arranging computations. Advantages of SEPSIM come from its brevity and simplicity. It may be employed for many process systems with computers of just modest core capacity without resorting to overlays. Input of information is logical and simple so as to minimize the curse of input "bugs". Similarly, the output is complete and well ordered. Information printed is identified. Input data is printed along with the output to facilitiate the latter's use. Finally, the structure

of the Executive is simple so that it may be easily altered to meet special needs.

SEPSIM is by no means a static development. There are two basic versions of the Executive currently offered, both performing the same task:

WATFIV version - for use only on computer systems with a WATFIV Fortran IV processor, this version uses WATFIV extensions to the Fortran language, resulting in slightly easier use than would otherwise be possible.

Standard version - for use on computer systems with any Fortran IV processor, this version uses the American standardized Fortran language (USASI or ANSI Fortran).

The WATFIV version is customarily preferred on systems where it can be used. The Standard version was developed to permit more widespread use of SEPSIM. It is at least as efficient as the WATFIV version, but requires slightly more effort to understand, owing to its more intricate use of the standard Fortran statements. Due to its more widespread use, the Standard version of SEPSIM receives more attention for new improvements than the WATFIV version. Thus, for example, the input/output operations of the two versions are quite different.

As a user, you may wish to change one of these versions of the Executive to adapt it to your special needs. To assist you in doing this, comprehensive documentation has been built into the Executive, but further, a listing of the current versions and a logical flow diagram for the program are included in this manual.

Either version of the SEPSIM executive is very efficient in terms of computer time and storage. The "object program" requires only about 20K for storage, and with present dimensions the arrays require about 10K. Typical waste treatment processes, consisting of 6 process units, require an additional 10K for process subroutine storage, and execute in under one second on an IBM 360.

A.2 Structure And Operation (WATFIV Version)

A.2.1 General:

An understanding of how the Executive operates can assist you in mastering data required for a SEPSIM run and how it must be organized. A thorough understanding is essential if the Executive is to be altered.

SEPSIM is a modular executive program and it consists of the following components:

Mainline Program -

a) reads in data

b) relates units to appropriate model subroutines

c) initiates calculations

d) identifies recycle (or feedback) in networks and sets up iterative calculations

e) orders sequence of calculations

f) tests for convergence of iterative calculations

g) transfers information to and from storage

h) determines when calculations are complete

i) calls other SEPSIM components.

NØMEN Subroutine -

Sole function is to set up model subroutine names in a vector used by the mainline program to relate process units with models.

SELECT Subroutine -

This is a calling subroutine which calls model subroutines when they are required for computations by the mainline program.

RPRINT Subroutine -

a) reads in definitions of the abbreviations used in output printing

b) prints well formatted results, a portion of the input data and the list of definitions in a).

Model Subroutines -

Subroutines for all the models named in the calling statements in SELECT are provided...these are not usable process subroutines, but so-called "dummies" required by programming technicalities.

The NØMEN and SELECT subroutines were built into SEPSIM as sub-programs to permit different numbers of model subroutines to be used as well as to allow different names to be employed without reprogramming the mainline part of SEPSIM. NØMEN splits out the last three alphanumeric characters in the model names and places these in the vector NAME(I). This vector is used by the mainline program to give a model subroutine index to each unit in the process network under study.

SELECT, as the listing in section A.6 shows, starts with a computed GØ TØ statement which sets up the calling of specific model subroutines. The index, NDX, which is defined in the mainline program just before SELECT is called is used in the computed GØ TØ statement so that it functionally selects the model subroutine to be used.

SELECT and NØMEN have provision for 50 subroutine names in the current version; however, only 42 are actually used. The number of model subroutines is controlled by the dimension statements, but any change in dimension will necessitate changes in SELECT and NØMEN. New names can be introduced or names replaced by adding the name to the NØMEN INTEGER statement and adding a call statement to SELECT or, if a replacement is involved, replacing names in the INTEGER and in the SELECT CALL statements. This is discussed in detail in Section A.4.5.

Since users may want to set up output printing to satisfy their special requirements, the printing function has been separated from the mainline program. A user may write his own RPRINT subroutine, employ the RPRINT furnished with SEPSIM or modify it to suit his needs.

The RPRINT subroutine currently used with SEPSIM prints out all of the stream information and the equipment parameters at the end of the simulation. These matrices will contain normally all the results sought for in a simulation or design. As you can see from the sample print-out in section A.6, the components in the stream matrix are identified by a suitable abbreviation. Similarly, the parameters in the equipment matrix are also identified. To assist the location of streams the process matrix is also printed out. This matrix is, of course, part of the input data.

A list of definitions of the abbreviations used in the print-out (or any other documentation) can be placed at the head of the print-out sheet if the user wishes. The user must submit this documentation at the end of his input data. RPRINT reads these definitions after it is called and prints them out immediately. RPRINT will function without the list so that the inclusion of definitions in the print-out is a user option. We recommend use of the option because it contributes appreciably to the comprehension of the print-out.

Whenever a process model subroutine is actually required for a simulation, it must be made to replace the dummy subroutine of the same name provided by the executive.

A.2.2 Important Arrays:

Simulation and design frequently requires large amounts of information. The information must be stored and must be readily accessible to the various subroutines which form the modular executive. SEPSIM meets these requirements by providing storage blocks in core through a COMMON statement. The user does not have to dimension this storage, but he can change block size by altering the DIMENSION statements. The storage blocks are:

(a) Stream Matrix - SN (75,25)

Every stream in the process network is represented by a row in the SN matrix. The DIMENSION statements in the current version allow for networks of up to 75 streams. The columns can be used to represent any information about the streams that the user may like, with the exceptions that column 1 must contain the stream number (this number designates a specific stream in the network) and that column 2 should be left blank. The column dimension of 25 thus permits up to 23 entries for each stream. One possible way to use these entries is shown in Table 1. Column use is referred to as the stream information or property vector. The vector used in the WATCRAP waste treatment plant simulations is shown in Table A-1. Notice that the vector contains the flow rate, concentrations carried by the stream and the condition (Temperature). Properties such as enthalpy or density could also be included.

(b) Equipment Matrix - EN (20,20)

Every unit in the process network (with the exception of Dummy units) is represented by a subroutine performing calculations required for the unit. Likewise, each process unit has a corresponding row in the EN matrix containing all the equipment dependent parameters needed or produced by the subroutine. Such parameters would be vessel dimensions, operating conditions and constants in mathematical models. They could also be design criteria or performance results if a design model is used. Two similar units can thus use the same subroutine if the differences between them are only the values of these parameters. Furthermore, two identical units can be represented by the same EN

TABLE A-1: STREAM VECTOR FOR WASTE TREATMENT APPLICATIONS

Column	Description
1	Stream number
2	
3	Volumetric flow (millions of gallons per day)
4	Suspended Nonbiodegradable Carbon
5	Dissolved Nonbiodegradable Carbon
6	Suspended Organic Carbon (mg./l.)
7	Dissolved Organic Carbon
8	Suspended Organic Nitrogen
9	Dissolved Nitrogen
10	Suspended Organic Phosphorus
11	Dissolved Phosphorus
12	Suspended Fixed Matter
13	Dissolved Fixed Matter
14	Suspended Biological Oxygen Demand (BOD)
15	Dissolved BOD
16	Total Suspended Solids
17	Temperature, degrees (^{o}F)
18	Volatile Suspended Solids
19	Alkalinity

vector, assuming that any equipment results produced by the subroutine will also be identical.

The first column is reserved for the equipment number, and the second for the vector length. Thus, the dimensions of EN allow 18 parameters for each equipment vector. In all, 20 equipment vectors can be handled in the current version of SEPSIM. Table A-2 shows a row from one of the process unit subroutines used in the WATCRAP simulation[1]. Note that the last two entries in Table A-2 are process performance information calculated by the subroutine. The EN vector may be used also to store cost information and results. Note that elements of EN

(1) Silveston, P.L., "Digital Computer Simulation of Waste Treatment Plants Using the WATCRAP-PACER System", Water Pollution Control 69, No. 6, 686 (1970).

calculated during the simulation are not tested for convergence.

TABLE A-2: EQUIPMENT VECTOR FOR THE WATCRAP SIMULATION OF A TRICKLING FILTER

Column	Parameter
1	Equipment Number
2	Number of Parameters in Equipment Vector (e.g. 10 here)
3	Specific Surface Area of Filtration Media
4	Depth of Filter Bed
5	Filter Bed Diameter
6	Rate Constant for Biological Activity on Carbon
7	Rate Constant for Biological Activity on Nitrogen
8	Minimum BOD Value Obtainable
9	Fractional Reduction in BOD
10	Fractional Reduction in Nitrogen

(c) Additional Data Matrix - AEN (2,40)

In the unlikely event that a process unit needs more parameters than a row in the EN matrix can carry, the AEN matrix may be used for storage of the additional data. Column 1 must contain the AEN row number (i.e. 1 or 2). We have made use of the AEN matrix to store a table of operating data which is fitted in the process unit subroutine to provide an empirical model for that process unit. Thirty-nine data points may be stored in each AEN row with the dimensions now used. More than one subroutine could use AEN in one simulation.

(d) Erasable Working Storage Matrices - PAPER (2,10) and NPAPER (20)

These two matrices are placed in COMMON to provide storage for calculations done within a model subroutine. PAPER provides 20 entries while NPAPER provides an equal number of integer or alphanumeric entries. Since the matrices are not erased when a new subroutine is called, they can be used to transfer information between subroutines or between successive passes during iterative calculations. Some care is necessary to prevent unintentional erasing of numbers in PAPER if this transfer property is used because more than one subroutine may use PAPER for inter-

mediate calculations. If the same elements in PAPER are used, numbers first transferred into PAPER will be replaced by any numbers subsequently transferred.

(e) Stream Input and Output Matrices

The user-written subroutines can operate directly on the SN matrix, but to promote their use in more than one process network they should be written so that they do not. To avoid direct use of SN, SEPSIM places the appropriate SN values for the NIN process unit input streams in STRMI (5,25) and the NØUT output streams in STRMØ (5,25) when the unit model is to perform its calculation. Each process model subroutine should be written in terms of STRMI and STRMØ. NIN and NØUT may not exceed 5. After the transfer into STRMI and STRMØ, a model subroutine will be called to compute STRMØ from the given STRMI. The values of STRMØ from the previous iteration are also available for this calculation. The newly calculated values of STRMØ replace the transferred values and may enter a convergence test performed by SEPSIM using the values in SN for the streams in question. After the convergence test, the STRMØ values replace the corresponding entries in the SN matrix.

(f) Process Matrix - NPROCS (14,50)

The key to the operation of SEPSIM lies with the process matrix. This is the matrix which encodes the process network and controls the sequence of computations in a design or a simulation. The matrix contains 14 columns:

PROCESS MATRIX

		Subroutine		Input Streams					Output Streams				
K	NE	Names	III	1	2	3	4	5	1	2	3	4	5

Each row of the matrix determines the application of a process model subroutine to modify the process stream properties.

The first column in the matrix is referred to as the K column. This column, the 4th column (the III column) and the order of the process matrix rows control the calculational sequence. This is discussed in detail in Section A.4.4. The second column contains the equipment number NE. This number identifies the equipment vector to be used in the calculation,

and is submitted in the data as the first element of the vector. The third column contains the name of the subroutine used to model the process unit. Columns 5 to 9 contain the assigned numbers of the process unit input streams, while columns 10 to 14 contain those of the process unit output streams. There are no rules in numbering streams, except that each stream should have a different number.

(g) Equipment Parameter Names - NAMEN (20,20)

This array simply stores the 4-character symbols to be placed beside each member of EN that appears in the printout. We mention it here to explain how it is handled and facilitate the comparison, made in Section A.3, with the way it is handled in the standard version.

A different row of NAMEN must be available for each process model subroutine used in a simulation. The programmer who writes the process model subroutine determines its equipment parameter names, using a DATA statement in the subroutine. But the user, generally a different person unknown to the programmer, determines the array EN. So usually the rows of NAMEN and EN do not correspond in order. The exact correspondence is established by the statement KEY(NE) = (some integer), included in the subroutine, where the value given to KEY(NE) is the row of NAMEN in which the parameter names are stored (by the DATA statement) for any equipment vector EN(NE,-) used with this subroutine. The user must make sure that each subroutine used in a simulation assigns a different value in the KEY(NE) statement, and that if this is modified the DATA statement is modified to match.

A.2.3 Logical Flow:

The operation of the executive is illustrated best by an outline of its logical flow shown as Figure A-1. If you prefer to follow the listing, it is given in section A.6.1. Table A-3 is an explanation of the internal control parameters of the mainline program which may help you to understand Figure A-1 or the listing.

The main program begins by calling the NØMEN subroutine, which sets up the vector NAME (I) from a list of allowable subroutine names. After this has been accomplished, all storage arrays are initialized to

zero. All numbers which were in the arrays are wiped out. Input values for the stream matrix (SN) are read in next. These values will be the stream vectors for all the feed streams and, at the user's option, guess values for other streams in the network. Following the SN matrix, the equipment matrix (EN), the additional equipment matrix (AEN) and the vector of convergence tolerances are read into their storage blocks in order.

The read-in functions end with the input of the process matrix. The process matrix is read a single line at a time. The first four columns provide values for the loop number (K), the equipment number (NE), the model index (NDX) and the iterative calculation indicator (III). The last three characters of the model name in column 3 of the process matrix are compared with the vector NAME (I) in an IF statement. When a match is found, NDX is set equal to I. As we have indicated previously, NDX is used in SELECT to call a specific model subroutine. Thus, we have replaced the subroutine name in the process matrix by the "location" of the subroutine.

The Executive's final function before beginning the calculations is to set the indicators shown in Table A-3 to zero.

The Executive assumes that the process units are sequentially ordered in the process matrix according to the main flow of information. SEPSIM reads the first row of this matrix to begin calculations. If the first column contains a zero, this unit will not be in a recycle loop. The executive will call the appropriate subroutine via the SELECT subroutine, execute the calculations and transfer the resulting stream values to the SN matrix, filling new rows of this matrix. When a recycle loop is encountered ($K \neq 0$), INDC is set equal to K, KØUT = 1, the subroutine is called and executed and the resulting stream values tested for convergence with the vector EPS, which is part of the input data. Since they will not converge for the first iteration, IFLUN (IN) will be set to 1. A look at Figure A-1 shows that we will go back to (B) and read in another row of the process matrix. Suppose that we have a nested loop so that the next row will contain a value of $K \neq$ INDC. This is used to indicate nesting of recycle loops and we now let LOOP (IN) = INDC and IN = 1. We reset INDC to the K of the nested loop, set IFLUNK = 1 and KØUT = 1 and call and execute the appropriate subroutine. Convergence will not be found so IFLUN(1) will be set to 1 and another row of the matrix will be

called.

When the last row of the now active inner loop is reached, K = INDC. Then KØUT is incremented to 2. This permits us to return to the first terminal of the nested loop. We iterate the inner loop until convergence is achieved. When this occurs we set INDC to its previous value, decrease IN and KØUT and proceed with calculating any further process units in the outer or primary loop. The end of this loop is found when K = INDC and we return to the beginning of the outer loop. We now iterate on the primary loop, but in each cycle through this loop we must converge the inner or nested loop.

Convergence of the inner loop is indicated by IFLUN(1) = 0, if the outer has also converged, the next pass through the iterative loop sets IFLUNK = 0. We go through the loop again with both indicators showing zero. When the last unit in the outer loop (III = 1) is reached we set INDC = 0. We now return at (C) in Figure A-1 and proceed with the calculations by reading in another row of the matrix.

TABLE A-3: INTERNAL CONTROL INDICATORS IN SEPSIM

Indicator	Explanation
INDC	Number of last calculational loop SEPSIM has started to calculate. If no loop has been started INDC = 0. Note that loops are numbered in SEPSIM by K.
KØUT	Position in loop. KØUT = 0; no loop is being calculated. KØUT = 1; a loop is active. KØUT = 2; end of a loop has been reached.
IN	Nesting level of a loop. SEPSIM allows IN = 10.
IFLUN(IN)	If currently active loop of nesting level IN is to be repeated IFLUN(IN) = 1. If not, IFLUNK(IN) = 0.
IFLUNK	If the outer loop in which the currently active loop is nested is itself to be repeated IFLUNK = 1. If not, IFLUNK = 0.
LOOP(IN)	Identifies loop of nesting level IN.

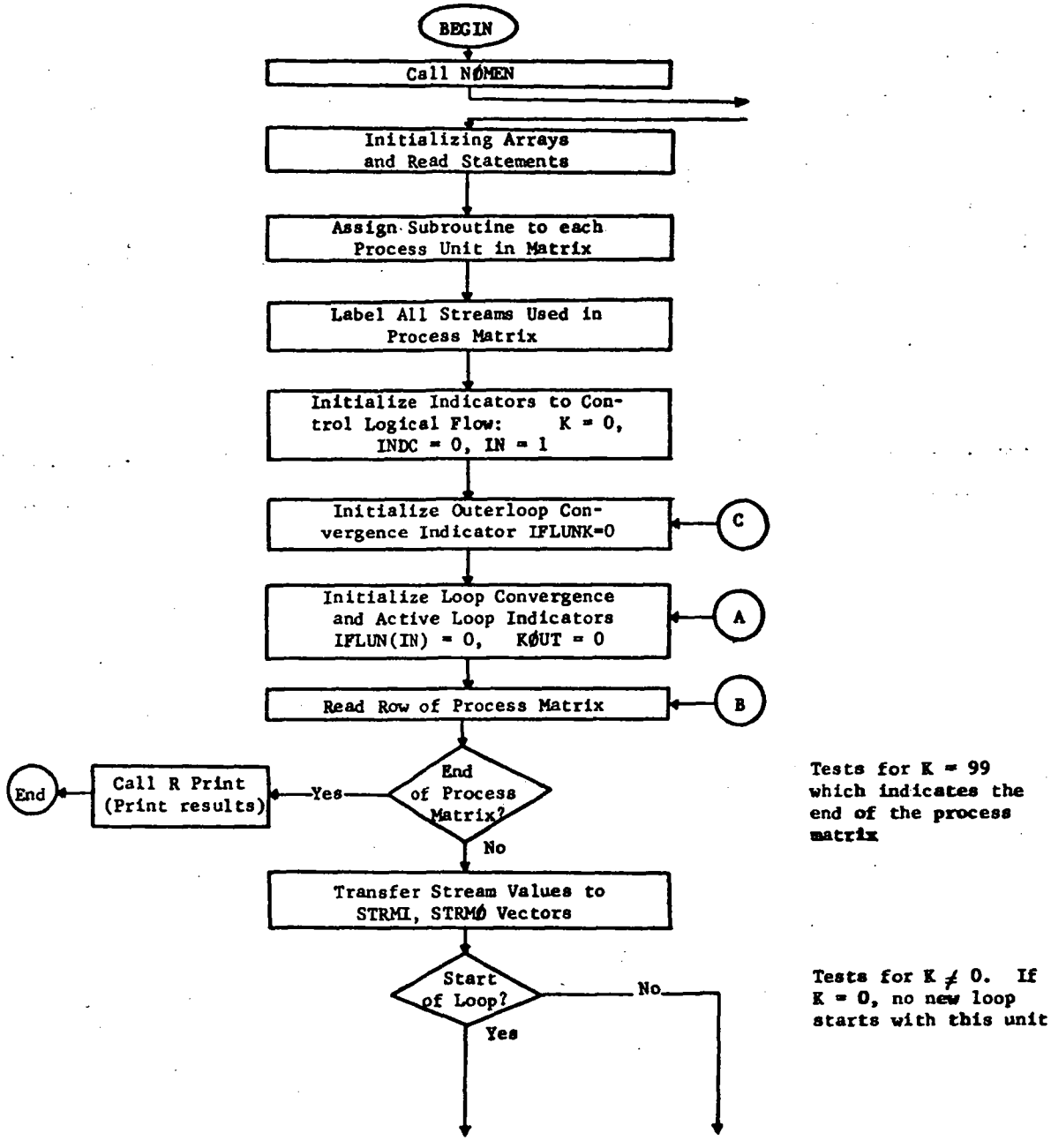
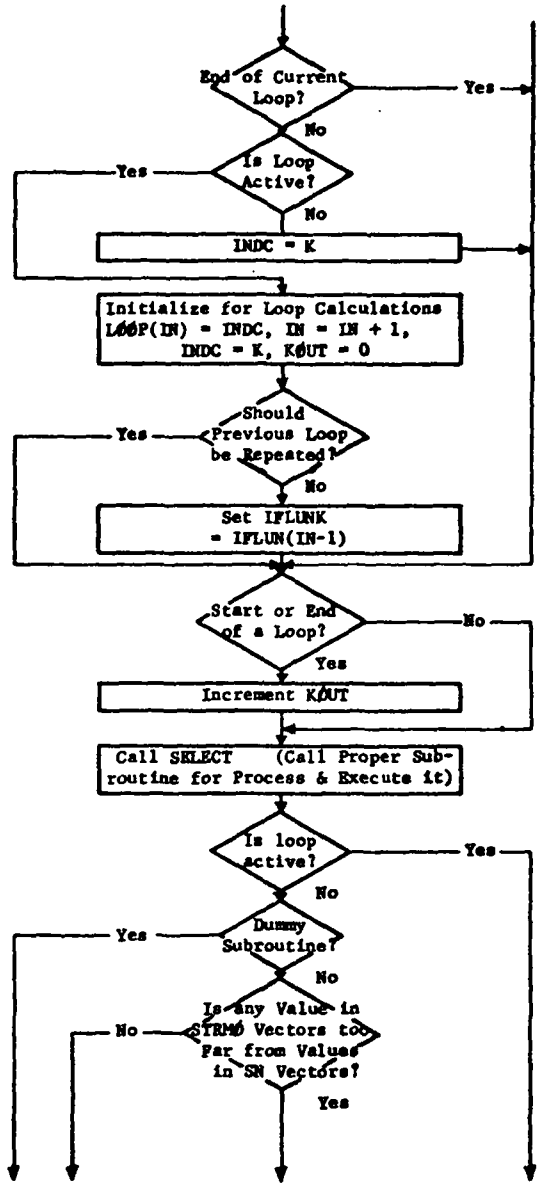


FIGURE A-1. LOGICAL FLOW DIAGRAM FOR SEPSIM.



Tests for K = INDC. If K = INDC, the end of the active loop has been reached.

Tests for INDC = 0.

Tests for IFLUNK = 1. Outer loop is repeated if IFLUNK = 1.

Tests for K = INDC. If K = INDC, the innermost nested loop has been located and will be iterated until convergence reached.

Tests for III = 2. If III = 2, no loop is active and convergence tests can be skipped.

Tests 3rd column for DUMMY.

Convergence test using EPS vector

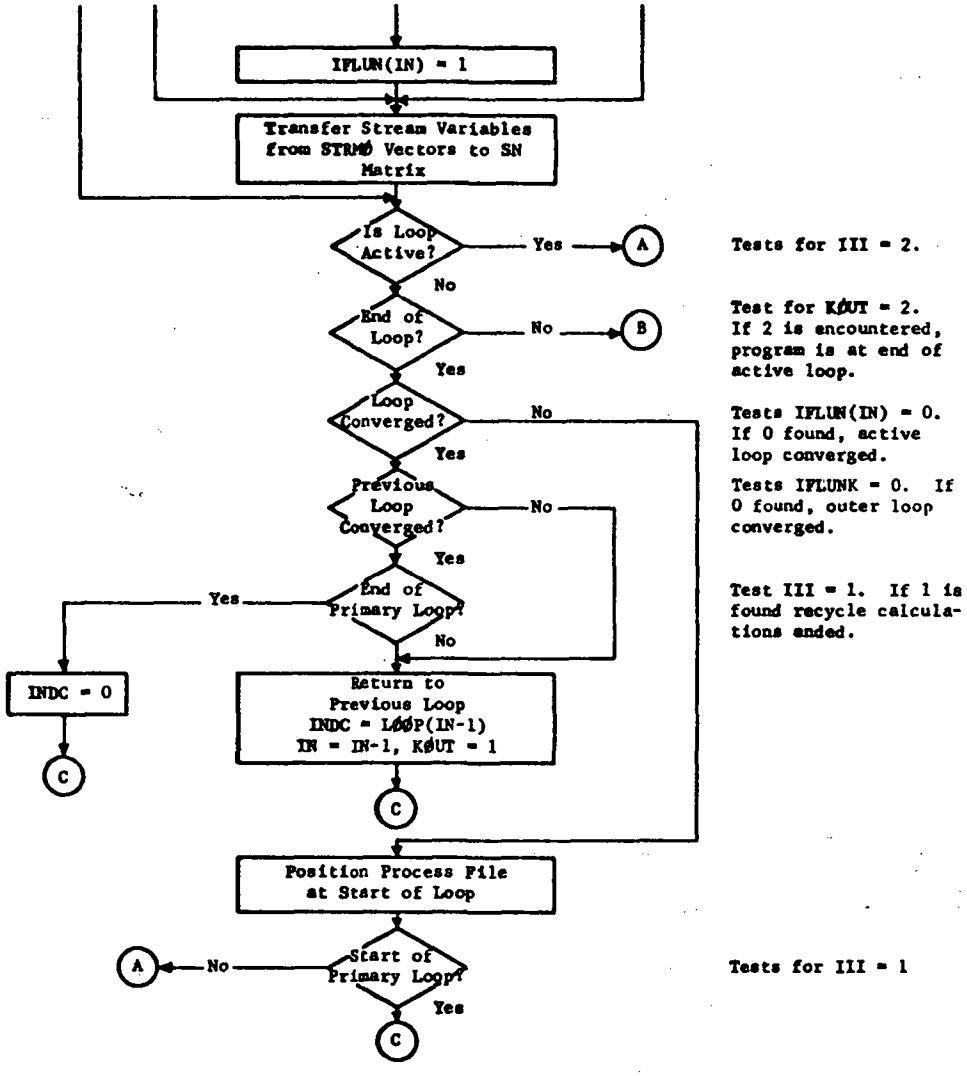


FIGURE A-1. LOGICAL FLOW DIAGRAM FOR SEPSIM

A.3 Structure and Operation (Standard Version)

A.3.1 General:

In outline, the modular components of this executive program are:

program, main

- reads and prints given data
- relates process units with proper process models
- initiates calculations
- identifies iterative loops in calculation sequence
- tests for convergence at appropriate points in calculation sequence
- transfers stream information between storage and process model subroutines
- prints results when calculations are complete

subroutine SELECT

- calls process model subroutine corresponding to number code given by main program when it wants a process model subroutine called.

subprogram BLOCK DATA (associated with SELECT)

- defines process model subroutine names that are to correspond to the number code used in the main program.

subroutines, process models

- a subroutine is provided for each model mentioned in the above two components...these are not usable process model subroutines, but so-called "dummies" required by programming technicalities.

The most important difference between the main program in this version and that in the WATFIV version is that here all data is printed out as soon as it is read in, thus greatly facilitating the search for the errors that are often made in initially setting up the data. This, however, rules out the possibility of having all printing operations in one neat subprogram, as done in the WATFIV version; so here the results, i.e. the final values of the stream and equipment information, are also printed out by the main program. Usually no other quantities are of interest as results; if there were, then the statements for printing out the results would have to be modified.

Although the statements for printout are not as accessible for modification in this version, this is not difficult to overcome. Printing formats

provided are appropriate for the majority of purposes, such as for inclusion in reports.

Another important difference is that in the Standard version the vectors of equipment information have no restrictions on their length (see Section A.3.2 discussion of EN).

A minor improvement in the Standard version is that the model subroutines define the equipment parameter names (see NAMEN in Section A.3.2) in such a way that no two differently-named subroutines can possibly try to use the same storage space for this purpose, as could happen in the WATFIV version.

Other improvements include the printout of stream and equipment information in more detail, identifying each element by number as well as by name.

Also, it is possible in this version to perform more than one simulation in one computer run.

The subroutine NØMEN in the WATFIV version is replaced in this version by a BLOCK DATA subprogram, which achieves the same purpose but in the manner specified by standard Fortran. Just this BLOCK DATA subprogram, along with the subroutine SELECT with which it is (conceptually) associated, and the set of dummy subroutines, must be modified in a matching way if the user wants to change the list of process subroutine names provided with SEPSIM. The modification required is simply that an unwanted subroutine name must be replaced, by the desired new name, in the one place where it occurs in SELECT, BLOCK DATA, and the set of dummies. This is discussed in detail in Section A.4.5.

Whenever a process model subroutine is actually required for a simulation, it must be made to replace the dummy subroutine of the same name provided by the executive. The most direct way of doing this is to physically replace the one set of computer cards with the other. In many computer systems the same thing may be accomplished automatically by storing the dummies in a special kind of "auxiliary" file which the computer searches, after reading in the real subroutines, to obtain only the dummy subroutines that it has determined are necessary from compiling subroutine SELECT. The user should find out whether a method such as this is available and worthwhile to him.

A.3.2 Important Arrays:

This is the same as for the WATFIV version (see Section A.2.2), with two exceptions regarding the arrays EN and NAMEN.

(a) As stated in Section A.2.2, the equipment parameter array EN and the equipment parameter name array NAMEN are determined by different (possibly isolated) people, the user and the programmers, respectively, so that the rows in each array do not correspond, in general, in order. In the standard version, we provide a row of NAMEN for every possible process model subroutine rather than just for every possible equipment vector, thus avoiding the danger of different subroutines trying to use the same row of NAMEN for different equipment vectors.

In this version the dimensions of NAMEN are (50,20): 50 to provide a different row for every possible process subroutine, and 20 to provide for names of up to the first 20 elements of an equipment vector. Each row of NAMEN is reserved for the process model subroutine that corresponds in order as the process model subroutines are listed in subroutine SELECT. A programmer who writes a process model subroutine also writes a DATA statement defining the equipment parameter names in the row of NAMEN that corresponds to his subroutine name. He places this DATA statement in a BLOCK DATA subprogram as required by standard Fortran. Thus each process model subroutine used in this version of SEPSIM is accompanied by a BLOCK DATA subprogram to define the equipment parameter names. The main program determines from the process matrix NPROCS which row of NAMEN belongs to each equipment vector.

(b) In the Standard version an equipment vector may occupy any number of consecutive rows of the array EN(20,20). The first element of the vector is submitted as the equipment vector number, NE, and names the row of EN where the vector begins. The second element of the vector is submitted as its total length, LN, and determines how many rows of EN the vector requires. When you use this feature, be careful that different vectors do not overlap in EN. Thus with present dimensions a vector with NE = 7 and LN = 42 requires 3 rows in EN and no vector with NE = 8 or 9 can be submitted although only the first 2 elements of the 3rd row are used. Moreover, you must allow enough room at the "bottom" of the EN array: for example a vector with LN = 42 must have NE = 18 or less.

A subroutine using a vector occupying 3 rows in EN would be

written in terms of EN(NE,-), EN(NE+1,-) and EN(NE+2,-). This permits more flexible use of subroutines than if they were written in terms of AEN. AEN is now reserved for additional data used by more than one subroutine and not normally included in results.

A.3.3 Logical Flow:

This is similar to the WATFIV version (see Section A.2.3), with the exception that there is no NØMEN, and that output steps are split up before and after the simulation routine in the main program to show all quantities as soon as they are obtained. The calculational procedure is exactly as for the WATFIV version, illustrated by Figure A-1 and Table A-3. The program listing for the standard version is given in Section A.6.2.

A.4 Use of SEPSIM

A.4.1 General:

Certainly the first job to undertake in using SEPSIM is to carefully define the purposes of the simulation or design. What information is to be obtained? How is this information to be used? What portion, if not all, of the process system is to be considered? What accuracy is required? From these questions it should be possible to construct a flow sheet of the process to be considered and determine the information vector to be employed.

The information vector such as shown in Table A-1 must be given careful attention. It must contain the system information, e.g., flows and compositions, desired from a simulation or used as criteria in a design. It must also contain stream information needed to calculate the desired data. For example, pH may be of no particular interest in a process study, however pH of the feed streams to a unit may influence conversion and thus the composition of the output from the unit. In this case, pH should appear in the vector. Since it is poor practice to change the structure of the vector between calculations for the different process units, the vector must be long enough to hold all the information even if some of the compositions are not changed in a process unit or are inapplicable in portions of the process. Unfortunately, this makes the vector quite long if the process contains streams of widely different character such as gas and liquid. This can be overcome, if such "extra" variables are associated only with certain process units, by storing them in another

array such as EN or PAPER. However, it must be born in mind that only STRMØ variables are tested for convergence.

It is necessary to have mathematical models available for all the process units in the network. A discussion of the wide variety of possible models is outside the scope of this manual. Each process model subroutine must transmit information in the stream vector from the process unit's input to its output via one or more Fortran statements. For example, a model for a settler must contain statements which specify the reduction in suspended solids. A settler does not effect pH. Therefore, if pH is in the stream vector, the model must have a statement: output pH = input pH. If this is not done, the vector describing the output of the process unit will always contain the same pH value with which it is initialized at the beginning of the calculations.

The subroutine for a model must be written in terms of the STRMI (I,J) vectors. I must only be given values from 1 to NIN, where NIN is the number of input streams to the process unit. All the results of calculations performed in the model must be expressed as elements in the STRMØ (K,J) vectors. Again the K index must run consecutively from K = 1 to NØUT which is the number of streams leaving the process unit. These indispensable requirements for the model subroutines are illustrated in Figure A-2. The figure is a SEPSIM subroutine for a rock media trickling filter, without the declarative and initializing statements whose form depends on the version of SEPSIM used. Notice in statements 1, 55 and 4 the use of STRMI (I,3) and STRMI (I,J) variables. PAPER (I,J) is used to store intermediate calculations. For example, statement 4 sums the input streams. Statement 5 calculates the average composition and stores it in PAPER (2,J). At the end of the subroutine, elements of the STRMØ vector which do not change in the process are obtained from PAPER (2,J).

Models for process units should be made as general as possible so that one model suffices for similar process units and may be reused for another design or simulation. This is achieved by separating out the model parameters, such as dimensions or design criteria, and treating these as input data. The EN matrix is used for these parameters as described earlier. Generality is accomplished by writing the model with the parameters as variable elements of the EN vector. Figure A-2 also illustrates the use of an EN vector element. The fractional reduction of

BOD is calculated from parameters contained in the EN row for the filter in statements following Statement 5. The 5th column of the row, for example, contains the diameter of the trickling filter being simulated, while the 6th contains a rate constant of the kinetic model. The statements in the subroutine thus are written using EN (NE,5) and EN (NE,6). The row of the EN matrix which furnishes the values for EN(NE,5) or EN (NE,6), for example, is located by the main program using the process matrix.

If additional parameters are needed for a model, a vector from the AEN matrix which contains 40 elements may be used. Numbers are obtained from this vector by using either AEN(1,L) or AEN(2,L) depending on which of the two rows in the AEN matrix is to be used. Just as for the EN vector, L represents the column in which the desired number is stored. In the Standard version additional parameters are more easily represented by EN(NE+1,L), etc.

Notice the careful documentation of the subroutine in Figure A-2. Documentation is essential if others are to use the subroutine or if it is to be used over a period of time. Documentation shows the contents of the equipment vector used with the subroutine; it provides suggested values for model constants as well as model source and modifications which have been made. A subroutine is written for a specific stream vector and must be rewritten if this vector is changed. Thus, the vector used should appear in the documentation.

It will be noticed that the first executable statement in Figure A-2 causes printout conditional upon the value of KSETS, whose value is submitted as data. A subroutine can include any action conditional upon KSETS. Thus the user can be given the option to command a special action, such is the use of an alternative formula, as well as the printout of intermediate results to examine the calculational sequence or the rate of convergence.

```
      SUBROUTINE TRFLTR
C
C     THIS IS A TRICKLING FILTER MODEL
C
C
C     THIS SUBROUTINE SIMULATES THE PREFORMANCE OF A ROCK MEDIA
C     BIOLOGICAL FILTER.  THE MODEL IS TAKEN FROM ROESLER & SMITH,
C     'MATHEMATICAL MODEL FOR A TRICKLING FILTER', REPORT OF THE
C     CINCINNATI WATER RESEARCH LABORATORY,F.W.P.C.A., CINCINNATI
C     HOWLAND'S FORMULA IS USED
C
C           BOD(O) = BOD(I)*EXP(-K*AP*D/(HQ**ZN))
C
C     SILVESTON'S MODIFICATION ASSUMES DBOD IS PREFERENTIALLY DESTROYED
C     UP TO A LIMIT DBODMIN.  SUSPENDED MATTER DOES NOT INCREASE IN THE
C     PROCESS.  SUSPENDED ORGANIC NITROGEN IS PARTIALLY AVAILABLE FOR
C     DENITRIFICATION.  DENITRIFICATION CONVERTS AMMONIA TO NITROGEN
C     AND IS GOVERNED BY THE SAME TYPE OF EQUATION AS IS BOD REMOVAL.
C     SUSPENDED ORGANIC PHOSPHOROUS IS PARTIALLY CONVERTED TO A SOLUBLE
C     FORM.  ALKALINITY IS UNCHANGED,WHILE THE TEMPERATURE IS ASSUMMED
C     TO DROP BY 1/2 DEGREE.  IN THE ABOVE FORMULA,
C     ***************************************************************
C     K = K20*1.035**(T-20)
C     K20 IS A CONSTANT **** ROESLER & SMITH RECOMMEND 0.0233
C     AP = SPECIFIC SURFACE AREA OF THE MEDIA **** USE 150 FOR 1/4'' ROCK
C     80 FOR 1/2'' ROCK, 55 FOR 3/4''ROCK, 40 FOR 1''ROCK, 20 FOR 1 3/4''
C     ROCK, AND 12 FOR 3''ROCK
C     D = BED DEPTH IN FEET
C     HQ = HYDRAULIC LOADING IN MGD(U.S.)/ACRE
C     ZN = 0.91 - 6.45/AP     ACCORDING TO ROESLER & SMITH
C     OTHER VARIABLES USED IN THE SUBROUTINE ARE,
C     DBODMIN = MINIMUM DBOD ATTAINABLE **** SILVESTON RECOMMENDS A VALUE
C     OF 10 FOR INPUT BOD IN EXCESS OF 100
C     DELBOD = CHANGE IN TOTAL BOD
C     FREBOD = FRACTIONAL REDUCTION IN TOTAL BOD
C     FRENIT = FRACTIONAL REDUCTION IN NITROGEN
C     DELON = CHANGE IN DISSOLVED NITROGEN
C     KN20 = COEFFICIENT FOR NITROGEN CONVERSION **** ROESLER & SMITH
C     RECOMMEND 0.0079
C     ***************************************************************
C                 SUBROUTINE WRITTEN BY
C                 P.L.SILVESTON AND A.  ROUKENS DE LANGE
C                 DEPT. OF CHEMICAL ENGINEERING
C                 UNIVERSITY OF THE WITWATERSRAND
C                 JOHANNESBURG, SOUTH AFRICA
C                 VERSION 1         MAY, 1969
C                 MODIFIED BY PLS **** FEBRUARY, 1970
C
C     THE SUBROUTINE WAS PREPARED AS A MODEL FOR STUDENT EXERCISES
```

```
C     ************************************************************************
C     THE LONG STREAM VECTOR OF WATCRAP-PACER IS EMPLOYED
C
C     1. STREAM NO.                          11. DP - DISSOLVED PHOSPHOROUS
C     2.                                     12. SFM - SUSPENDED FIXED MATTER
C     3. FLOW (MGD)                          13. DFM - DISSOLVED FIXED MATTER
C     4. SNBC - SUSPENDED NONBIO-            14. SBOD - SUSPENDED BIOLOGICAL
C          DEGRADABLE CARBON (MG/L)               OXYGEN DEMAND
C     5. DNBC - DISSOLVED NONBIO-            15. DBOD - DISSOLVED BIOLOGICAL
C          DEGRADABLE CARBON (MG/L)               OXYGEN DEMAND
C     6. SOC - SUSPENDED ORGANIC CARBON      16. TSS - TOTAL SUSPENDED SOLIDS
C     7. DOC - DISSOLVED ORGANIC CARBON      17. TEMPERATURE
C     8. SON - SUSPENDED ORGANIC             18. VSS - VOLATILE SUSPENDED
C          NITROGEN                               SOLIDS
C     9. DN - DISSOLVED NITROGEN             19. ALKALINITY
C     10. SOP - SUSPENDED ORGANIC
C          PHOSPHOROUS
C
C     ************************************************************************
C
C                FN VECTOR
C
C     1. EQUIPMENT NO.                       8. DBODMIN
C     2. EQUIPMENT FLAG                      9. FREBOD
C     3. AP                                  10. FRENIT
C     4. D
C     5. DIAMETER
C     6. K20
C     7. KN20
C     ************************************************************************
C     DEBUGGING PRINTOUT
      IF (KSETS)90,90,95
   95 PRINT 96, NE
   96 FORMAT(1HO, 10X31HCALCULATION REACHED TRFLTR, NE =,I4/)
   90 CONTINUE
C     PREVENT DIVISION BY ZERO
      IF(STRMI(1,3))1,1,2
    1 STRMI(1,3) = 1.
C     FIND MIXED INPUT CONCENTRATIONS
    2 CONTINUE
      Q = 0.0
      DO 3 I = 1,2
      DO 3 J = 4,19
    3 PAPER(I,J) = 0.0
      DO 55 I = 1,NIN
   55 Q = Q + STRMI(2,3)
      DO 5 J = 4,19
      DO 4 I = 1,NIN
    4 PAPER(1,J) = PAPER(1,J) + STRMI(I,3)*STRMI(I,J)
    5 PAPER(2,J) = PAPER(1,J)/Q
      BODI = PAPER(2,14) + PAPER(2,15)
C     CALCULATION OF FRACTIONAL REDUCTION OF BOD
      A = (3.145*(EN(NE,5)**2.))/(4.*160.*16.5**2.)
C     NOTE THAT Q IS IN MGD(U.S.)
      HQ = Q/A
      ZN = 0.91 - 6.45/EN(NE,3)
      ZK = EN(NE,6)*1.035**(PAPER(2,17) - 20.)
      FRBOD = 1. - EXP(-ZK*EN(NE,3)*EN(NE,4)/(HQ**ZN))
```

```
      DLBOD = BODI*FRBOD
      EN(NE,9) = FRBOD
C     FIND THE CHANGE IN DBOD AND SBOD
      DIFF = PAPER(2,15) - DLBOD
      IF(DIFF-EN(NE,8)) 8,8,6
    8 STRMO(1,15) = EN(NE,8)
      STRMO(1,14)=BODI-EN(NE,8)-DLBOD
      GO TO 7
    6 STRMO(1,15) = PAPER(2,15) - DLBOD
      STRMO(1,14) = PAPER(2,14)
C     FIND NITROGEN REMOVAL
C     ASSUME PART OF THE SUSPENDED NITROGEN IS AVAILABLE FOR REDUCTION
    7 PAPER(3,9)=PAPER(2,9)+PAPER(2,8)*(1.-STRMO(1,14)/PAPER(2,14))
C     CORRECT RATE CONSTSANT FOR TEMPERATURE
      ZKN = EN(NE,7)*1.141**(PAPER(2,17) - 20.)
C     OBTAIN FRACTIONAL REDUCTION IN DISSOLVED NITROGEN
      FRNIT = 1. - EXP(-ZKN*EN(NE,3)*EN(NE,4)/(HO**ZN))
      EN(NE,10) = FRNIT
      DELDN = PAPER(3,9)*FRNIT
      STRMO(1,9) = PAPER(3,9) - DELDN
      STRMO(1,8) = PAPER(2,8)*STRMO(1,14)/PAPER(2,14)
C     PHOSPHOROUS COMPOUNDS ARE SOLUBILIZED BY THE FILTER
      STRMO(1,10) = PAPER(2,10)*STRMO(1,14)/PAPER(2,14)
      STRMO(1,11) = PAPER(2,11) + PAPER(2,10) - STRMO(1,10)
C     ASSUME FIXED MATTER DOES NOT CHANGE
      STRMO(1,12) = PAPER(2,12)
      STRMO(1,13) = PAPER(2,13)
C     ASSUME NONBIODEGRADABLE CARBON IS UNCHANGED
      STRMO(1,4) = PAPER(2,4)
      STRMO(1,5) = PAPER(2,5)
C     ORGANIC CARBON CHANGES BECAUSE OF THE REDUCTION IN BOD
C     FOLLOWING ROESLER & SMITH ASSUMEBOD = 1.87*CARBON
      STRMO(1,6) = (STRMO(1,14) + 1.87*STRMO(1,4))/1.87
      STRMO(),7) = (STRMO(1,15) + 1.87*STRMO(1,5))/1.87
C     FLOW RATE DOES NOT CHANGE
      STRMO(1,3) = Q
C     NOW WE FIND THE SUSPENDED SOLIDS TERMS
C     ASSUME SBOD = SUSPENDED SOLIDS
      STRMO(1,18) = STRMO(1,14) + STRMO(1,4) + STRMO(1,8)
      STRMO(1,16) = STRMO(1,18) + STRMO(1,12) + STRMO(1,10)
C     TEMPERATURE DROPS BY 1/2 DEGREES
      STRMO(1,17) = PAPER(2,17) - 0.5
C     ALKALINITY IS UNCHANGED
      STRMO(1,19) = PAPER(2,19)
C     ************************************************************************
      RETURN
      END
```

FIGURE A-2. SAMPLE SEPSIM SUBROUTINE

A.4.2 Process Subroutine Requirements (WATFIV Version):

In addition to the general requirements described in Section A.4.1, a process subroutine must meet three more requirements.

(a) Declarative statements must be included to dimension the arrays used and to locate them and other variables in the storage block which is used in CØMMØN with the main program. This is conveniently accomplished by using the statements shown in Figure A-3(a).

(b) Statements must be included to store the equipment parameter names in some row of the array NAMEN and link this row with any rows of EN which may be used with the subroutine. This is most conveniently done with a DATA statement (using Implied DØ) and a statement assigning the NAMEN row number to KEY(NE), as illustrated in Figure A-3(b) for an equipment vector of length 7 with names stored in row 3 of NAMEN. If the NAMEN row number is defined as zero in the KEY(NE) statement, RPRINT assumes the DATA statement has been omitted and does not attempt to print NAMEN out.

(c) A statement must be included to define the second element of any equipment vector, used with the subroutine, as the length of the vector. This is necessary because this element is used in RPRINT to control printout of EN and it is not customarily submitted, for this version, as data. The requirement is met simply by assigning the length of the vector to EN(NE,2), as illustrated in Figure A-3(c) for a vector of length 7. Since RPRINT converts this "floating point" number to a "fixed point" integer, it is a good idea to assign it with a fraction added on, as illustrated, to ensure that internal conversion errors do not result in a round-off to the next lower number.

(a) Declarative Statements

```
DIMENSIØN NAME(50),NAME2(50),TITLE(24),AEN(2,40),PAPER(2,10)
DIMENSIØN SN(75,25),EN(20,20),NPAPER(20)
DIMENSIØN NPRØCS(14,50),EPS(30),LØØP(10),IFLUN(10)
DIMENSIØN STRMI(5,25),STRMØ(5,25)
DIMENSIØN NAMEN(20,20),NAMESN(25),NAMDEF(15),KEY(20)
CØMMØN SN,EN,STRMI,STRMØ,AEN,NIN,NØUT,NE
CØMMØN NAME,NAME2,TITLE,PAPER,NPAPER,NPRØCS,EPS,LØØP,IFLUN,NUMPR
CØMMØN KSETS,KRUN,NELMAX,NEMAX,NSLMAX,NSMAX,NØAEN
CØMMØN NAMEN,NAMESN,NAMDEF,KEY,NØNAME
```

(b) Definition of Equipment Parameter Names

```
DATA (NAMEN(3,I),I=1,7)/'NO. ', 'NTRY','VOL.','K1. ','K2 ',
* 'VRED','DETN'/
KEY(NE)=3
```

(c) Definition of Equipment Vector Length

```
EN(NE,2)=7.001
```

FIGURE A-3: Samples for Meeting Additional Requirements on Process Subroutines (WATFIV Version)

A.4.3 Process Subroutine Requirements (Standard Version)

In addition to the general requirements described in Section A.4.1, a process subroutine must meet two more requirements.

(a) A declarative statement must be included to dimension the arrays used and to locate them and other variables in the labelled block PRØDAT which is used in CØMMØN with the main program. This is conveniently accomplished by using the statements shown in Figure A-4(a).

(b) A short BLØCK DATA subprogram must be added after the end of the subroutine to store the 4-character equipment parameter names in the row of NAMEN that corresponds to the subroutine name. This correspondence is easily found by referring to the list of subroutines in SELECT. Figure A-4(b) illustrates a suitable BLØCK DATA subprogram for a subroutine named MIXER3 which uses an equipment vector of length 4. For brevity the symbol NAMEN can be replaced by the symbol B. First the CØMMØN block labelled EQPNAM,which contains the storage space used by NAMEN or B, is completely defined. Then a DATA statement defines the 4 equipment parameter names to be used, and the elements of B in which they are to be stored. Since MIXER3 is the first subroutine in SELECT, the first row of B is used. Just the first four elements of the row should be defined. Note that Standard Fortran does not permit Implied DØ in DATA statements - each element must be explicitly stated.

For equipment vectors of length up to 20, every element must have a name defined, if only by blanks. For equipment vectors of length over 20, just the first 20 elements must have names defined.

(a) Declarative Statement

```
      CØMMØN/PRØDAT/STRMI(5,25), SN(75,25), PAPER(2,10), AEN(2,40),
     *              STRMØ(5,25), EN(20,20), NPAPER(20),  KSETS, NE
```

(b) Definition of Equipment Parameter Names

```
      BLØCK DATA
      CØMMØN/EQPNAM/B(50,20)
      DATA B(1,1),B(1,2),B(1,3),B(1,4)/4HEQVE,4HLNTH,4HMAG ,4H DIV/
      END
```

FIGURE A-4: Samples for Meeting Additional Requirements on Process Subroutines (Standard Version)

A.4.4 Flowsheet Analysis:

With a stream vector chosen and a set of compatible model subroutines on hand, the next step in either a design or a simulation is to number each significant process unit and stream in the flow sheet. For convenience, process units should be numbered in the main calculational sequence to be employed, which normally follows the main direction of influence of one unit upon another in the process. Also, for convenience, there should be no gaps in the process unit or stream number sequence. Each number will denote the vector in SN or EN where information concerning the stream or equipment, respectively, is stored. Two or more process units can have the same number if they use the same equipment vector; but no two streams can have the same number.

Next, the structure of the network must be examined to construct the process matrix. Loops of various types (nested, interlocking, etc.) can be spotted for any network, in principle, by listing the process units in a column and sketching in the network connections. This is best illustrated. Figure A-5 shows a waste treatment process which will be used as an example for this section. The units, in order by number, are a primary clarifier, digester, trickling filter, secondary clarifier, junction box and chlorinator. Every unit in this example uses a different model, which is indicated by the abbreviated name in the figure. Streams have also been numbered. Stream splitting or confluence must always be represented as a distinct process unit, and a subroutine must be available to relate the outflows to the inflows, just as for any other unit. Hence the junction box (the 5th unit) in this process.

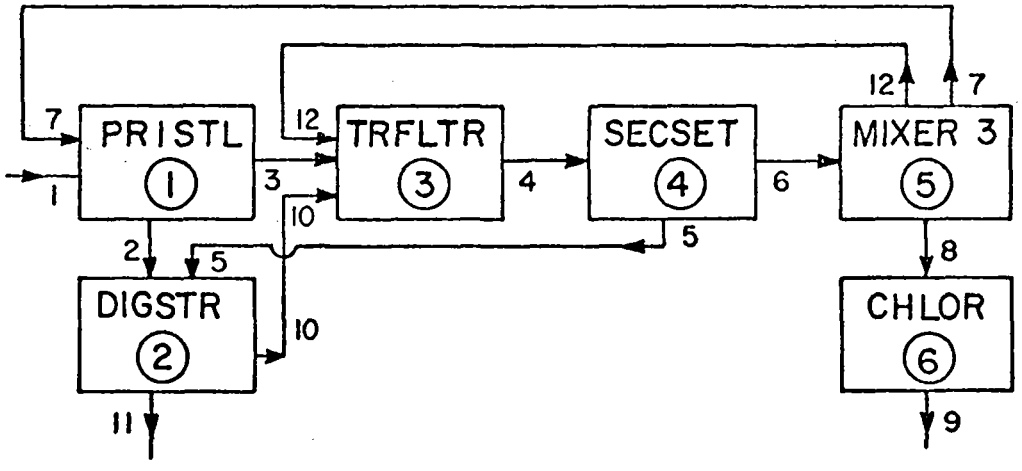
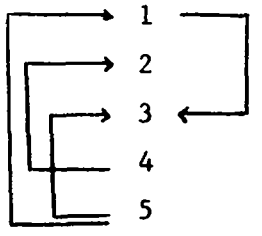


FIGURE A-5: PROCESS FLOW SHEET EXAMPLE

Listing the process units and sketching the network connections:

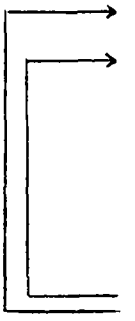


NE	NAME
1	PRISTL
2	DIGSTR
3	TRFLTR
4	SECSET
5	MIXER3
6	CHLOR

For clarity we have omitted the connections between consecutive units, and placed feedback streams and feedforward streams on the left and right sides, respectively. In what follows, we shall modify the structure shown above, without changing its meaning, to obtain a process matrix acceptable to the SEPSIM executive.

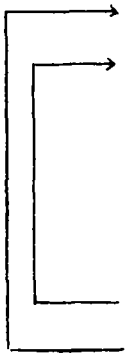
At this point one must bear in mind that the purpose of this is to encode the desired calculational sequence in terms which SEPSIM can understand. First, recall that SEPSIM accepts only nested feedback loops in the process matrix. The executive does not accept interlocking loops such as those embracing the 2nd and 4th units and the 3rd and 5th units. Finally, SEPSIM does not accept two or more feedback loops beginning or ending at the same unit, as at the 5th unit. The present example will illustrate how to express such features in terms acceptable to SEPSIM.

In order to converge the inside interlocking loops a desirable iteration sequence would be 234534,234534, etc., where we have denoted each process unit by its number since they all have different numbers. The point is that to obtain good convergence it would be best to alternate between one loop and the other, and this is done most conveniently by the above sequence. After these inside loops have converged, calculations should begin again at the first unit. The 6th unit should be calculated after all feedback loops have converged. So far we are ignoring the feedforward loop. The desired calculation sequence is now represented by this list:



NE	NAME
1	PRISTL
2	DIGSTR
3	TRFLTR
4	SECSET
5	MIXER3
3	TRFLTR
4	SECSET
6	CHLOR

In order to express the fact that two loops terminate in the second-last row, a DUMMY process unit is introduced as a terminal for the outside loop:

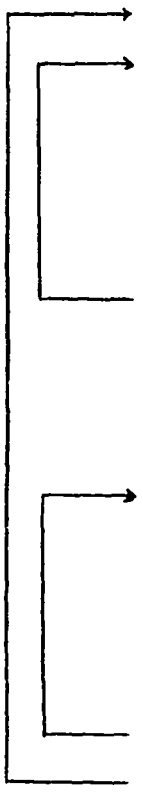


NE	NAME
1	PRISTL
2	DIGSTR
3	TRFLTR
4	SECSET
5	MIXER3
3	TRFLTR
4	SECSET
0	DUMMY
6	CHLOR

We now have a list that, with the appropriate addition of the other required columns of the process matrix, would express the calculational sequence described above in terms acceptable to SEPSIM. When the sequence meets a DUMMY row, this is not interpreted as an instruction to do any calculation but merely to go on to the next loop. This DUMMY has nothing to do with dummy subroutines.

Now suppose we wanted to take the feedforward loop into account in the calculational sequence. This would be desirable if it were thought that this loop had a significant influence on the DIGSTR unit through the TRFLTR and SECSET units. This would not normally be true in this example, but the technique generally used can nonetheless be illustrated. To take this influence into account it would be desirable to perform the calcula-

tions for the TRFLTR and SECSET units, after the PRISTL unit and before the DIGSTR unit, in every other iteration of the outside loop in the above list. This would require the above list to be expanded as follows:



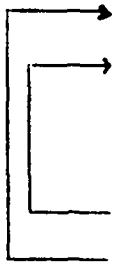
NE	NAME
1	PRISTL
2	DIGSTR
3	TRFLTR
4	SECSET
5	MIXER3
3	TRFLTR
4	SECSET
1	PRISTL
3	TRFLTR
4	SECSET
2	DIGSTR
3	TRFLTR
4	SECSET
5	MIXER3
3	TRFLTR
4	SECSET
0	DUMMY
6	CHLOR

It can be seen that the shorter list has simply been written twice, the second time with the desired modification, resulting in 18 rows. With its present dimensions SEPSIM can accept up to 50 rows in the process matrix.

The network connections implied in the lists prepared for the process matrix often have no counterpart in the real process network. Such connections, invented solely to express the calculational sequence, are customarily called "dummy streams".

If the process structure is too complicated or if it is not convenient to analyse a process network to determine the optimal calculational sequence, simpler iteration patterns can be used and the convergence obtained is often acceptable. The first simplification is to ignore feedforward streams. Next, for instance, the interlocking loops in the present example could be treated as if all process units affected were involved in just one

loop:



NE	NAME
1	PRISTL
2	DIGSTR
3	TRFLTR
4	SECSET
5	MIXER3
0	DUMMY
6	CHLOR

Going further, any feedback loop that is nested within another loop could be ignored. The maximum simplification is to encompass all the process units in arbitrary order in one large iteration loop, for instance:

NE	NAME
1	PRISTL
3	TRFLTR
4	SECSET
5	MIXER3
2	DIGSTR
6	CHLOR

This last method often yields acceptable convergence for simple processes, but wastes computer time.

When the desired calculational sequence has been expressed by a list with feedback loops, as described in the above discussion, it is a simple matter to set up the process matrix. For the present example a suitable process matrix for the third list given in this section, in which the DUMMY was first introduced, is shown in Table A-4. The columns NE and NAME are the same in the process matrix and in the list. The feedback loops in the list are expressed in the process matrix by the two columns called K and III. K is used to indicate the loop nesting level and to match the two ends of each loop. The values of K must obey the following rules:

(a) Rows which are not loop terminals have K = 0.

(b) The two terminals of a loop have the same value of K.

(c) A loop that is nested within another loop must have a higher value of K.

(d) K must not be 99 or a negative number.

For convenience unnecessarily high K values should be avoided.

The column called III is used to indicate rows that are terminals of outside loops and rows that are not involved in any loop. The values of III must obey the following rules:

(a) Rows that are part of loops nested within other loops have III = 0.
(b) Rows that are terminals of loops not nested within another loop have III = 1.
(c) All other rows, that is, those not involved in any loop, have III = 2 (this causes the convergence test to be bypassed).

Thus only three values of III are possible.

TABLE A-4: Sample Process Matrix

				SN for STRMI					SN for STRMØ				
K	NE	NAME	III	1	2	3	4	5	1	2	3	4	5
1	1	PRISTL	1	1	7	0	0	0	3	2	0	0	0
2	2	DIGSTR	0	2	5	0	0	0	10	11	0	0	0
0	3	TRFLTR	0	3	10	12	0	0	4	0	0	0	0
0	4	SECSET	0	4	0	0	0	0	6	5	0	0	0
0	5	MIXER3	0	6	0	0	0	0	12	7	8	0	0
0	3	TRFLTR	0	3	10	12	0	0	4	0	0	0	0
2	4	SECSET	0	4	0	0	0	0	6	5	0	0	0
1	0	DUMMY	1	0	0	0	0	0	0	0	0	0	0
0	6	CHLOR	2	8	0	0	0	0	9	0	0	0	0

While NE is the row of EN and NAME is the process model subroutine, to be used for the calculation demanded by the row of the process matrix, the five columns headed "SN for STRMI" and the five headed "SN for STRMØ" give the rows of SN that correspond to the rows of STRMI and STRMØ, respectively, in the process model subroutine. The row numbers of SN are assumed to be as assigned in the flowsheet in Figure A-5, and the ordering

of the process unit input streams (for STRMI) and the output streams (for STRMØ) must be obtained by inspection of the process model subroutine to be used. Taking the first row as an example, the input streams in Figure A-5 for the PRISTL unit are numbered 7 and 1, while the output streams are numbered 3 and 2. These numbers designate the rows of the SN matrix where the properties of these streams will be stored. The ordering of SN stream numbers 1 and 7 in columns 1 and 2, respectively, under the heading "SN for STRMI" in Table A-4 implies that the process model subroutine called PRISTL uses the 1st row of STRMI for sewage flowing into the process system, and the 2nd row of STRMI for recycle input from elsewhere in the plant. Assuming that the subroutine uses the 1st row of STRMØ for the supernatant effluent and the 2nd row of STRMØ for the settled sludge, the corresponding SN stream numbers 3 and 2 go in columns 1 and 2, respectively, under the heading "SN for STRMØ" in Table A-4. Note that these columns are for real process network connections, not dummy streams. Unused rows of STRMI and STRMØ are indicated by zero entries. SEPSIM determines NIN and NØUT by the location of the first zero entries in a row under "SN for STRMI" and "SN for STRMØ", respectively.

In this example each process unit has a different equipment vector number and a different model subroutine. In general this may not be true; it is possible that some process units may have not only the same model subroutine but also the same equipment vector. In such a case we suggest labelling the units, during construction of the process matrix, by letters of the alphabet so that they can be distinguished. In the process matrix itself, the only way to distinguish them is by the stream connections in the 10 right-hand columns.

A.4.5 Process Model Subroutine Names:

The 3rd column in the Process Matrix contains the names of the SEPSIM subroutines used to model the process units in the network. Names for subroutines are restricted to the 42 names currently listed in the SEPSIM executive. The current list is shown in Table A-5. It reflects the original application of SEPSIM to the simulation of waste treatment systems. Use of names which suggest the physical nature of the process units was felt to be more convenient than a general coding such as represented by the UNAME group at the end of Table A-5.

If you find these standard subroutine names awkward, the list is easily altered by replacing one or more names (except DUMMY) in the executive by your choice of names. This must be done in each of the three places in the executive where the name occurs: in the dummy subroutines, in SELECT, and in NØMEN or SELECT's BLØCK DATA, as appropriate depending on whether you have the WATFIV or the Standard Version. It is also possible to add new names to the list of 42, up to a maximum total of 49 with SEPSIM's present dimensions. This is done by inserting the new name into the blanks provided in NØMEN or SELECT's BLØCK DATA, as appropriate, and inserting a CALL statement with the suitable numerical label in place of the corresponding CØNTINUE or RETURN statement (as appropriate), and adding a suitable dummy to the list of dummy subroutines. For instance, a suitable

TABLE A-5: CURRENT SEPSIM SUBROUTINE NAMES

Subroutine Name	Suggested Use	Subroutine Name	Suggested Use
MIXER 3	Junction or Splitter	STRIP	Ammonia Stripper
PRISTL	Primary Clarifier	XCHAN	Ion Exchanger
TRFLTR	Trickling Filter	XCIN	Incinerator
ACSLD1	Activated Sludge Reactor	XTRANS	Reverse Osmosis
ACSLD2	Sludge Holding Vessel	DSTIL1	Distillation
DIGSTR	Digester	FLASH	Flash Distillation
CHLOR	Chlorinator	XTRAC2	Extraction
SECSET	Secondary Clarifier	CRYST	Crystallization
RFLTER	Sand Filter	BLOW2	Compressor
VACFL	Vacuum Filter	COOL4	Heat Exchanger
MECFIL	Mechanical Filter	REACT1	Reactor
DRYER	Dryer	UNAME0	Arbitrary
THICK	Thickener	UNAME1	Arbitrary
WASHR	Elutriator	UNAME2	Arbitrary
XFLOT	Flotation Tank	UNAME3	Arbitrary
BIOXP	Oxidation Pond	UNAME4	Arbitrary
COAG	Coagulation Contactor	UNAME5	Arbitrary
XFLOC	Flocculation Contactor	UNAME6	Arbitrary
PHCONT	CO_2 Absorber	UNAME7	Arbitrary
ADSORP	Adsorption Column	UNAME8	Arbitrary
DIALS	Dialysis or Electrodialysis Unit	UNAME9	Arbitrary

dummy for a new subroutine name DIFFUZ would be:

```
      SUBRØUTINE DIFFUZ
      RETURN
      END
```

Subroutine names may have up to 6 characters; as far as NØMEN or SELECT's BLØCK DATA are concerned (as appropriate), every name has 6 characters some of which may be blank. The main program distinguishes between subroutines by the last 3 of the 6 characters of their names. Therefore the convention is used that a name shorter than 6 characters is right-justified in the 6 spaces provided for it. This also means that all names of subroutines must be distinguishable by their last 3 characters, and no name can end with MMY.

A.5 Rules for Data Input

To run a simulation with SEPSIM you must have the executive, the process model subroutines the simulation requires, plus a set of data. In this section the data required is described and the formats are given that will allow the main program to read it in.

A.5.1 WATFIV Version:

The data deck will be described in detail and then summarized in Table A-6 showing the formats.

(1) First a title is read in, consisting of 72 alphanumeric characters, any of which can be blank. This is for documentation: it helps the user identify data decks by just looking at the top card.

(2) Then the vector NAMESN, which contains the stream vector element names, is read in. Each name has 4 characters, any of which can be blank.

(3) Then the control variables are read in, in the following order:

KSETS: The subroutine action signal.

KRUN: For documentation, distinguishing data decks that have the same title. Must be greater than zero.

NELMAX: The length of the longest equipment vector in EN. Must be 20 or less with present SEPSIM dimensions.

NEMAX: The highest equipment identification number, i.e., the highest row number (NE) used, in EN. Must be 20 or less.

NSLMAX: The length of the stream vector. Must be 15 or less.

NSMAX: The highest stream identification number, i.e., the highest row number used in SN. Must be 75 or less.

NØAEN: The length of the longest row of data in AEN. Must be 40 or less; or zero if there is no data in AEN.

(4) Next, the initial values for the SN matrix are read in. Let NCS be the number of cards required to enter a stream vector, with each card containing 8 elements except, possibly, for the last card. Then NCS cards are read in for each stream vector. Streams which are external inputs (feed streams) to the process system must be fully given here. All other streams should be given rough estimates of their final values, if possible, in order to speed convergence; otherwise they can be entered as zero. The first element of each vector is the stream number, and the second must be blank.

After all the SN vectors are read in, the procedure is stopped with NCS cards in which at least the first entry, as formatted for a stream vector, is blank or zero.

(5) Then the equipment vectors in EN are read in. Let NCE be the number of cards required to enter the longest vector in EN, with each card containing 8 elements except, possibly, the last card. NCE cards must be read in for each equipment vector; if a short vector does not actually require NCE cards, blank cards must be added to make up the NCE. The first element of each vector is the equipment vector number, and the second must be blank.

After all the EN vectors are read in, the procedure is stopped with NCE cards in which at least the first entry, as formatted for an equipment vector, is blank or zero.

(6) Then the additional data rows in AEN are read in, in the same way as for EN, but with NCA cards for each vector instead of NCE, where NCA is the number of cards required to enter the longest row in AEN. Similarly, the first element of each vector is the row in AEN where it is stored (i.e. either 1 or 2) and NCA cards beginning with a blank are added to end the procedure. If AEN is not used, this step is omitted.

(7) Next the vector EPS of convergence tolerances is read in: one element for each element of the stream vector. The format is such that NCS cards will be required. The first 2 elements of EPS can be blank or zero, as the corresponding elements of the

stream vectors are never tested for convergence. Typical values for the rest would be 0.1 (i.e. 10%) for a first run, decreasing in subsequent runs.

(8) Then the process matrix is read in, one card for each row. The subroutine name must be right-adjusted in the 6 spaces provided for it.

After the process matrix is read in, the procedure is stopped with a card containing the number 99 where K would be.

(9) A card is then read to obtain NDEF, the number of cards following which contain documentation that is to be printed out, such as parameter definitions. Must be zero or larger.

(10) Finally NDEF cards are read to obtain the documentation that is to be printed out. Each card contains 60 characters, any of which can be blank.

TABLE A-6: FORMATS FOR SEPSIM DATA DECK (WATFIV VERSION)

No. of Cards	Variables	Format
1	alphanumeric title	24A3
1	NAMESN(1 to 15)	15A4
1	KSETS,KRUN,NELMAX,NEMAX,NSLMAX,NSMAX,NØAEN	8I3
NCS for each stream	SN	8F10.3
NCS	zero or blank	8F10.3
NCE for each equipment vector	EN	8F10.3
NCE	zero or blank	8F10.3
NCA for each additional eqpt. vector (zero if AEN is not used)	AEN	8F10.3
NCA (zero if AEN is not used)	zero or blank	8F10.3
NCS	EPS	8F10.3
one for each row of process matrix	K,NE,NAME,III,SN_1^{in}...SN_5^{in},SN_1^{out}...SN_5^{out}	2I4,2X, 2A3,11I4
1	99	I4
1	NDEF	free(integer)
NDEF	alphanumeric documentation	15A4

A.5.2 Standard Version:

The data deck will be described in detail and then summarized in Table A-7 showing the formats.

(1) First a title is read in, consisting of 80 alphanumeric characters, any of which can be blank. This is for documentation purposes: it appears at the beginning of the printout and helps the user identify data decks by just looking at the top card.

(2) Then the following variables are read in, in the order given:

KRUN: for documentation, appearing as "run number" in the printout.

KSETS: the subroutine action signal.

NEMAX: the highest equipment vector identification number, i.e. the highest value of NE, used for EN. Must be 20 or less.

NSLMAX: the length of the stream vector. Must be 25 or less.

NSMAX: the highest stream vector identification number, i.e. the highest value of NS occurring in SN. Must be 75 or less.

(3) Next the process matrix is read in, one card for each row. The subroutine name must be right-adjusted in the 6 spaces provided for it.

After the process matrix is read in, the procedure is ended with a card containing the number 99 where K would be.

(4) Then the equipment vectors in EN are read in. For each vector, only as many cards as it requires are used. The first element of each vector is the equipment vector number (NE), and the second must be the length of the vector. The vectors need not be entered in numerical order. If a vector will occupy more than one row of EN, each new row must start with a new card.

After all the EN vectors are read in, the procedure is ended by one blank card.

(5) Next the rows of AEN are read in, using only as many cards as required for each row. The first element of each row is the row number. The second element must be the vector length, which must be 40 or less.

After all the AEN rows are read in, the procedure is ended by one blank card.

(6) The vector NAMESN, which contains the stream vector element names, is then read in. Let NCS be the number of cards required to enter a stream vector, if each card contains 8 elements except, possibly, for the last card. Then NCS cards are read to obtain NSLMAX names for NAMESN. Each name has 4 characters, any of which can be blank.

(7) Then the initial values for the SN matrix are read in, NCS cards for each stream vector. Streams which are external inputs (feed streams) to the process system must be fully given. All other streams should be given rough estimates of their final values, if possible, in order to speed convergence; otherwise they may be entered as zero. The first element of each vector is the stream number, and the second element must be blank (The second entry in each SN vector is never used by SEPSIM. The actual stream parameters are started in the third entry because this is what is required in some other simulation executive programs, and we want to promote the compatibility of process subroutines with different simulation executive programs). The stream vectors need not be entered in numerical order.

After all the SN vectors are read in, the procedure is ended with NCS cards in which at least the first entry, as formatted for a stream vector, is blank or zero.

(8) Next the vector EPS of convergence tolerances is read in: one element for each element of the stream vector. This will require NCS cards in all. The first 2 elements of EPS can be blank or zero, as the corresponding elements of the stream vectors are never tested for convergence. Typical values for the rest would be 0.1 (10%) for a first run, decreasing in subsequent runs.

(9) Finally NDEF is read in, followed by NDEF cards containing alphanumeric documentation, such as parameter definitions, to be printed out in addition to the data already read in and printed out. Each of the NDEF cards contains 80 characters, any of which can be blank.

(10) The data deck must be ended by a card indicating whether another data deck follows for another simulation in the same computer run. If this card has the word MØRE in the first 4 columns, SEPSIM will start reading another data deck starting with the title card (see (1) above); otherwise the computer run is ended.

TABLE A-7: FORMATS FOR SEPSIM DATA DECK (STANDARD VERSION)

No. of Cards	Variables	Format
1	alphanumeric title	20A4
1	KRUN,KSETS,NEMAX,NSLMAX,NSMAX	5I3
one for each row of process matrix	K,NE,NAME,III,SN_1^{in}...SN_5^{in},SN_1^{out}...SN_5^{out}	2I4,2X, 2A3,11I4
1	99	I4
as required for each equipment vector	EN	8F10.3
1	blank or zero	8F10.3
as required for each additional data row	AEN	8F10.3
1	blank or zero	8F10.3
NCS	NAMESN	8(A4,6X)
NCS for each stream vector	SN	8F10.3
NCS	blank or zero	8F10.3
NCS	EPS	8F10.3
1	NDEF	I4
NDEF	alphanumeric documentation	20A4
1	indicator whether to continue with following data deck	A4

A.6 Source Program Listing of SEPSIM Executive

A.6.1 WATFIV Version:

The following 9 pages reproduce the source program listing.

```
C     SEPSIM
C
C     A SHORT EXECUTIVE PROGRAM FOR SIMULATION OF
C           CHEMICAL PROCESSES
C
C     THIS PROGRAM IS INTENDED TO ASSIST IN
C     ORGANIZING AND EXECUTING PROCESS SIMULATION. IT
C     ORIGINATED FROM A NEED FOR A
C     PROGRAM WHICH COULD BE RUN ON A COMPUTER WITH A SMALL
C     FAST ACCESS STORAGE CAPABILITY AND ONE WHOSE
C     LOGIC COULD BE DESCRIBED EASILY FOR TEACHING
C     SIMULATION. THE PROGRAM IS SUITABLE FOR HANDLING
C     SIMPLE NETWORKS
C
C     LOGIC FOR HANDLING NESTED LOOPS HAS BEEN ADAPTED FROM
C     A PROCESS DESIGN EXECUTIVE WRITTEN BY ROBERT SMITH (U.S.
C     DEPT. OF INTERIOR, F.W.P.C.A. PUBLICATION # WP-20-14).
C     NAMES OF ARRAYS, VECTORS, TRANSFER OF
C     DATA TO AND FROM MODEL SUBROUTINES HAVE BEEN TAKEN
C     FROM THE PACER SIMULATION EXECUTIVE DEVELOPED BY PROF.
C     PAUL SHANNON (D...  ... COLLEGE, NEW HAMPSHIRE). THE
C     PURPOSE OF THIS WAS TO PERMIT THE USE OF SUBROUTINES WRITTEN
C     FOR PACER WITH SEPSIM. RECENT SEPSIM MODIFICATIONS
C     MAKE THIS NOLONGER POSSIBLE, ALTHOUGH SUBROUTINES FOR BOTH
C     EXECUTIVES REMAIN VERY SIMILAR.
C
C     NUMEROUS COMMENT STATEMENTS HAVE BEEN ADDED TO EXPLAIN
C     THE STRUCTURE OF SEPSIM TO THE USER. FOR FURTHER DETAILS
C     ON LOGIC OR ON THE USE OF THIS EXECUTIVE, CONSULT
C     THE SEPSIM USER'S MANUAL
C
C
C     MODIFIED AND UPDATED AUGUST 1969, FURTHER MODIFICATION BY PLS
C      JANUARY 1970 AND MAY 1973
C
C              SEPSIM COMMON AND DIMENSION DECK
C
      DIMENSION NAME(50),NAME2(50),TITLE(24),AEN(2,40),PAPER(2,10)
      DIMENSION SN(75,25),EN(20,20),NPAPER(20)
      DIMENSION NPROCS(14,50),EPS(30),LOOP(10),IFLUN(10)
      DIMENSION STRMI(5,25),STRMO(5,25)
      DIMENSION NAMEN(20,20),NAMESN(25),NAMDEF(15),KEY(20)
      COMMON SN,EN,STRMI,STRMO,AEN,NIN,NOUT,NE
      COMMON NAME,NAME2,TITLE,PAPER,NPAPER,NPROCS,EPS,LOOP,IFLUN,NUMPR
      COMMON KSETS,KRUN,NELMAX,NEMAX,NSLMAX,NSMAX,NOAEN
      COMMON NAMEN,NAMESN,NAMDEF,KEY,NONAME
      INTEGER NONAME/'XXXX'/
C
C     A TYPICAL COLUMN OF THE PROCESS MATRIX IS AS FOLLOWS
C     1. IDENTIFICATION OF START AND END OF RECYCLE LOOP
C     2. EQUIPMENT IDENTIFICATION NUMBER
C       3. MODEL SUBROUTINE NAME (REPLACED BY A NUMBER
C                 AT THE BEGINNING OF THE PROGRAM).
C       4. CLASSIFICATION OF PROCESS UNIT WITH RESPECT TO
C                 RECYCLE LOOPS
C     5. FIRST INPUT STREAM
C     ETC. UP TO 9
```

```
C      10. FIRST OUTPUT STREAM
C      ETC. UP TO 14
C
C      SIMULATION CALCULATIONS ARE CONTROLLED THROUGH THIS MATRIX
C      NAMING OF SUBROUTINES
       CALL NOMEN
       READ(5,9330) TITLE
 9330  FORMAT(24A3)
C
C       READ NAMES OF STREAM VECTOR PARAMETERS
C
       READ8000,(NAMESN(I),I=1,15)
 8000  FORMAT(15A4)
C      READ DIMENSION AND CONTROL PARAMETERS
C
       READ 9303,KSETS,KRUN,NELMAX,NEMAX,NSLMAX,NSMAX,NOAEN
 9303  FORMAT(8I3)
C      INITIALIZING ARRAYS USED IN COMPUTATION
C
       DO 6 J=1,20
   6   KEY(J)=0
       IF(KRUN)9999,9310,9320
 9310  PRINT9311
 9311  FORMAT(//47HNO MORE RUNS WERE FOUND. THE JOB WAS TERMINATED)
 9320  CONTINUE
       DO 1002 I=1,NSLMAX
       DO 1001 J=1,3
       STRMI(J,I)=0.
 1001  STRMO(J,I)=0.
       DO 1002 J=1,NSMAX
 1002  SN(J,I)=0.
       DO 1006 I=1,NELMAX
       DO 1006 J=1,NEMAX
 1006  EN(J,I)=0.
C
C      INPUT OF STREAM AND EQUIPMENT MATRICES
C
 1050  READ 9001,(STRMI(1,I),I=1,NSLMAX)
       J=STRMI(1,1)
       IF(J)9999,1100,1051
 1051  DO 1052 I=1,NSLMAX
 1052  SN(J,I)=STRMI(1,I)
       GOTO 1050
 9001  FORMAT(8F10.3)
C
 1100  READ 9001,(STRMI(1,I),I=1,NELMAX)
       J=STRMI(1,1)
       IF(J)9999,1149,1101
 1101  DO 1102 I=1,NELMAX
 1102  EN(J,I)=STRMI(1,I)
       GOTO 1100
C
C      INPUT OF ADDITIONAL EQUIPMENT MATRIX
C
 1149  IF(NOAEN)9999,1170,1150
 1150  READ 9001,(STRMI(1,I),I=1,NOAEN)
       J=STRMI(1,1)
       IF(J)9999,1170,1151
 1151  DO 1152 I=1,NOAEN
 1152  AEN(J,I)=STRMI(1,I)
       GOTO 1150
C
C      INPUT OF TOLERANCE VECTOR
C
 1170  READ 9001,(EPS(I),I=1,NSLMAX)
C
C      INPUT OF PROCESS MATRIX
C      ANY UNUSED STREAMS MAY BE LEFT BLANK
C
       DO 1200 I=1,50
```

```
C      IF MORE THAN 50 PROCESS UNITS NEEDED, CHANGE I, STATEMENT 1210
C      AND THE NPROC AND  FN DIMENSIONS
       READ 9003,NPROCS(1,I),NPROCS(2,I),NAMPRC,(NPROCS(J,I),J=4,14)
 9003 FORMAT(2I4,5X,A3,1I14)
C      CHECKING FOR END OF PROCESS MATRIX
       IF(NPROCS(1,1)-88)1210,1250,1210
C      GUARDING AGAINST TOO MANY PROCESS STEPS
 1210 IF(I-50)1211,1211,9999
C      IDENTIFYING PROCESS TYPE
 1211 DO 1201 J=1,50
       IF(NAMPRC-NAME(J))1201,1202,1201
 1201 CONTINUE
       GOTO 9999
 1202 NPROCS(3,I)=J
 1200 CONTINUE
 1250 CONTINUE
       NUMPR=I-1
C
C
C      LABEL ALL STREAMS USED
C
       DO 1300 I=1,NUMPR
       DO 1301 J=5,9
       K=NPROCS(J,I)
       IF(K)9999,1302,1301
 1301 SN(K,1)=K
 1302 DO 1303 J=10,14
       K=NPROCS(J,I)
       IF(K)9999,1300,1303
 1303 SN(K,1)=K
 1300 CONTINUE
C
C      SET UP INDICATORS TO CONTROL LOGICAL FLOW
C
       K=0
       INDC=0
       IN=1
       I=0
C
   58 IFLUNK=0
C
   55 IFLUN(IN)=0
       KOUT=0
C
C
C      CALL IN A NEW COLUMN OF PROCESS MATRIX
C
   53 I=I+1
       IF(I-NUMPR)1399,1399,220
 1399 K=NPROCS(1,I)
       NE=NPROCS(2,I)
       NDX=NPROCS(3,I)
       III=NPROCS(4,I)
       IF(NDX-50)9339,59,9999
C
C      TRANSFER INPUT STREAM VECTORS TO STRMI MATRIX
C
 9339 DO 1400 J=5,9
       JIS=NPROCS(J,I)
       IF(JIS)9999,1402,1401
 1401 NIN=J-4
       DO 1403 JJ=1,NSLMAX
 1403 STRMI(NIN,JJ)=SN(JIS,JJ)
 1400 CONTINUE
C
C      TRANSFER OUTPUT STREAM VECTORS TO STRMO MATRIX
C
 1402 DO 1410 J=10,14
       JOS=NPROCS(J,I)
```

```
      IF(JOS)9999,1412,1411
 1411 NOUT=J-9
      DO 1413 JJ=1,NSLMAX
 1413 STRMO(NOUT,JJ)=SN(JOS,JJ)
 1410 CONTINUE
 1412 CONTINUE
   59 IF(K)591,77,591
C     IF PROCESS IS NOT START OR END OF LOOP, SKIP FOLLOWING
  591 IF(K-INDC)592,77,592
C     IF PROCESS IS END OF CURRENT LOOP, SKIP FOLLOWING
  592 IF(INDC)594,593,594
C     IF NO LOOP IS ACTIVE, MAKE ONE ACTIVE AND SKIP FOLLOWING
  593 INDC=K
      GOTO 77
C     ELSE DO HOOKKEEPING FOR NESTING OF LOOPS
  594 LOOP(IN)=INDC
      IN=IN+1
      INDC=K
      KOUT=0
      IF(IFLUNK-1)595,77,595
C     IF ANY EMBRACING LOOP HAS NOT CONVERGED, SKIP FOLLOWING
  595 IFLUNK=IFLUN(IN-1)
C     RESET CONVERGENCE INDICATOR OF OUTERMOST LOOP
C
C
C     THIS IS WHERE EVERYTHING HAS SKIPPED TO
C
   77 IF(K-INDC)598,597,598
C     IF PROCESS IS START OR END OF LOOP, INCREMENT KOUT
C     KOUT IS 1 AT THE START OF A LOOP, 2 AT THE END
  597 KOUT=KOUT+1
C     CALL APPROPRIATE SUBROUTINE
  598 CALL SELECT(NDX)
C
 1000 IF(III-2)1011,80,1011
C     IF III=2 BYPASS CONVERGENCE TEST
 1011 IF(NDX-50)3921,120,9999
C     IF DUMMY BYPASS CONVERGENCE TEST AND STREAM REPLACEMENT
C
C     TEST FOR CONVERGENCE
C
 3921 DO 3002 J=1,NOUT
      JOS=STRMO(J,1)
      DO 3002 L=3,NSLMAX
      IF(STRMO(J,L))3001,3002,3001
 3001 IF(EPS(L)-ABS((STRMO(J,L)-SN(JOS,L))/STRMO(J,L)))70,3002,3002
 3002 CONTINUE
      GOTO 80
   70 IFLUN(IN)=1
C
C     REPLACE STREAM VECTORS BY CALCULATED VALUES
C
 80   DO 3010 J=1,NOUT
      JOS=STRMO(J,1)
      DO 3010 L=3,NSLMAX
 3010 SN(JOS,L)=STRMO(J,L)
      IF(III-2)120,55,120
C     IF NOT IN ANY LOOP GO DIRECTLY TO NEXT PROCESS
C
  120 IF(KOUT-2)53,1428,53
C     IF NOT END OF LOOP GO TO NEXT PROCESS
 1428 IF(IFLUN(IN))1204,1251,1204
C     IF THIS LOOP HAS NOT CONVERGED THEN REPEAT IT
 1251 IF(IFLUNK)121,1252,121
C     IF PREVIOUS LOOP HAS NOT CONVERGED THEN REPEAT IT
 1252 IF(III-1)121,160,121
```

```
C      IF THIS LOOP WAS PRIMARY THEN RESET ALL INDICATORS
C      AND GO TO NEXT PROCESS
C
C      FIND START OF CURRENT LOOP
 1204  I=0
  150  I=I+1
       IF(NPROCS(1,I)-INDC)150,1205,150
 1205  I=I-1
       IF(NPROCS(4,I+1)-1)55,58,55
C
C      RESET INDICATORS TO THOSE OF PREVIOUS LOOP
  121  INDC=LOOP(IN-1)
       KOUT=1
       IN=IN-1
       GOTO 53
C
  160  INDC=0
       GOTO 58
C      PRINTOUT SUBROUTINE CALLED HERE
C
  220  CONTINUE
       CALL RPRINT
 1910  RETURN
 9999  PRINT 9998
 9998  FORMAT(38H1IRREGULARITY IN DATA - JOB TERMINATED)
       STOP
       END
C
       SUBROUTINE RPRINT
C      PRINTOUT OF SEPSIM RESULTS
C
C      SEPSIM COMMON AND DIMENSION DECK
       DIMENSION NAME(50),NAME2(50),TITLE(24),AEN(2,40),PAPER(2,10)
       DIMENSION SN(75,25),EN(20,20),NPAPER(20)
       DIMENSION NPROCS(14,50),EPS(30),LOOP(10),IFLUN(10)
       DIMENSION STRMI(5,25),STRMO(5,25)
       DIMENSION NAMEN(20,20),NAMESN(25),NAMDEF(15),KEY(20)
       COMMON SN,EN,STRMI,STRMO,AEN,NIN,NOUT,NE
       COMMON NAME,NAME2,TITLE,PAPER,NPAPER,NPROCS,EPS,LOOP,IFLUN,NUMPR
       COMMON KSETS,KRUN,NELMAX,NEMAX,NSLMAX,NSMAX,NOAEN
       COMMON NAMEN,NAMESN,NAMDEF,KEY,NONAME
       PRINT 902
       DO 1 I=1,NUMPR
       K=NPROCS(3,I)
     1 PRINT 903,NPROCS(1,I),NPROCS(2,I),NAME2(K),NAME(K),
      *(NPROCS(J,I),J=4,14)
       READ,NDEF
       IF(NDEF)200,200,201
  201  PRINT199
  199  FORMAT(' ',///,20X,'V A R I A B L E  D E F I N I T I O N S')
       PRINT912
       DO 203 NCOUNT=1,NDEF
       READ202,NAMDEF
  202  FORMAT(15A4)
  203  PRINT204,NAMDEF
  204  FORMAT('0',10X,15A4)
  200  CONTINUE
       PRINT 904
       PRINT911
       DO 2 I=1,NEMAX
       IF(EN(1,1))2,2,3
    3  PRINT900,EN(I,1)
       NTRY=IFIX(EN(I,2))
       KEYS=KEY(I)
       IF(KEYS)20,20,21
   21  PRINT905,(NAMEN(KEYS,J),EN(I,J),J=1,NTRY)
```

```
      GO TO 2
   20 PRINT905,(NONAME,EN(I,J),J=1,NTRY)
    2 CONTINUE
      IF(NOAEN)4,4,5
    5 PRINT 901,TITLE,KRUN
      PRINT 906
      DO 6 I=1,4
      IF(AEN(I,1))6,6,7
    7 PRINT 905,(AEN(I,J),J=1,NOAEN)
    6 CONTINUE
    4 CONTINUE
    9 PRINT 908
      PRINT912
      DO 12 I=1,NSMAX
      IF(SN(I,1))12,12,13
   13 PRINT910,SN(I,1)
      PRINT905,(NAMESN(J),SN(I,J),J=3,NSLMAX)
   12 CONTINUE
      RETURN
  900 FORMAT('-',6X,'PROCESS NUMBER',F4.0)
  901 FORMAT(1H0,24A3/60X,3HRUN,I4//)
  902 FORMAT(1H1,22X,37H1 N P U T  P R O C E S S  M A T R I X//1H0,
     *8HLOOP NO.,2X,9HEQPT. NO.,2X,12HPROCESS NAME,2X,9HLOOP IND.,
     *3X,13HINPUT STREAMS,4X,14HOUTPUT STREAMS/)
  903 FORMAT(3X,I3,8X,I3,8X,2A3,8X,I2,5X,5I3,3X,5I3)
  904 FORMAT('-',25X,34HOUTPUT EQUIPMENT PARAMETERS MATRIX/)
  905 FORMAT('0',10X,A4,'=',F12.4,10X,A4,'=',F12.4)
  906 FORMAT(1H0,19X,44HINPUT ADDITIONAL EQUIPMENT PARAMETERS MATRIX/)
  908 FORMAT('1',25X,33HRESULTS - STREAM VARIABLES MATRIX/)
  910 FORMAT('-',6X,'STREAM NUMBER',F4.0)
  911 FORMAT(' ',24X,'-----------------------------------------------')
  912 FORMAT(' ',18X,'-----------------------------------------------')
      END
C
      SUBROUTINE SELECT(NDX)
C     THIS SUBROUTINE CALLS THE SUBRCUTINE CORRESPONDING TO NDX
C
      GOTO(2001,2002,2003,2004,2005,2006,2007,2008,2009,2010,
     *     2011,2012,2013,2014,2015,2016,2017,2018,2019,2020,
     *     2021,2022,2023,2024,2025,2026,2027,2028,2029,2030,
     *     2031,2032,2033,2034,2035,2036,2037,2038,2039,2040,
     *     2041,2042,2043,2044,2045,2046,2047,2048,2049,2050),NDX
 2001 CALL MIXER3
      GOTO 1000
 2002 CALL PRISTL
      GOTO 1000
 2003 CALL TRFLTR
      GO TO 1000
 2004 CALL ACSLD1
      GOTO 1000
 2005 CALL ACSLD2
      GOTO 1000
 2006 CALL DIGSTR
      GOTO 1000
 2007 CALL CHLOR
      GOTO 1000
 2008 CALL SECSET
      GOTO 1000
 2009 CALL BFLTER
      GOTO 1000
 2010 CALL VACFL
      GO TO 1000
 2011 CALL MECFIL
      GOTO 1000
 2012 CALL DRYER
      GOTO 1000
```

```
2013 CALL THICK
     GOTO 1000
2014 CALL WASHR
     GOTO 1000
2015 CALL XFLOT
     GOTO 1000
2016 CALL BIOXP
     GO TO 1000
2017 CALL COAG
     GOTO 1000
2018 CALL XFLOC
     GOTO 1000
2019 CALL PHCONT
     GOTO 1000
2020 CALL ADSORP
     GOTO 1000
2021 CALL DIALS
     GOTO 1000
2022 CALL STRIP
     GOTO 1000
2023 CALL XCHAN
     GOTO 1000
2024 CALL XCIN
     GOTO 1000
2025 CALL XTRANS
     GOTO 1000
2026 CALL DSTIL1
     GOTO 1000
2027 CALL FLASH
     GOTO 1000
2028 CALL XTRAC2
     GOTO 1000
2029 CALL CRYST
     GOTO 1000
2030 CALL BLOW2
     GOTO 1000
2031 CALL COOL4
     GOTO 1000
2032 CALL REACT1
     GOTO 1000
2033 CALL UNAME0
     GOTO 1000
2034 CALL UNAME1
     GOTO 1000
2035 CALL UNAME2
     GOTO 1000
2036 CALL UNAME3
     GOTO 1000
2037 CALL UNAME4
     GOTO 1000
2038 CALL UNAME5
     GOTO 1000
2039 CALL UNAME6
     GO TO 1000
2040 CALL UNAME7
     GOTO 1000
2041 CALL UNAME8
     GOTO 1000
2042 CALL UNAME9
2043 CONTINUE
2044 CONTINUE
2045 CONTINUE
2046 CONTINUE
2047 CONTINUE
2048 CONTINUE
2049 CONTINUE
```

```
 2050 CONTINUE
 1000 RETURN
      END
C
      SUBROUTINE NOMEN
C
C     FORTRAN IV
C
C     THIS SUBROUTINE INITIALIZES THE NAMES OF SUBROUTINES NEEDED FOR
C     THE ARRAYS NAME AND NAME2
C
C     SEPSIM COMMON AND DIMENSION DECK
C
      DIMENSION NAME(50),NAME2(50),TITLE(24),AEN(2,40),PAPER(2,10)
      DIMENSION SN(75,25),EN(20,20),NPAPER(20)
      DIMENSION NPROCS(14,50),EPS(30),LOOP(10),IFLUN(10)
      DIMENSION STRMI(5,25),STRMO(5,25)
      DIMENSION NAMEN(20,20),NAMESN(25),NAMDEF(15),KEY(20)
      COMMON SN,EN,STRMI,STRMO,AEN,NIN,NOUT,NE
      COMMON NAME,NAME2,TITLE,PAPER,NPAPER,NPROCS,EPS,LOOP,IFLUN,NUMPR
      COMMON KSETS,KRUN,NELMAX,NEMAX,NSLMAX,NSMAX,NOAEN
      COMMON NAMEN,NAMESN,NAMDEF,KEY,NONAME
      INTEGER SNAMES(100)/'MIX','ER3','PRI','STL','TEF','LER','ACS','LD1
     *','ACS','LD2','DIG','STR',' CH','LOK','SEC','SFT','DFL','TER',' VA
     *','CFL','MEC','FIL',' DR','YER',' TH','ICK',' WA','SHR',' XF','LOT
     *',' BI','OXP','  C','OAG',' XF','LOC','PHC','ONT','ADS','ORP',' DI
     *','ALS',' ST','RIP',' XC','HAN','  X','CIN','XTR','ANS','DST','IL1
     *',' FL','ASH','XTR','AC2',' CR','YST',' BL','OW2',' CO','OL4','REA
     *','CT1','UNA','ME0','UNA','ME1','UNA','ME2','UNA','ME3','UNA','ME4
     *','UNA','ME5','UNA','ME6','UNA','ME7','UNA','ME8','UNA','ME9','
     *','   ','   ','   ','   ','   ','   ','   ','   ','   ','   ','
     *','   ','   ',' DU','MMY'/
      DO 1 I=1,50
      NAME(I)=SNAMES(1+I)
 1    NAME2(I)=SNAMES(1+I-1)
      RETURN
      END
C
C THE FOLLOWING SUBROUTINES ARE DUMMIES TO PACIFY UNUSED CALL STATEMENTS
C IN SUBROUTINE SELECT...
C
      SUBROUTINE UNAME0
      RETURN
      END
      SUBROUTINE UNAME1
      RETURN
      END
      SUBROUTINE UNAME2
      RETURN
      END
      SUBROUTINE UNAME3
      RETURN
      END
      SUBROUTINE UNAME4
      RETURN
      END
      SUBROUTINE UNAME5
      RETURN
      END
      SUBROUTINE UNAME6
      RETURN
      END
      SUBROUTINE UNAME7
      RETURN
      END
      SUBROUTINE UNAME8
```

```
      RETURN
      END
      SUBROUTINE UNAME9
      RETURN
      END
      SUBROUTINE REACT1
      RETURN
      END
      SUBROUTINE COOL4
      RETURN
      END
      SUBROUTINE BLOW2
      RETURN
      END
      SUBROUTINE CRYST
      RETURN
      END
      SUBROUTINE XTRAC2
      RETURN
      END
      SUBROUTINE FLASH
      RETURN
      END
      SUBROUTINE DSTIL1
      RETURN
      END
      SUBROUTINE XTRANS
      RETURN
      END
      SUBROUTINE XCIN
      RETURN
      END
      SUBROUTINE XCHAN
      RETURN
      END
      SUBROUTINE STRIP
      RETURN
      END
      SUBROUTINE DIALS
      RETURN
      END
      SUBROUTINE ADSORP
      RETURN
      END
      SUBROUTINE PHCONT
      RETURN
      END
      SUBROUTINE XFLOC
      RETURN
      END
      SUBROUTINE COAG
      RETURN
      END
      SUBROUTINE BFLTER
      RETURN
      END
      SUBROUTINE MIXER3
      RETURN
      END
      SUBROUTINE PRISTL
      RETURN
      END
      SUBROUTINE ACSLD1
      RETURN
      END
      SUBROUTINE DIGSTR
```

```
      RETURN
      END
      SUBROUTINE BIOXP
      RETURN
      END
      SUBROUTINE XPLOT
      RETURN
      END
      SUBROUTINE WASHR
      RETURN
      END
      SUBROUTINE THICK
      RETURN
      END
      SUBROUTINE DRYER
      RETURN
      END
      SUBROUTINE MECFIL
      RETURN
      END
      SUBROUTINE VACFL
      RETURN
      END
      SUBROUTINE SECSET
      RETURN
      END
      SUBROUTINE CHLOR
      RETURN
      END
      SUBROUTINE ACSLD2
      RETURN
      END
      SUBROUTINE TRFLTR
      RETURN
      END
C
C
C
C
```

A.6.2 Standard Version:

The following 10 pages reproduce the source program listing.

```
C     SEPSIM                                                                SPM00010
C                                                                           SPM00020
C     A SHORT EXECUTIVE PROGRAM FOR SIMULATION OF                           SPM00030
C           CHEMICAL PROCESSES                                              SPM00040
C                                                                           SPM00050
C     THIS PROGRAM IS INTENDED TO ASSIST IN                                 SPM00060
C     ORGANIZING AND EXECUTING PROCESS SIMULATION. IT                       SPM00070
C     ORIGINATED FROM A NEED FOR A                                          SPM00080
C     PROGRAM WHICH COULD BE RUN ON A COMPUTER WITH A SMALL                 SPM00090
C     FAST ACCESS STORAGE CAPABILITY AND ONE WHOSE                          SPM00100
C     LOGIC COULD BE DESCRIBED EASILY FOR TEACHING                          SPM00110
C     SIMULATION. THE PROGRAM IS SUITABLE FOR HANDLING                      SPM00120
C     SIMPLE NETWORKS                                                       SPM00130
C                                                                           SPM00140
C     LOGIC FOR HANDLING NESTED LOOPS HAS BEEN ADAPTED FROM                 SPM00150
C     A PROCESS DESIGN EXECUTIVE WRITTEN BY ROBERT SMITH (U.S.              SPM00160
C     DEPT. OF INTERIOR, F.W.P.C.A. PUBLICATION = WP-20-14).                SPM00170
C     NAMES OF ARRAYS, VECTORS, TRANSFER OF                                 SPM00180
C     DATA TO AND FROM MODEL SUBROUTINES HAVE BEEN TAKEN                    SPM00190
C     FROM THE PACER SIMULATION EXECUTIVE DEVELOPED BY PROF.                SPM00200
C     PAUL SHANNON (DARTMOUTH COLLEGE, NEW HAMPSHIRE). THE                  SPM00210
C     PURPOSE OF THIS WAS TO PERMIT THE USE OF SUBROUTINES WRITTEN          SPM00220
C     FOR PACER WITH SEPSIM. RECENT SEPSIM MODIFICATIONS                    SPM00230
C     MAKE THIS NOLONGER POSSIBLE, ALTHOUGH SUBROUTINES FOR BOTH            SPM00240
C     EXECUTIVES REMAIN VERY SIMILAR.                                       SPM00250
C                                                                           SPM00260
C     NUMEROUS COMMENT STATEMENTS HAVE BEEN ADDED TO EXPLAIN                SPM00270
C     THE STRUCTURE OF SEPSIM TO THE USER. FOR FURTHER DETAILS              SPM00280
C     ON LOGIC OR ON THE USE OF THIS EXECUTIVE, CONSULT                     SPM00290
C     THE SEPSIM USER'S MANUAL                                              SPM00300
C                                                                           SPM00310
C                                                                           SPM00320
C     MODIFIED AND UPDATED AUGUST 1969, FURTHER MODIFICATION BY PLS         SPM00330
C      JANUARY 1970 AND MAY 1973          , REVISED AGAIN BY JIM ALLAN      SPM00340
C IN FEB/74 AFTER EXPERIENCE IN THE SIMULATION WORKSHOP AT CCIW.            SPM00350
C     THIS REVISION MAY 1974 FOR PUBLICATION OF NEW USERS MANUAL.           SPM00360
C     A TYPICAL ROW    OF THE PROCESS MATRIX IS AS FOLLOWS                  SPM00370
C     1. IDENTIFICATION OF START AND END OF RECYCLE LOOP                    SPM00380
C     2. EQUIPMENT IDENTIFICATION NUMBER                                    SPM00390
C       3. MODEL SUBROUTINE NAME (REPLACED BY A NUMBER                      SPM00400
C                 AT THE BEGINNING OF THE PROGRAM).                         SPM00410
C       4. CLASSIFICATION OF PROCESS UNIT WITH RESPECT TO                   SPM00420
C                 RECYCLE LOOPS                                             SPM00430
C     5. FIRST INPUT STREAM                                                 SPM00440
C     ETC. UP TO 9                                                          SPM00450
C     10. FIRST OUTPUT STREAM                                               SPM00460
C     ETC. UP TO 14                                                         SPM00470
C                                                                           SPM00480
C     SIMULATION CALCULATIONS ARE CONTROLLED THROUGH THIS MATRIX            SPM00490
C*********************************************************************    SPM00500
C                                                                           SPM00510
```

```
C                                                                       SPM00520
C DECLARATION OF VARIABLES                                              SPM00530
C                                                                       SPM00540
C THE  COMMON BLOCK  PRODAT IS TO BE AVAILABLE TO PROCESS               SPM00550
C  SUBROUTINES... THIS STATEMENT MUST APPEAR IN THEM ALSO.              SPM00560
      COMMON/PRODAT/STRM1(5,25),  SN(75,25),  PAPER(2,10),  AEN(2,40),  SPM00570
     *             STRNO(5,25),  EN(20,20),  NPAPER(20),   KSETS, NE    SPM00580
C THE COMMON BLOCK EQPNAM IS TO BE AVAILABLE TO THE BLOCK DATA          SPM00590
C SUBPROGRAMS SUPPLIED WITH THE PROCESS SUBROUTINES... THIS STATEMENT   SPM00600
C MUST APPEAR IN THEM ALSO.                                             SPM00610
      COMMON/EQPNAM/NAMEN(50,20)                                        SPM00620
C THE COMMON BLOCK  NITNAM  IS TO BE AVAILABLE TO THE BLOCK DATA        SPM00630
C SUBPROGRAM SUPPLIED WITH SUBROUTINE SELECT...  THIS STATEMENT APPEARS SPM00640
C IN THAT BLOCK DATA SUBPROGRAM ALSO.                                   SPM00650
      COMMON/NITNAM/ NAME2(50),NAME(50)                                 SPM00660
C THE FOLLOWING ARRAYS ARE NOT NEEDED OUTSIDE THE MAIN PROGRAM.         SPM00670
      DIMENSION TITLE(20),     IFLUN(10),  NPROCS(14,50), NAMESN(25),   SPM00680
     *          NAMDEF(20),    EPS(40),     LOOP(10),  S(10),  X(10)   SPM00690
      DATA IQMORE/4HMORE/                                               SPM00700
C*************************************************************************SPM00710
C                                                                       SPM00720
10000 READ (5,202) TITLE                                                SPM00730
C     READ DIMENSION AND CONTROL PARAMETERS                             SPM00740
      READ (5,9003)KRUN,KSETS,NEMAX,NSLMAX,NSMAX                        SPM00750
      WRITE(6,901) TITLE,KRUN,KSETS,NEMAX,NSLMAX,NSMAX                  SPM00760
C     FIRST INITIALIZE TO ZERO SO THAT UNUSED ROWS WILL NOT BE UNDEFINEDSPM00770
      DO 1006 J=1,NEMAX                                                 SPM00780
 1006 EN(J,1)=0.                                                        SPM00790
C                                                                       SPM00800
C     INPUT OF PROCESS MATRIX                                           SPM00810
C                                                                       SPM00820
      DO 1200 I=1,50                                                    SPM00830
      READ (5,9003)NPROCS(1,I),NF,NAMPRC,(NPROCS(J,I),J=4,14)           SPM00840
C     CHECKING FOR END OF PROCESS MATRIX                                SPM00850
      IF(NPROCS(1,I)-99)1210,1250,1210                                  SPM00860
C     IDENTIFYING PROCESS TYPE                                          SPM00870
 1210 DO 1201 J=1,50                                                    SPM00880
      IF(NAMPRC-NAME(J))1201,1202,1201                                  SPM00890
 1201 CONTINUE                                                          SPM00900
      GOTO 9999                                                         SPM00910
 1202 NPROCS(3,I)=J                                                     SPM00920
      EN(NE,1)=FLOAT(J)                                                 SPM00930
      NPROCS(2,I)=NE                                                    SPM00940
 1200 CONTINUE                                                          SPM00950
 1250 NUMPR=I-1                                                         SPM00960
      PRINT 902                                                         SPM00970
      DO 1 I=1,NUMPR                                                    SPM00980
      K=NPROCS(3,I)                                                     SPM00990
    1 WRITE(6,903)NPROCS(1,I),NPROCS(2,I),NAME2(K),NAME(K),             SPM01000
     *(NPROCS(J,I),J=4,14)                                              SPM01010
C                                                                       SPM01020
C I/O OF EQUIPMENT VECTORS PERMITTING A VECTOR TO BE STORED IN MORE THANSPM01030
C ONE ROW OF EN...  M IS THE WIDTH OF A ROW IN EN, N IS THE WIDTH OF A  SPM01040
C ROW OF DATA ON A CARD...  ASSUMED THAT M GT N.                        SPM01050
      WRITE(6,904)                                                      SPM01060
 1100 M=20                                                              SPM01070
      N=8                                                               SPM01080
      READ(5,9001)RNE,   (EPS(I),I=2,N)                                 SPM01090
      NE=IFIX(RNE)                                                      SPM01100
      IF(NE.LE.0)GO TO 1149                                             SPM01110
      LN=IFIX(EPS(2))                                                   SPM01120
```

```
      DO 1102 I=2,N                                                    SPM01130
 1102 EN(NE,I)=EPS(I)                                                  SPM01140
      NDX=IFIX(EN(NE,1))                                               SPM01150
      IF(LN.LT.M)M=LN                                                  SPM01160
      IF(LN.LE.N)GO TO 1103                                            SPM01170
      N=N+1                                                            SPM01180
      READ(5,9001)(EN(NE,J),J=N,N)                                     SPM01190
      I=1                                                              SPM01200
 1103 WRITE(6,905)I,NAMEN(NDX,1),RNE,(J,NAMEN(NDX,J),EN(NE,J),J=2,M)   SPM01210
      IF(LN.LE.M)GO TO 1100                                            SPM01220
      K=M+M                                                            SPM01230
 1104 NE=NE+1                                                          SPM01240
      IF(LN.LT.K)M=LN-K+M                                              SPM01250
      READ(5,9001)(EN(NE,J),J=1,M)                                     SPM01260
      WRITE(6,9004)NE,(J,EN(NE,J),J=1,M)                               SPM01270
      IF(LN.LE.K)GO TO 1100                                            SPM01280
      K=K+M                                                            SPM01290
      GO TO 1104                                                       SPM01300
C                                                                      SPM01310
C     INPUT OF ADDITIONAL EQUIPMENT MATRIX                             SPM01320
C                                                                      SPM01330
 1149 READ(5,9001)RNE,    (EPS(I),I=2,N)                               SPM01340
      NE=IFIX(RNE)                                                     SPM01350
      IF(NE.LE.0)GO TO 1171                                            SPM01360
      LN=IFIX(EPS(2))                                                  SPM01370
      IF(LN.GT.8)READ(5,9001)(EPS(I),I=9,LN)                           SPM01380
      WRITE(6,906)NE,LN,(I,EPS(I),I=3,LN)                              SPM01390
      AEN(NE,1)=RNE                                                    SPM01400
      DO 1152 I=2,LN                                                   SPM01410
 1152 AEN(NE,I)=EPS(I)                                                 SPM01420
      GO TO 1149                                                       SPM01430
C                                                                      SPM01440
C     INPUT OF STREAM VECTOR PARAMETER NAMES NAMESN AND MATRIX SN      SPM01450
C     FIRST INITIALIZE TO ZERO SO THAT UNUSED ROWS WILL NOT BE UNDEFINEDSPM01460
 1171 DO 1002 J=1,NSMAX                                                SPM01470
 1002 SN(J,1)=0.                                                       SPM01480
C                                                                      SPM01490
      READ (5,8000) (NAMESN(I), I=1,NSLMAX)                            SPM01500
 1050 READ (5,9001)(EPS(I),I=1,NSLMAX)                                 SPM01510
      J=IFIX(EPS(1))                                                   SPM01520
      IF(J)9999,1053,1051                                              SPM01530
 1051 DO 1052 I=1,NSLMAX                                               SPM01540
 1052 SN(J,I)=EPS(I)                                                   SPM01550
      GOTO 1050                                                        SPM01560
 1053 WRITE(6,907)                                                     SPM01570
      DO212 I=1,NSMAX                                                  SPM01580
      NS=IFIX(SN(I,1))                                                 SPM01590
      IF(NS.LE.0) GO TO 212                                            SPM01600
      WRITE(6,905)(J,NAMESN(J),SN(NS,J),J=1,NSLMAX)                    SPM01610
 212  CONTINUE                                                         SPM01620
C                                                                      SPM01630
C     INPUT OF TOLERANCE VECTOR                                        SPM01640
C                                                                      SPM01650
      READ(5,9001)(EPS(I),I=1,NSLMAX)                                  SPM01660
      WRITE(6,909)(NAMESN(I),EPS(I),I=1,NSLMAX)                        SPM01670
C                                                                      SPM01680
```

```
C I/O FOR SUPPLIED MESSAGES FOR PRINTOUT                                SPM01690
      READ (5,130) NDEF                                                 SPM01700
      IF(NDEF)200,200,201                                               SPM01710
  201 WRITE(6,199)                                                      SPM01720
      DO 203 NCOUNT=1,NDEF                                              SPM01730
      READ(5,202)NAMDEF                                                 SPM01740
  203 WRITE(6,204)NAMDEF                                                SPM01750
  200 CONTINUE                                                          SPM01760
C                                                                       SPM01770
C     INITIALIZING ARRAYS USED IN COMPUTATION                           SPM01780
      DO 1001 I=1,NSLMAX                                                SPM01790
      DO 1001 J=1,5                                                     SPM01800
      STRMI(J,I)=0.                                                     SPM01810
 1001 STRMO(J,I)=0.                                                     SPM01820
C INITIALIZING ARRAYS FOR EXCLUSIVE USE OF PROCESS SUBROUTINES          SPM01830
      DO 1005 I=1,2                                                     SPM01840
      DO 1005 J=1,10                                                    SPM01850
 1005 PAPER(I,J)=0.0                                                    SPM01860
      DO 1007 I=1,20                                                    SPM01870
 1007 NPAPER(I)=0                                                       SPM01880
C*************************************************************************SPM01890
C                                                                       SPM01900
      WRITE(6,2000)                                                     SPM01910
C NOW SIMULATION BEGINS                                                 SPM01920
C                                                                       SPM01930
C     SET UP INDICATORS TO CONTROL LOGICAL FLOW                         SPM01940
C                                                                       SPM01950
      K=0                                                               SPM01960
      INDC=0                                                            SPM01970
      IN=1                                                              SPM01980
      I=0                                                               SPM01990
C                                                                       SPM02000
   58 IFLUNK=0                                                          SPM02010
C                                                                       SPM02020
   55 IFLUN(IN)=0                                                       SPM02030
      KOUT=0                                                            SPM02040
C                                                                       SPM02050
C     CALL IN A NEW COLUMN OF PROCESS MATRIX                            SPM02060
C                                                                       SPM02070
   53 I=I+1                                                             SPM02080
      IF(I-NUMPR)1399,1399,220                                          SPM02090
 1399 K=NPROCS(1,I)                                                     SPM02100
      NE=NPROCS(2,I)                                                    SPM02110
      NDX=NPROCS(3,I)                                                   SPM02120
      III=NPROCS(4,I)                                                   SPM02130
      IF(NDX-50)9339,59,9999                                            SPM02140
C                                                                       SPM02150
C     TRANSFER INPUT STREAM VECTORS TO STRMI MATRIX                     SPM02160
C                                                                       SPM02170
 9339 DO 1400 J=5,9                                                     SPM02180
      JIS=NPROCS(J,I)                                                   SPM02190
      IF(JIS)9999,1402,1401                                             SPM02200
 1401 NIN=J-4                                                           SPM02210
      DO 1403 JJ=1,NSLMAX                                               SPM02220
 1403 STRMI(NIN,JJ)=SN(JIS,JJ)                                          SPM02230
 1400 CONTINUE                                                          SPM02240
```

```
C                                                                       SPM02250
C     TRANSFER OUTPUT STREAM VECTORS TO STRMO MATRIX                    SPM02260
C                                                                       SPM02270
 1402 DO 1410 J=10,14                                                   SPM02280
      JOS=NPROCS(J,1)                                                   SPM02290
      IF(JOS)9999,1412,1411                                             SPM02300
 1411 NOUT=J-9                                                          SPM02310
      DO 1413 JJ=1,NSLMAX                                               SPM02320
 1413 STRMO(NOUT,JJ)=SN(JOS,JJ)                                         SPM02330
 1410 CONTINUE                                                          SPM02340
 1412 CONTINUE                                                          SPM02350
   59 IF(K)591,77,591                                                   SPM02360
C     IF PROCESS IS NOT START OR END OF LOOP, SKIP FOLLOWING            SPM02370
  591 IF(K-INDC)592,77,592                                              SPM02380
C     IF PROCESS IS END OF CURRENT LOOP, SKIP FOLLOWING                 SPM02390
  592 IF(INDC)594,593,594                                               SPM02400
C     IF NO LOOP IS ACTIVE, MAKE ONE ACTIVE AND SKIP FOLLOWING          SPM02410
  593 INDC=K                                                            SPM02420
      GOTO 77                                                           SPM02430
C     ELSE DO BOOKKEEPING FOR NESTING OF LOOPS                          SPM02440
  594 LOOP(IN)=INDC                                                     SPM02450
      IN=IN+1                                                           SPM02460
      INDC=K                                                            SPM02470
      KOUT=0                                                            SPM02480
      IF(IFLUNK-1)595,77,595                                            SPM02490
C     IF ANY EMBRACING LOOP HAS NOT CONVERGED, SKIP FOLLOWING           SPM02500
  595 IFLUNK=IFLUN(IN-1)                                                SPM02510
C     RESET CONVERGENCE INDICATOR OF OUTERMOST LOOP                     SPM02520
C                                                                       SPM02530
C                                                                       SPM02540
C     THIS IS WHERE EVERYTHING HAS SKIPPED TO                           SPM02550
C                                                                       SPM02560
   77 IF(K-INDC)598,597,598                                             SPM02570
C     IF PROCESS IS START OR END OF LOOP, INCREMENT KOUT                SPM02580
C     KOUT IS 1 AT THE START OF A LOOP, 2 AT THE END                    SPM02590
  597 KOUT=KOUT+1                                                       SPM02600
C     CALL APPROPRIATE SUBROUTINE                                       SPM02610
  598 CALL SELECT(NDX)                                                  SPM02620
C                                                                       SPM02630
      IF(III-2)1011,80,1011                                             SPM02640
C     IF III=2 BYPASS CONVERGENCE TEST                                  SPM02650
 1011 IF(NDX-50)3021,120,9999                                           SPM02660
C     IF DUMMY BYPASS CONVERGENCE TEST AND STREAM REPLACEMENT           SPM02670
C                                                                       SPM02680
C     TEST FOR CONVERGENCE                                              SPM02690
C                                                                       SPM02700
 3021 DO 3002 J=1,NOUT                                                  SPM02710
      JOS=STRMO(J,1)                                                    SPM02720
      DO 3002 L=3,NSLMAX                                                SPM02730
      IF(STRMO(J,L))3001,3002,3001                                      SPM02740
 3001 IF(EPS(L)-ABS((STRMO(J,L)-SN(JOS,L))/STRMO(J,L)))70,3002,3002     SPM02750
 3002 CONTINUE                                                          SPM02760
      GOTO 80                                                           SPM02770
   70 IFLUN(IN)=1                                                       SPM02780
C                                                                       SPM02790
C     REPLACE STREAM VECTORS BY CALCULATED VALUES                       SPM02800
```

```
C                                                                       SPM02810
 80    DO 3010 J=1,NOUT                                                 SPM02820
       JOS=STRMO(J,1)                                                   SPM02830
       DO 3010 L=3,NSLMAX                                               SPM02840
 3010  SN(JOS,L)=STRMO(J,L)                                             SPM02850
       IF(III-2)120,55,120                                              SPM02860
C      IF NOT IN ANY LOOP GO DIRECTLY TO NEXT PROCESS                   SPM02870
C                                                                       SPM02880
  120  IF(KOUT-2)53,1428,53                                             SPM02890
C      IF NOT END OF LOOP GO TO NEXT PROCESS                            SPM02900
 1428  IF(IFLUN(IN))1204,1251,1204                                      SPM02910
C      IF THIS LOOP HAS NOT CONVERGED THEN REPEAT IT                    SPM02920
 1251  IF(IFLUNK)121,1252,121                                           SPM02930
C      IF PREVIOUS LOOP HAS NOT CONVERGED THEN REPEAT IT                SPM02940
 1252  IF(III-1)121,160,121                                             SPM02950
C      IF THIS LOOP WAS PRIMARY THEN RESET ALL INDICATORS               SPM02960
C      AND GO TO NEXT PROCESS                                           SPM02970
C                                                                       SPM02980
C      FIND START OF CURRENT LOOP                                       SPM02990
 1204  I=0                                                              SPM03000
  150  I=I+1                                                            SPM03010
       IF(NPROCS(1,I)-INDC)150,1205,150                                 SPM03020
 1205  I=I-1                                                            SPM03030
       IF(NPROCS(4,I+1)-1)55,58,55                                      SPM03040
C                                                                       SPM03050
C      RESET INDICATORS TO THOSE OF PREVIOUS LOOP                       SPM03060
  121  INDC=LOOP(IN-1)                                                  SPM03070
       KOUT=1                                                           SPM03080
       IN=IN-1                                                          SPM03090
       GOTO 53                                                          SPM03100
C                                                                       SPM03110
  160  INDC=0                                                           SPM03120
       GOTO 58                                                          SPM03130
  220  CONTINUE                                                         SPM03140
C                                                                       SPM03150
C***********************************************************************SPM03160
C      PRINTOUT OF SEPSIM RESULTS                                       SPM03170
       WRITE(6,908)                                                     SPM03180
       DO 12 I=1,NSMAX                                                  SPM03190
       NS=IFIX(SN(I,1))                                                 SPM03200
       IF(NS.LE.0) GO TO 12                                             SPM03210
       WRITE(6,905)(J,NAMESN(J),SN(NS,J),J=1,NSLMAX)                    SPM03220
   12  CONTINUE                                                         SPM03230
       WRITE(6,910)                                                     SPM03240
       NE=1                                                             SPM03250
   15  NDX=IFIX(EN(NE,1))                                               SPM03260
       IF(NDX.LE.0)GO TO 17                                             SPM03270
       LN=IFIX(EN(NE,2))                                                SPM03280
       M=20                                                             SPM03290
       IF(LN.LT.M)M=LN                                                  SPM03300
       RNE=FLOAT(NE)                                                    SPM03310
       I=1                                                              SPM03320
       WRITE(6,905)I,NAMEN(NDX,1),RNE,(J,NAMEN(NDX,J),EN(NE,J),J=2,M)   SPM03330
       IF(LN.LE.M)GO TO 17                                              SPM03340
       K=M+M                                                            SPM03350
   16  NE=NE+1                                                          SPM03360
```

```
      IF(LN.LT.K)N=LN-K+M                                                SPM03370
      WRITE(6,9004)NE,(J,EN(NE,J),J=1,M)                                 SPM03380
      IF(LN.LE.K)GO TO 17                                                SPM03390
      K=K+M                                                              SPM03400
      GO TO 16                                                           SPM03410
   17 IF(NE.EQ.NEMAX)GO TO 18                                            SPM03420
      NE=NE+1                                                            SPM03430
      GO TO 15                                                           SPM03440
   18 READ(5,911)MORE                                                    SPM03450
      IF(MORE.EQ.IOMORE)GO TO 10000                                      SPM03460
      STOP                                                               SPM03470
 9999 WRITE(6,9998)                                                      SPM03480
      STOP                                                               SPM03490
C*************************** FORMATS ***************************************SPM03500
  180 FORMAT(I4)                                                         SPM03510
  199 FORMAT(1H0/1H0,20X,37H***** D O C U M E N T A T I O N ***** /      SPM03520
     *       1H0,20X,37H------------------------------------ //)         SPM03530
  202 FORMAT(20A4)                                                       SPM03540
  204 FORMAT(1H ,20A4)                                                   SPM03550
  901 FORMAT(1H1,20A4/41H0THIS IS RUN NUMBER                    ,I3/     SPM03560
     *                41H KSETS, SIGNAL FOR SUBROUTINE ACTION, IS ,I3/  SPM03570
     *                41H HIGHEST EQUIPMENT MATRIX ROW IS         ,I3/  SPM03580
     *                41H LENGTH OF STREAM VECTOR IS              ,I3/  SPM03590
     *                41H HIGHEST STREAM NUMBER IS                ,I3)  SPM03600
  902 FORMAT(1H1,22X,37HI N P U T  P R O C E S S  M A T R I X//1H0,      SPM03610
     *8HLOOP NO.,2X,9HFOPT. NO.,2X,12HPROCESS NAME,2X,9HLOOP IND.,      SPM03620
     *3X,13HINPUT STREAMS,4X,14HOUTPUT STREAMS/)                         SPM03630
  903 FORMAT(3X,I3,8X,I3,8X,2A3,8X,I2,5X,5I3,3X,5I3)                     SPM03640
  904 FORMAT(1H0/1H0 ,25X,29H INPUT DATA EQUIPMENT VECTORS/              SPM03650
     *       1H0 ,25X,29H ----------------------------/)                 SPM03660
  905 FORMAT(1H /(1H ,7X,3(3X,I2,1X,A4,1H=,F10.3)))                      SPM03670
  906 FORMAT(1H0,10X,26HADDITIONAL INPUT DATA AEN(,I1,3H,3-,I2,1H)/      SPM03680
     *      (1H ,8X,5(1X,I2,1X,1PE10.3)))                               SPM03690
  907 FORMAT(1H0/1H0,25X,31HINITIAL VALUES - STREAM VECTORS /            SPM03700
     *       1H0,25X,31H------------------------------ /)               SPM03710
  908 FORMAT(1H0/1H0,25X,24HRESULTS - STREAM VECTORS /                   SPM03720
     *       1H0,25X,24H-------------------------/)                     SPM03730
  909 FORMAT(1H0/(14H TOLERANCE ON ,A4,3H IS,F10.5))                     SPM03740
  910 FORMAT(1H0/1H0 ,25X,30H OUTPUT DATA EQUIPMENT VECTORS/             SPM03750
     *       1H0 ,25X,30H -----------------------------/)               SPM03760
  911 FORMAT(A4)                                                         SPM03770
 2000 FORMAT(1H0/50H0THE SIMULATION WILL NOW START WITH THE ABOVE DATA/  SPM03780
     *1H0/1H0)                                                          SPM03790
 8000 FORMAT (8(A4,6X))                                                 SPM03800
 9001 FORMAT(8F10.3)                                                    SPM03810
 9003 FORMAT(2I4,5X,A3,1I14)                                            SPM03820
 9004 FORMAT(1H ,10X,19HADDITIONAL ROW, NE=,I3/                         SPM03830
     *      (1H ,8X,5(1X,I2,1X,1PE10.3)))                               SPM03840
 9303 FORMAT(8I3)                                                       SPM03850
 9998 FORMAT(38H1IRREGULARITY IN DATA - JOB TERMINATED)                 SPM03860
C*******************************************************************SPM03870
      END                                                               SPM03880
      SUBROUTINE SELECT(NDX)                                            SPM03890
C                                                                       SPM03900
C     THIS SUBPOUTINE CALLS THE SUBROUTINE CORRESPONDING TO NDX         SPM03910
C                                                                       SPM03920
```

```
      GO TO( 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,SPM03930
     *       21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,SPM03940
     *       41,42,43,44,45,46,47,48,49,50),NDX                          SPM03950
   01 CALL MIXER3                                                        SPM03960
              RETURN                                                     SPM03970
   02 CALL PRISTL                                                        SPM03980
              RETURN                                                     SPM03990
   03 CALL TRFLTR                                                        SPM04000
              RETURN                                                     SPM04010
   04 CALL ACSLD1                                                        SPM04020
              RETURN                                                     SPM04030
   05 CALL ACSLD2                                                        SPM04040
              RETURN                                                     SPM04050
   06 CALL DIGSTR                                                        SPM04060
              RETURN                                                     SPM04070
   07 CALL CHLOR                                                         SPM04080
              RETURN                                                     SPM04090
   08 CALL SECSET                                                        SPM04100
              RETURN                                                     SPM04110
   09 CALL BFLTER                                                        SPM04120
              RETURN                                                     SPM04130
   10 CALL VACFL                                                         SPM04140
              RETURN                                                     SPM04150
   11 CALL MECFIL                                                        SPM04160
              RETURN                                                     SPM04170
   12 CALL DRYER                                                         SPM04180
              RETURN                                                     SPM04190
   13 CALL THICK                                                         SPM04200
              RETURN                                                     SPM04210
   14 CALL WASHR                                                         SPM04220
              RETURN                                                     SPM04230
   15 CALL XFLOT                                                         SPM04240
              RETURN                                                     SPM04250
   16 CALL BIOXP                                                         SPM04260
              RETURN                                                     SPM04270
   17 CALL COAG                                                          SPM04280
              RETURN                                                     SPM04290
   18 CALL XFLOC                                                         SPM04300
              RETURN                                                     SPM04310
   19 CALL PHCONT                                                        SPM04320
              RETURN                                                     SPM04330
   20 CALL ADSORP                                                        SPM04340
              RETURN                                                     SPM04350
   21 CALL DIALS                                                         SPM04360
              RETURN                                                     SPM04370
   22 CALL STRIP                                                         SPM04380
              RETURN                                                     SPM04390
   23 CALL XCHAN                                                         SPM04400
              RETURN                                                     SPM04410
   24 CALL XCIN                                                          SPM04420
              RETURN                                                     SPM04430
   25 CALL XTRANS                                                        SPM04440
              RETURN                                                     SPM04450
   26 CALL DSTIL1                                                        SPM04460
              RETURN                                                     SPM04470
   27 CALL FLASH                                                         SPM04480
```

```
                RETURN                                                  SPM04490
     28 CALL XTRAC2                                                     SPM04500
                RETURN                                                  SPM04510
     29 CALL CRYST                                                      SPM04520
                RETURN                                                  SPM04530
     30 CALL BLOW2                                                      SPM04540
                RETURN                                                  SPM04550
     31 CALL COOL4                                                      SPM04560
                RETURN                                                  SPM04570
     32 CALL REACT1                                                     SPM04580
                RETURN                                                  SPM04590
     33 CALL UNAME0                                                     SPM04600
                RETURN                                                  SPM04610
     34 CALL UNAME1                                                     SPM04620
                RETURN                                                  SPM04630
     35 CALL UNAME2                                                     SPM04640
                RETURN                                                  SPM04650
     36 CALL UNAME3                                                     SPM04660
                RETURN                                                  SPM04670
     37 CALL UNAME4                                                     SPM04680
                RETURN                                                  SPM04690
     38 CALL UNAME5                                                     SPM04700
                RETURN                                                  SPM04710
     39 CALL UNAME6                                                     SPM04720
                RETURN                                                  SPM04730
     40 CALL UNAME7                                                     SPM04740
                RETURN                                                  SPM04750
     41 CALL UNAME8                                                     SPM04760
                RETURN                                                  SPM04770
     42 CALL UNAME9                                                     SPM04780
     43         RETURN                                                  SPM04790
     44         RETURN                                                  SPM04800
     45         RETURN                                                  SPM04810
     46         RETURN                                                  SPM04820
     47         RETURN                                                  SPM04830
     48         RETURN                                                  SPM04840
     49         RETURN                                                  SPM04850
     50         RETURN                                                  SPM04860
        END                                                             SPM04870
        BLOCK DATA                                                      SPM04880
C                                                                       SPM04890
C    THIS SUBPROGRAM INITIALIZES VARIABLES IN COMMON BLOCK              SPM04900
        COMMON/NITNAM/ NAME2(50),NAME(50)                               SPM04910
C    FOR SUBROUTINE NAMES TO BE IDENTIFIED WITH THE VALUES OF NDX.      SPM04920
C                                                                       SPM04930
        DATA NAME2 /                3HMIX,3HPRI,3HTRF,3HACS,3HACS,3HDIG,SPM04940
       *3H CH,3HSEC,3HBFL,3H VA,3HMEC,3H DR,3H TH,3H WA,3H XF,3H BI,3H  C,SPM04950
       *3H XF,3HPHC,3HADS,3H DI,3H ST,3H XC,3H  X,3HXTR,3HDST,3H FL,3HXTR,SPM04960
       *3H CR,3H BL,3H CO,3HREA,3HUNA,3HUNA,3HUNA,3HUNA,3HUNA,3HUNA,3HUNA,SPM04970
       *3HUNA,3HUNA,3HUNA,3H    ,3H    ,3H    ,3H    ,3H    ,3H    ,3H    ,3H DU/SPM04980
        DATA NAME /                 3HER3,3HSTL,3HLTR,3HLD1,3HLD2,3HSTR,SPM04990
       *3HLOR,3HSET,3HTFR,3HCFL,3HFIL,3HYER,3HICK,3HSHR,3HLOT,3HOXP,3HOAG,SPM05000
       *3HLOC,3HONT,3HORP,3HALS,3HRIP,3HHAN,3HCIN,3HANS,3HIL1,3HASH,3HAC2,SPM05010
       *3HYST,3HOW2,3HOL4,3HCT1,3HME0,3HME1,3HME2,3HME3,3HME4,3HME5,3HME6,SPM05020
       *3HME7,3HME8,3HMED,3H    ,3H    ,3H    ,3H    ,3H    ,3H    ,3HMMY/SPM05030
C                                                                       SPM05040
```

```
C*************************************************************************SPM05050
      END                                                                 SPM05060
C                                                                         SPM05070
C  ALL OF THE FOLLOWING SUBPROGRAMS ARE DUMMIES TO PACIFY UNUSED          SPM05080
C  CALL STATEMENTS IN SUBPROGRAM SELECT(NDX)                              SPM05090
C                                                                         SPM05100
      SUBROUTINE MIXER3                                                   SPM05110
      RETURN                                                              SPM05120
      END                                                                 SPM05130
      SUBROUTINE PRISTL                                                   SPM05140
      RETURN                                                              SPM05150
      END                                                                 SPM05160
      SUBROUTINE TRFLTR                                                   SPM05170
      RETURN                                                              SPM05180
      END                                                                 SPM05190
      SUBROUTINE ACSLD1                                                   SPM05200
      RETURN                                                              SPM05210
      END                                                                 SPM05220
      SUBROUTINE ACSLD2                                                   SPM05230
      RETURN                                                              SPM05240
      END                                                                 SPM05250
      SUBROUTINE DIGSTR                                                   SPM05260
      RETURN                                                              SPM05270
      END                                                                 SPM05280
      SUBROUTINE CHLOR                                                    SPM05290
      RETURN                                                              SPM05300
      END                                                                 SPM05310
      SUBROUTINE SECSET                                                   SPM05320
      RETURN                                                              SPM05330
      END                                                                 SPM05340
      SUBROUTINE BFLTER                                                   SPM05350
      RETURN                                                              SPM05360
      END                                                                 SPM05370
      SUBROUTINE VACFL                                                    SPM05380
      RETURN                                                              SPM05390
      END                                                                 SPM05400
      SUBROUTINE MECFIL                                                   SPM05410
      RETURN                                                              SPM05420
      END                                                                 SPM05430
      SUBROUTINE DRYER                                                    SPM05440
      RETURN                                                              SPM05450
      END                                                                 SPM05460
      SUBROUTINE THICK                                                    SPM05470
      RETURN                                                              SPM05480
      END                                                                 SPM05490
      SUBROUTINE WASHR                                                    SPM05500
      RETURN                                                              SPM05510
      END                                                                 SPM05520
      SUBROUTINE XFLOT                                                    SPM05530
      RETURN                                                              SPM05540
      END                                                                 SPM05550
      SUBROUTINE BIOXP                                                    SPM05560
      RETURN                                                              SPM05570
      END                                                                 SPM05580
      SUBROUTINE COAG                                                     SPM05590
      RETURN                                                              SPM05600
```

```
END                                                                SPM05610
SUBROUTINE XFLOC                                                   SPM05620
RETURN                                                             SPM05630
END                                                                SPM05640
SUBROUTINE PHCONT                                                  SPM05650
RETURN                                                             SPM05660
END                                                                SPM05670
SUBROUTINE ADSORP                                                  SPM05680
RETURN                                                             SPM05690
END                                                                SPM05700
SUBROUTINE DIALS                                                   SPM05710
RETURN                                                             SPM05720
END                                                                SPM05730
SUBROUTINE STRIP                                                   SPM05740
RETURN                                                             SPM05750
END                                                                SPM05760
SUBROUTINE XCHAN                                                   SPM05770
RETURN                                                             SPM05780
END                                                                SPM05790
SUBROUTINE XCIN                                                    SPM05800
RETURN                                                             SPM05810
END                                                                SPM05820
SUBROUTINE XTRANS                                                  SPM05830
RETURN                                                             SPM05840
END                                                                SPM05850
SUBROUTINE DSTIL1                                                  SPM05860
RETURN                                                             SPM05870
END                                                                SPM05880
SUBROUTINE FLASH                                                   SPM05890
RETURN                                                             SPM05900
END                                                                SPM05910
SUBROUTINE XTRAC2                                                  SPM05920
RETURN                                                             SPM05930
END                                                                SPM05940
SUBROUTINE CRYST                                                   SPM05950
RETURN                                                             SPM05960
END                                                                SPM05970
SUBROUTINE BLOW2                                                   SPM05980
RETURN                                                             SPM05990
END                                                                SPM06000
SUBROUTINE COOL4                                                   SPM06010
RETURN                                                             SPM06020
END                                                                SPM06030
SUBROUTINE REACT1                                                  SPM06040
RETURN                                                             SPM06050
END                                                                SPM06060
SUBROUTINE UNAME0                                                  SPM06070
RETURN                                                             SPM06080
END                                                                SPM06090
SUBROUTINE UNAME1                                                  SPM06100
RETURN                                                             SPM06110
END                                                                SPM06120
SUBROUTINE UNAME2                                                  SPM06130
RETURN                                                             SPM06140
END                                                                SPM06150
SUBROUTINE UNAME3                                                  SPM06160
```

```
      RETURN                                                            SPM06170
      END                                                               SPM06180
      SUBROUTINE UNAME4                                                 SPM06190
      RETURN                                                            SPM06200
      END                                                               SPM06210
      SUBROUTINE UNAME5                                                 SPM06220
      RETURN                                                            SPM06230
      END                                                               SPM06240
      SUBROUTINE UNAME6                                                 SPM06250
      RETURN                                                            SPM06260
      END                                                               SPM06270
      SUBROUTINE UNAME7                                                 SPM06280
      RETURN                                                            SPM06290
      END                                                               SPM06300
      SUBROUTINE UNAME8                                                 SPM06310
      RETURN                                                            SPM06320
      END                                                               SPM06330
      SUBROUTINE UNAME9                                                 SPM06340
      RETURN                                                            SPM06350
      END                                                               SPM06360
```

A.7 Sample Printout

The following 2 pages illustrate a typical printout for a SEPSIM run using the WATFIV Version. The printout using the Standard Version is very similar but includes all data submitted to the program, such as control parameters, titles, etc.

I N P U T P R O C E S S M A T R I X

LOOP NO.	EQPT. NO.	PROCESS NAME	LOOP IND.	INPUT STREAMS	OUTPUT STREAMS
1	1	PRISTL	1	1 2 0 0 0	3 5 0 0 0
1	2	ACSLD1	1	3 0 0 0 0	4 2 0 0 0
0	3	DIGSTR	2	5 0 0 0 0	6 0 0 0 0

V A R I A B L E D E F I N I T I O N S

STREAM VARIABLES DEFINITIONS----------

FLOW = VOLUMETRIC FLOW RATE IN MGD.

S.S. = SUSPENDED SOLIDS(G/L.)

DBOD = SOLUBLE BIO. OXYGEN DEMAND (MG/L.)

SBOD = SUSPENDED BIO. OXYGEN DEMAND

TBOD = TOTAL BIO. OXYGEN DEMAND

V.SS = VOLATILE SUSPENED SOLIDS (MG/L.)

EQUIPMENT PARAMETERS DEFINITIONS ----------

DIA = DIAMETER OF SETTLER (FT)

NTKS = NO. OF SETTLING TANKS

BOD. = SETTLING CONSTANT FOR SUSPENDED B O D

CST. = CONSTANT IN MODEL FOR FRACTIONAL REMOVAL

URPS = RATIO OF SOLIDS CONC'N IN SLUDGE AND FEED

VOL. = VOLUME OF AERATOR VESSEL (MILL. GAL.)

VRSS = RATIO OF SOLIDS CONC'N IN SETTLER BOTTOMS AND FEED

CELL = CONC'N OF ACTIVE CELLS (MG/L.)

RATE = MAXIMUM SPECIFIC RATE CONSTANT IN MONOD EQN.

YLD. = YIELD COEFFICIENT FOR CELLS

SAT = SATURATION CONSTANT (MG/L.)

RESP = ENDOGENOUS RESPIRATION CONSTANT

XRSS = RATIO OF SOLIDS CONC'N IN SETTLER OVERFLOW TO FEED

VS/M = VOLATILE TO TOTAL SUSPENDED SOLIDS RATIO

VSS = VOLATILE SUSPENDED SOLIDS CONC'N (MG/L.)

NTKS = NO. OF AERATION VESSELS IN PARALLEL

AREA = AREA OF FINAL CLARIFIER

MLSS = MIXED LIQUOR SUSPENDED SOLIDS CONC'N (MG/L.)

TEMP = TEMPERATURE

RCLE = SLUDGE RECYCLE/FEED RATIO

VOL. = VOLUME OF DIGESTER (MILL. GAL.)

K1 = RATE CONSTANT IN DIGESTER MODEL

K2 = SECOND RATE CONSTANT

VRED = VOLATILE SOLIDS REDUCTION IN DIGESTER (%)

DETN = DETENTION TIME (DAYS)

OUTPUT EQUIPMENT PARAMETERS MATRIX

PROCESS NUMBER 1.

NO. =	1.0000	NTRY=	10.0000
DIA =	30.0000	NTKS=	4.0000
BOD.=	6565.0000	CST.=	0.8200
URPS=	25.0000	S.S.=	11643.0000
CST.=	0.8200	URPS=	25.0000

PROCESS NUMBER 2.

NO. =	2.0000	NTRY=	17.0000
VOL.=	3.9400	VRSS=	2.3600
CELL=	878.7681	RATE=	2.4800
YLD.=	0.7000	SAT.=	365.0000
RESP=	0.1710	XRSS=	0.0075
VS/M=	0.6240	VSS =	1167.8840
NTKS=	7.0000	AREA=	0.0000
MLSS=	1871.4940	TEMP=	0.0000
RCLE=	7.7803		

PROCESS NUMBER 3.

NO. =	3.0000	NTRY=	7.0010
VOL.=	3.9400	K1. =	700.0000
K2. =	0.2800	VRED=	50.0000
DETN=	15.9128		

RESULTS - STREAM VARIABLES MATRIX

STREAM NUMBER 1.

FLOW=	12.0000	S.S.=	321.0000
DBOD=	124.8000	SBOD=	187.2000
TBOD=	312.0000	V.SS=	156.0000

STREAM NUMBER 2.

FLOW=	0.7964	S.S.=	4416.7220
DBOD=	25.1821	SBOD=	65.7866
TBOD=	80.9787	V.SS=	2756.2070

STREAM NUMBER 3.

FLOW=	12.5488	S.S.=	260.0002
DBOD=	118.6001	SBOD=	107.7980
TBOD=	226.3981	V.SS=	143.9318

STREAM NUMBER 4.

FLOW=	11.7524	S.S.=	14.0362
DBOD=	25.1821	SBOD=	6.4044
TBOD=	31.5865	V.SS=	8.7591

STREAM NUMBER 5.

FLOW=	0.2476	S.S.=	16494.8700
DBOD=	118.6001	SBOD=	3820.9810
TBOD=	3939.5810	V.SS=	9131.2850

STREAM NUMBER 6.

FLOW=	0.0000	S.S.=	0.0000
DBOD=	0.0000	SBOD=	0.0000
TBOD=	0.0000	V.SS=	0.0000

A.8 Background Information and Legal Notice

SEPSIM (A Short Executive Program for SIMulation of Process Networks) was developed under the auspices of the South African Council for Scientific and Industrial Research by Mr. D. P. Laurie of the Numerical Analysis Division, National Research Institute for Mathematical Sciences (NRIMS), C.S.I.R., and Dr. P.L. Silveston who at that time (1969) was a visiting lecturer at the Department of Chemical Engineering, University of the Witwatersrand.

The original version of the USER'S MANUAL was prepared by Mr. Laurie and Dr. Silveston in 1970. Revision of SEPSIM and the current version of the USER'S MANUAL are the work of Mr. Ken Birkett, Mr. F. James Allan, and Dr. P.L. Silveston of B & P Silveston, Engineers, 550 Glasgow St., Kitchener, Ontario. The latest Standard version has benefitted from experience in a simulation workshop conducted under the auspices of E.P.S. at the Canada Centre for Inland Waters, January 1974.

The executive program is the property of the Council for Scientific and Industrial Research. However, they have generously released the program for public use, on condition that the following legal notice for public use appear in any release of the program or in any manual dealing with the program.

"The current version of this manual was prepared to assist users in the application of the executive program SEPSIM whose development was sponsored by the South African Council for Scientific and Industrial Research. Neither the Council, nor any person acting on behalf of them:

A. Makes any warrenty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this manual.

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information or method described in this manual."

Additional information and copies of SEPSIM can be obtained from B & P Silveston, Engineers, at a nominal charge to cover costs.

Should you encounter problems in SEPSIM use or modification,

please feel free to write to B & P Silveston, Engineers. Your comments on your use of SEPSIM-application, successes or problems, would be most welcome.

APPENDIX B

INSTRUCTIONS FOR TESTER

B USER'S MANUAL FOR TESTER

B.1 Introduction

Preparation of model subroutines is normally one of the most difficult tasks in computer-aided simulation or design. The task is compounded when executive routines are used because the subroutine must be written in a "language" compatible with the executive. This language must be learnt.

TESTER can be thought of as a personal tutor whose job is to help you learn the SEPSIM language.

The program deals with the most frequently made errors in writing model subroutines and draws on five years of teaching students how to write simulation models. It should prove to be a valuable aid in debugging your subroutine programming attempts.

TESTER has been designed specifically for the SEPSIM Executive. To use it and these instructions, you should first review Appendix A - User's Manual for SEPSIM. There are two versions of TESTER: one for subroutines written for the WATFIV Version of SEPSIM, and one for subroutines written for the Standard Version.

B.2 Function

TESTER performs the following checks and issues the following messages:

(1) Checks to see if the name of your model subroutine is "legal", that is, whether it is one of the subroutine names listed in the SEPSIM Executive. If the name is not in the list, the following message is printed;

SUBROUTINE NAME ..... IS ILLEGAL.

TESTER then lists all legal names as they have been defined in its DATA statements which occur, in the WATFIV Version, just after its beginning declarative statements, and in the Standard Version, in its associated BLØCK DATA subprogram. If the list of subroutine names were to be modified in SEPSIM, these DATA statements would have to be modified in the same way.

(2) Prints out the documentation that should be included in a subroutine for the SEPSIM Model Library.

(3) Reads in STRMI, initial STRMØ and estimated final STRMØ Vectors,

and the EN vector (plus estimated final values for EN in the Standard version). TESTER checks for zero or negative values in these data, and prints out warnings if there are such values. Then the additional data AEN is read in (if any).

(4) All input data is printed out complete with parameter names so that you may check that the data has been submitted as desired.

At this point your subroutine is executed. TESTER continues with further checks:

(5) After execution a message is printed which asks you to check from the print-out whether you have included debugging print-out, to be commanded through the value of KSETS, for runs under the executive.

(6) TESTER prints out a warning if your subroutine has changed either of the first two elements of the EN or any stream vector, which is illegal.

(7) Prints values of STRMØ calculated by your subroutine, letting you check on the performance of your model. In the standard version the final values of EN are also printed out.

(8) Values of STRMØ calculated by your subroutine are checked to see if there are negative or zero entries. Warnings are issued if there are such entries asking you to check to see that they are correct.

(9) If the calculated values for the variables in the STRMØ vectors, and the given estimated values, which are called the STMEST vectors, differ by more than 100% of the smaller, warnings are printed asking you to check for the source(s) of the problem. In the Standard version EN is also checked in this way.

(10) TESTER sets the STRMI and STRMØ vectors to zero and executes your subroutine a second time. If execution aborts, a TESTER message indicates that you have failed to protect your program against division by zero.

B.3 Use of TESTER

B.3.1 General:

TESTER runs as a main program which calls the subroutine being tested twice: the first time with stream vectors initialized as directed

by the user, and the second time with them initialized to zero. Before calling the subroutine the first time, TESTER reads in and checks such things as the numbers and size of the stream and equipment vectors, as well as the proposed subroutine name (submitted as data).

To run a subroutine with TESTER it should meet the same requirements as with SEPSIM, with one exception: the SUBROUTINE statement should not contain the proposed name which is to be used with SEPSIM, but should read SUBROUTINE TSTING.

Also, in the WATFIV version, the statement assigning the NAMEN row number to KEY(NE) must be replaced by the statement:

DATA KEY(1)/row number/

If the row number is defined as zero in this statement, TESTER assumes there are no equipment parameter names defined and does not attempt to print them out.

In the Standard Version the subroutine's BLØCK DATA subprogram must correctly define the appropriate members of NAMEN, just as with SEPSIM.

B.3.2 Rules for Data Input:

The data deck must be made up according to the following rules, which are summarized later in Table B-1 and B-2 showing the formats.

(1) The first card contains the proposed subroutine name which is to be used with SEPSIM, right-justified in the 6 spaces provided for it.

(2) The second card contains these control parameters:

NIN: the number of input streams to the model.

NØUT: the number of output streams from the model.

NSLMAX: the length of the stream vectors.

NELMAX: the length of the equipment vector. (Omit in Standard version).

KSETS: the subroutine action signal.

(3) The next set of cards contains the equipment vector. The first element of the vector must be the value of NE used to identify the vector. The second element must be the vector length, in the Standard version; in the WATFIV version this element can be blank. In the Standard version, if the length is more than 20,

so that more than one row of EN is required, each new row must start on a new card.

(4) Standard version only: a set of cards giving estimated final values of the EN vector.

(5) Then the additional data AEN is read in, a set of cards for each row. The first element of each row must be the row number (i.e. 1 or 2), and the second element must be the total length of the row (i.e. 40 or less). Use only as many cards as required (e.g. zero if there is no additional data AEN).

(6) A blank card is then required to stop the reading of AEN, (must be included even if there is no AEN).

(7) The next set of cards contains the names of the stream vector parameters (abbreviated to 4 characters or less), in order from the first to the NSLMAX th. Use only as many cards as required to make NSLMAX entries with 8 entries per card, that is, NCS cards in all.

(8) The next sequence of cards contains the values to which the input and output stream vectors are to be initialized the first time the subroutine is called, as well as estimates of the values the subroutine will calculate for the output stream vectors:

   (a) for each input stream, a set of NCS cards giving NSLMAX initial values.

   (b) for each output stream, two sets of NCS cards, the first giving NSLMAX initial values, the second giving NSLMAX estimated final values.

TABLE B-1: SUMMARY OF TESTER DATA DECK (WATFIV VERSION)

No. of Cards	Variables	Format
1	the proposed name of the subroutine	2A3
1	NIN,NØUT,NSLMAX,NELMAX,KSETS	5I10
as required	equipment vector	8F10.3
as required	additional data AEN	8F10.3
1	blank or zero	8F10.3
NCS	NAMESN, the names of the stream vector parameters	8(A4,6X)
NCS for each input stream	initial values of each STRMI vector	8F10.3
2xNCS for each output stream	initial/and estimated final, values of each STRMØ vector	8F10.3/ 8F10.3

TABLE B-2: SUMMARY OF TESTER DATA DECK (STANDARD VERSION)

No. of Cards	Variables	Format
1	the proposed name of the subroutine	2A3
1	NIN,NØUT,NSLMAX,KSETS	4I10
as required	equipment vector initial values	8F10.3
as above	estimated equipment vector final values	8F10.3
as required	additional data AEN	8F10.3
1	blank or zero	8F10.3
NCS	NAMESN, the names of the stream vector parameters	8(A4,6X)
NCS for each input stream	initial values of each STRMI vector	8F10.3
2xNCS for each output stream	initial/and estimated final, values of each STRMØ vector	8F10.3/ 8F10.3

B.4 TESTER Source Program Listing

B.4.1 WATFIV Version

The following 4 pages reproduce the source program listing.

```
C************** TESTER ************                                    TSW00010
C THIS PROGRAM IS INTENDED TO TEST PROCESS MODEL SUBROUTINES           TSW00020
C  BEFORE THEY ARE USED WITH THE EXECUTIVE.                            TSW00030
C  WRITTEN BY R.W.BIRKETT OF THE UNIVERSITY OF WATERLOO , MAY 1973.    TSW00040
C REVISED BY F.J. ALLAN  OF B. AND P. SILVESTON, ENGINEERS,  FEB/74.   TSW00050
C                                                                      TSW00060
C SEPSIM COMMON AND DIMENSION DECK                                     TSW00070
C                                                                      TSW00080
      DIMENSION NAME(50),NAME2(50),TITLE(24),AEN(2,40),PAPER(2,10)     TSW00090
      DIMENSION SN(75,25),EN(20,20),NPAPER(20)                         TSW00100
      DIMENSION NPROCS(14,50),EPS(30),LOOP(10),IFLUN(10)               TSW00110
      DIMENSION STRMI(5,25),STRMO(5,25)                                TSW00120
      DIMENSION NAMEN(20,20),NAMESN(25),NAMDEF(15),KEY(20)             TSW00130
      COMMON SN,EN,STRMI,STRMO,AEN,NIN,NOUT,NE                         TSW00140
      COMMON NAME,NAME2,TITLE,PAPER,NPAPER,NPROCS,EPS,LOOP,IFLUN,NUMPR TSW00150
      COMMON KSETS,KRUN,NEIMAX,NEMAX,NSLMAX,NSMAX,NOAEN                TSW00160
      COMMON NAMEN,NAMESN,NAMDEF,KEY,NONAME                            TSW00170
C THE FOLLOWING DATA STATEMENTS INITIALIZE VARIABLES                   TSW00180
C  FOR SUBROUTINE NAMES USED AS A STANDARD BY THE MAIN PROGRAM.        TSW00190
C                                                                      TSW00200
      DATA NAME2 /                    3HMIX,3HPRI,3HTRF,3HACS,3HACS,3HDIG,TSW00210
     *3H CH,3HSEC,3HREL,3H VA,3HMEC,3H DR,3H TH,3H WA,3H XF,3H BI,3H  C,TSW00220
     *3H XF,3HPHC,3HADS,3H DI,3H ST,3H XC,3H  X,3HXTR,3HDST,3H FL,3HXTR,TSW00230
     *3H CR,3H BL,3H CO,3HREA,3HUNA,3HUNA,3HUNA,3HUNA,3HUNA,3HUNA,3HUNA,TSW00240
     *3HUNA,3HUNA,3HUNA,3H    ,3H    ,3H    ,3H    ,3H    ,3H    ,3H  ,3H DU/TSW00250
      DATA NAME /                     3HFR3,3HSTL,3HLTR,3HLD1,3HLD2,3HSTF,TSW00260
     *3HLOR,3HSET,3HTER,3HCEL,3HFIL,3HYER,3HICA,3HSHR,3HLOT,3HOXP,3HOAG,TSW00270
     *3HLOC,3HONT,3HORP,3HALS,3HRIP,3HHAN,3HCIN,3HANS,3HILI,3HASH,3HAC2,TSW00280
     *3HYST,3HOW2,3HOL4,3HCT1,3HME0,3HME1,3HME2,3HME3,3HME4,3HME5,3HME6,TSW00290
     *3HME7,3HME8,3HME9,3H    ,3H    ,3H    ,3H    ,3H    ,3H    ,3HMMY/TSW00300
      DIMENSION NAMPRC(2),STMEST(5,25)                                 TSW00310
      DIMENSION SI(5,2),SO(5,2)                                        TSW00320
      DATA NONAME/4HXXXX/                                              TSW00330
C                                                                      TSW00340
```

```
      WRITE(6,95)                                                       TSW00350
C  READ IN USERS SUBROUTINE NAME                                        TSW00360
      READ(5,96)NAMPRC(1),NAMPRC(2)                                     TSW00370
      WRITE(6,961) NAMPRC(1),NAMPRC(2)                                  TSW00380
C  TEST USER SUBROUTINE NAME TO SEE IF IT IS A LEGAL S E P S I M        TSW00390
C  NAME. PRINT WARNING IF IT IS NOT.                                    TSW00400
      DO 4 NDX=1,50                                                     TSW00410
      IF(NAMPRC(2).EQ.NAME(NDX))  GO TO 1                               TSW00420
    4 CONTINUE                                                          TSW00430
      GO TO 70                                                          TSW00440
    1 DO 2 I=1,50                                                       TSW00450
      IF(NAMPRC(1).EQ.NAME2(I)) GO TO 3                                 TSW00460
    2 CONTINUE                                                          TSW00470
      GO TO 70                                                          TSW00480
    3 IF(I.EQ.NDX.OR.(I.EQ.33.AND.NDX.GT.32.AND.NDX.LT.43))GO TO 5      TSW00490
   70 NDX=50                                                            TSW00500
      WRITE(6,100)NAMPRC(1),NAMPRC(2)                                   TSW00510
C  SHOW CORRECT SUBROUTINE NAMES                                        TSW00520
      WRITE(6,120)(NAME2(I),NAME(I),I=1,50)                             TSW00530
C  READ IN CONTROL PARAMETERS                                           TSW00540
    5 READ (5,97)  NIN,NOUT,NSLMAX,NELMAX,KSETS                        TSW00550
      WRITE(6,971) NIN,NOUT,NSLMAX,NELMAX,KSETS                         TSW00560
C  SHOW CORRECT DOCUMENTATION THAT IS REQUIRED IN USER SUBROUTINES       TSW00570
      WRITE(6,101)                                                      TSW00580
C READ EN VECTOR                                                        TSW00590
      READ (5,103)(EPS(I),I=1,NELMAX)                                   TSW00600
      RNE=EPS(1)                                                        TSW00610
      RLN=EPS(2)                                                        TSW00620
      NE=IFIX(RNE)                                                      TSW00630
      DO 48 I=1,NELMAX                                                  TSW00640
   48 EN(NE,I)=EPS(I)                                                   TSW00650
      KDX=KEY(1)                                                        TSW00660
      IF(KDX.GT.0)GO TO 49                                              TSW00670
      WRITE(6,109)(NONAME,EN(NE,I),I=1,NELMAX)                          TSW00680
      GO TO 51                                                          TSW00690
   49 WRITE (6,109)(NAMEN(KDX,1),EN(NE,I),I=1,NELMAX)                   TSW00700
      GO TO 51                                                          TSW00710
C I/O OF ADDITIONAL DATA AEN                                            TSW00720
   51 READ(5,103) (EPS(I),I=1,8)                                        TSW00730
      NAE=IFIX(EPS(1))                                                  TSW00740
      IF(NAE.LE.0)GO TO 52                                              TSW00750
      LN=IFIX(EPS(2))                                                   TSW00760
      IF(LN.GT.8)READ(5,103)(EPS(I),I=9,LN)                             TSW00770
      WRITE(6,906)NAE,LN,(I,EPS(I),I=3,LN)                              TSW00780
      DO 1252 I=3,LN                                                    TSW00790
 1252 AEN(NAE,I)=EPS(I)                                                 TSW00800
      GO TO 51                                                          TSW00810
C  READ NAMES OF STREAM VECTOR PARAMETERS                               TSW00820
   52 READ(5,99)(NAMESN(I),I=1,NSLMAX)                                  TSW00830
      DO 220 I=1,NIN                                                    TSW00840
```

```
      READ(5,103)(STRMI(I,J),J=1,NSLMAX)                                TSW00850
      SI(I,1)=STRMI(I,1)                                                TSW00860
  220 SI(I,2)=STRMI(I,2)                                                TSW00870
      DO 221 I=1,NOUT                                                   TSW00880
      READ (5,103) (STRMO(I,J),J=1,NSLMAX)                              TSW00890
      SO(I,1)=STRMO(I,1)                                                TSW00900
      SO(I,2)=STRMO(I,2)                                                TSW00910
  221 READ(5,103)(STMEST(I,J),J=1,NSLMAX)                               TSW00920
C DEFINE UNUSED STREAM VECTORS AS ZERO                                  TSW00930
      IF(NIN.EQ.5) GO TO 7                                              TSW00940
      NIN1=NIN+1                                                        TSW00950
      DO 6 J=NIN1,5                                                     TSW00960
      DO 6 I=1,NSLMAX                                                   TSW00970
    6 STRMI(J,I)=0.                                                     TSW00980
    7 IF(NOUT.EQ.5) GO TO 9                                             TSW00990
      NOUT1=NOUT+1                                                      TSW01000
      DO 8 J=NOUT1,5                                                    TSW01010
      DO 8 I=1,NSLMAX                                                   TSW01020
      STRMO(J,I)=0.                                                     TSW01030
    8 STMEST(J,I)=0.                                                    TSW01040
    9 WRITE (6,108)(NAMESN(J),(STRMI(I,J),I=1,5),(STRMO(I,J),I=1,5),J=1,TSW01050
     *                                                          NSLMAX)TSW01060
C  CHECK STRMI FOR NEGATIVE OR ZERO VALUES SUPPLIED IN DATA.            TSW01070
      DO 22 I=1,NIN                                                     TSW01080
      DO 22 J=1,NSLMAX                                                  TSW01090
      IF(STRMI(I,J)) 20,21,22                                           TSW01100
   20 WRITE(6,104)I,J                                                   TSW01110
      GO TO 22                                                          TSW01120
   21 WRITE(6,105)I,J                                                   TSW01130
   22 CONTINUE                                                          TSW01140
C  CHECK STMEST FOR NEGATIVE OR ZERO VALUES SUPPLIED AS DATA.           TSW01150
      DO 12 I=1,NOUT                                                    TSW01160
      DO 12 J=1,NSLMAX                                                  TSW01170
      IF(STMEST(I,J)) 30,31,12                                          TSW01180
   30 WRITE(6,106)I,J                                                   TSW01190
      GO TO 12                                                          TSW01200
   31 WRITE(6,107)I,J                                                   TSW01210
   12 CONTINUE                                                          TSW01220
      WRITE (6,951)                                                     TSW01230
      CALL TSTING                                                       TSW01240
      WRITE (6,95)                                                      TSW01250
      WRITE (6,952)                                                     TSW01260
C CHECK FOR USE OF FIRST TWO ELEMENTS OF EN VECTOR                      TSW01270
      IF(EN(NE,2).NE.KLN)WRITE(6,55)NE                                  TSW01280
      IF(EN(NE,1).NE.RNE)WRITE(6,54)NE                                  TSW01290
C  PRINT OUT RESULTS OF OUTPUT STREAM VECTOR CALCULATED IN THE USER     TSW01300
C  WRITTEN SUBROUTINE.                                                  TSW01310
      WRITE(6,110)(NAMESN(J),(STRMO(I,J),I=1,5),(STMEST(I,J),I=1,5),J=1,TSW01320
     *                                                          NSLMAX)TSW01330
C CHECK FOR CHANGES IN FIRST TWO ELEMENTS OF STREAM VECTORS             TSW01340
      DO 1311 J=1,2                                                     TSW01350
      DO 1310 I=1,NIN                                                   TSW01360
      IF(STRMI(I,J).NE.SI(I,J))WRITE(6,56)I,J                           TSW01370
 1310 CONTINUE                                                          TSW01380
      DO 1311 I=1,NOUT                                                  TSW01390
      IF(STRMO(I,J).NE.SO(I,J))WRITE(6,57)I,J                           TSW01400
 1311 CONTINUE                                                          TSW01410
C  CHECK FOR NEGATIVE OR ZERO VALUES IN STRMO FROM USER                 TSW01420
C  WRITTEN SUBROUTINE.                                                  TSW01430
      DO 14 I=1,NOUT                                                    TSW01440
      DO 14 J=3,NSLMAX                                                  TSW01450
      IF(STRMO(I,J)) 40,41,14                                           TSW01460
   40 WRITE(6,111)I,J,STRMO(I,J)                                        TSW01470
```

```
      GO TO 14                                                          TSW01450
   41 WRITE(6,112)I,J                                                   TSW01480
   14 CONTINUE                                                          TSW01500
C  COMPARE USER CALCULATED RESULTS IN STRMO TO ESTIMATED RESULTS        TSW01510
C  IN STMEST.                                                           TSW01520
      NCOUNT=0                                                          TSW01530
      DO 15 I=1,NOUT                                                    TSW01540
      DO 15 J=3,NSLMAX                                                  TSW01550
      A=STMEST(I,J)                                                     TSW01560
      B=STRMO(I,J)                                                      TSW01570
      C=ABS(A-B)                                                        TSW01580
      IF(A.GE.C.AND.B.GE.C)  GO TO 15                                   TSW01590
      WRITE (6,113)I,J                                                  TSW01600
      NCOUNT=1                                                          TSW01610
   15 CONTINUE                                                          TSW01620
C  IF RESULTS ARE IN DISAGREEMENT WITH ESTIMATES ,                      TSW01630
C  PRINT OUT A CHECK LIST.                                              TSW01640
      IF (NCOUNT)60,60,61                                               TSW01650
   61 WRITE(6,114)                                                      TSW01660
C  SET STRMI AND STRMO TO ZERO.                                         TSW01670
   60 DO 200 I=1,NIN                                                    TSW01680
      DO 200 J=3,NSLMAX                                                 TSW01690
  200 STRMI(I,J)=0.                                                     TSW01700
      DO 201 I=1,NOUT                                                   TSW01710
      DO 201 J=3,NSLMAX                                                 TSW01720
  201 STRMO(I,J)=0.                                                     TSW01730
      WRITE(6,115)                                                      TSW01740
      CALL TSTING                                                       TSW01750
      WRITE (6,95)                                                      TSW01760
      WRITE (6,2005)                                                    TSW01770
C..... FORMATS .....TSW01780
 0054 FORMAT(54H0THE SUBROUTINE HAS ILLEGALLY CHANGED THE VALUE OF EN(, TSW01790
     *          I2,3H1).)                                              TSW01800
 0055 FORMAT(54H0THE SUBROUTINE HAS ILLEGALLY CHANGED THE VALUE OF EN(, TSW01810
     *          I2,3H1).)                                              TSW01820
 0056 FORMAT(57H0THE SUBROUTINE HAS ILLEGALLY CHANGED THE VALUE OF STRMITSW01830
     *(,I2,1H,,I2,2H).)                                               TSW01840
 0057 FORMAT(57H0THE SUBROUTINE HAS ILLEGALLY CHANGED THE VALUE OF STRMOTSW01850
     *(,I2,1H,,I2,2H).)                                               TSW01860
  95  FORMAT(14H1TESTER OUTPUT )                                        TSW01870
  96  FORMAT(2A3)                                                       TSW01880
  97  FORMAT(5I10,7X,A3)                                                TSW01890
  99  FORMAT (8(A4,6X))                                                 TSW01900
 100  FORMAT(' ',5X,'SUBROUTINE NAME ',2A3,' IS ILLEGAL',/,'     PROPER TSW01910
     *NAMES ARE  ')                                                   TSW01920
 101  FORMAT(1H0,    ' COMMENTS AT START OF USER WRITTEN SUBROUTINE MUST TSW01930
     *INCLUDE '/                                                      TSW01940
     *       '0      SOURCE OF MODEL'/'       MODIFICATION OF MODEL'/' TSW01950
     *    TYPE OF PROGRAM'/'       PROGRAM DESCRIPTION'/'       DEFINITTSW01960
     *ION OF PARAMETERS'/'       AUTHOR NAMES AND ADDRESSES'/'       COMTSW01970
     *MENTS DESCRIBING EACH OPERATION IN YOUR PROGRAM')                TSW01980
 103  FORMAT(8F10.3)                                                    TSW01990
 104  FORMAT('0',5X,' WARNING.. STRMI(',2I3,')HAS NEGATIVE VALUE')      TSW02000
 105  FORMAT('0',5X,' WARNING.. STRMI(',2I3,') HAS VALUE OF ZERO')      TSW02010
 106  FORMAT('0',5X,'WARNING...STMEST(',2I3,') HAS NEGATIVE VALUE')     TSW02020
 107  FORMAT('0',5X,' WARNING...STMEST(',2I3,') HAS VALUE OF ZERO')     TSW02030
 108  FORMAT( 35H0GIVEN THE FOLLOWING STREAM VECTORS/1H0,4X,5HSTRMI,54X,TSW02040
     * 5HSTRMO /(1H ,A4,6X,5F10.3,9X,5F10.3) )                         TSW02050
 109  FORMAT(37H0GIVEN THE FOLLOWING EQUIPMENT VECTOR//(1H ,A4,F10.3))  TSW02060
 110  FORMAT( 63H0YOUR SUBROUTINE CALCULATED THE FOLLOWING OUTPUT STREAMTSW02070
     * VECTORS/1H0,4X,5HSTRMO,54X,16HESTIMATED VALUES/(1H ,A4,6X,5F10.3,TSW02080
     * 9X,5F10.3))                                                     TSW02090
 111  FORMAT('0',5X,'STRMO(',2I3,') HAS VALUE',F10.3,' CHECK TO SEE' /  TSW02100
```

```
     *' IF THIS NEGATIVE VALUE IS CORRECT')                                  TSW02110
112   FORMAT('0',5X,'STRMO(',213,') HAS VALUE ZERO.' / '     CHECK TO STSW02120
     *EE IF THIS IS CORRECT')                                                TSW02130
113   FORMAT(42H0ESTIMATED AND CALCULATED VALUES OF STRMO(,I2,1H,,I2,    TSW02140
     *61H) DIFFER BY MORE THAN 100 PER CENT OF THE SMALLER OF THE TWO.) TSW02150
114   FORMAT('0',5X,'CHECK THE FOLLOWING  ' / '    POOR ESTIMATES' /     TSW02160
     *'    ARE PARAMETERS IN CORRECT POSITIONS IN VECTORS ' / '    CHECKTSW02170
     * ARITHMETIC STATEMENTS FOR BRACKETS,WRONG SEQUENCE ETC' /          TSW02180
     *'    TRY WRITING EQUATIONS FROM FORTRAN STATEMENTS AND CHECK' /    TSW02190
     *'    CHECK INPUT DATA')                                            TSW02200
115   FORMAT('0           STREAM VECTORS HAVE BEEN SET TO ZERO AND '/    TSW02210
     *' PROGRAM WILL BE RE-EXECUTED.  IF EXECUTION HALTS BEFORE NEXT'/    TSW02220
     *' TESTER OUTPUT, YOU HAVE NOT PROTECTED YOUR PROGRAM AGAINST'/      TSW02230
     *' DIVISION BY ZERO-VALUED STREAM VECTOR COMPONENTS.')               TSW02240
120   FORMAT('0',5X,2A3,5X,2A3,5X,2A3,5X,2A3,5X,2A3)                      TSW02250
906   FORMAT(1H0,10X,26HADDITIONAL INPUT DATA AEN(,I1,3H,3-,I2,1H)/       TSW02260
     *      (1H ,8X,5(1X,I2,1X,1PE10.3)))                                TSW02270
951   FORMAT(57H0YOUR SUBROUTINE WILL NOW BE EXECUTED WITH THE ABOVE DATTSW02280
     *A)                                                                 TSW02290
952   FORMAT(79H YOUR SUBROUTINE HAS NOW BEEN EXECUTED - ANY PRINTOUT FRTSW02300
     *OM IT, ABOVE, SHOULD BE /80H AS EXPECTED WITH THE GIVEN VALUE OF KTSW02310
     *SETS.  FOR EXAMPLE, PRINTOUT OF STRMI(1,3) /80H FOR DEBUGGING MAY TSW02320
     *BE COMMANDED WITH THE DATA KSETS=1 IF THE SUBROUTINE CONTAINS /     TSW02330
     *27H THE FOLLOWING STATEMENTS../41H0       IF(KSETS.EQ.1)WRITE(6,1)STSW02340
     *TRMI(1,3)/36H   0001 FORMAT(12H STRMI(1,3)=,10E.3)/)               TSW02350
961   FORMAT(26H GIVEN SUBROUTINE NAME IS ,2A3)                           TSW02360
971   FORMAT(41H0GIVEN NUMBER OF INPUT STREAMS IS        ,I3/            TSW02370
     *       41H GIVEN NUMBER OF OUTPUT STREAMS IS       ,I3/            TSW02380
     *       41H GIVEN LENGTH OF STREAM VECTOR IS        ,I3/            TSW02390
     *       41H GIVEN LENGTH OF EQUIPMENT VECTOR IS     ,I3/            TSW02400
     *       41H GIVEN SUBROUTINE ACTION SIGNAL KSETS IS ,I3)            TSW02410
2005 FORMAT(79H YOUR SUBROUTINE HAS BEEN SUCCESSFULLY RE-EXECUTED WITH TSW02420
     *INITIAL VALUES OF ZERO./27H THIS IS THE END OF TESTER.)            TSW02430
      STOP                                                              TSW02440
      END                                                               TSW02450
```

B.4.2 Standard Version

The following 6 pages reproduce the source program listing.

```
C********** TESTER **********                                          TSN00010
C THIS PROGRAM IS INTENDED TO TEST PROCESS MODEL SUBROUTINES           TSN00020
C  BEFORE THEY ARE USED WITH THE EXECUTIVE.                            TSN00030
C  WRITTEN BY K.W.BIRKETT OF THE UNIVERSITY OF WATERLOO , MAY 1973.    TSN00040
C REVISED BY F.J. ALLAN  OF B. AND P. SILVESTON, ENGINEERS,  FEB/74.   TSN00050
C AND AGAIN IN MAY/74..                                                TSN00060
C                                                                      TSN00070
C DECLARATION OF VARIABLES                                             TSN00080
C                                                                      TSN00090
C THE COMMON BLOCK PRODAT IS TO BE AVAILABLE TO THE SUBROUTINE...      TSN00100
C  THIS STATEMENT MUST APPEAR IN IT ALSO.                              TSN00110
      COMMON/PRODAT/STRMI(5,25),  SN(75,25),  PAPER(2,10),  AEN(2,40), TSN00120
     *              STRMO(5,25),  EN(20,20),  NPAPER(20),   KSETS, NE  TSN00130
C THE COMMON BLOCK EQPNAM IS TO BE AVAILABLE TO THE BLOCK DATA         TSN00140
C SUBPROGRAM SUPPLIED WITH THE PROCESS SUBROUTINE... THIS STATEMENT    TSN00150
C MUST APPEAR IN IT ALSO.                                              TSN00160
      COMMON/EQPNAM/NAMEN(50,20)                                       TSN00170
C THE COMMON BLOCK NITNAM IS TO BE AVAILABLE TO THE BLOCK DATA         TSN00180
C SUBPROGRAM SUPPLIED WITH TESTER... THIS STATEMENT APPEARS IN IT ALSO. TSN00190
      COMMON/NITNAM/ NAME2(50),NAME(50)                                TSN00200
C THE FOLLOWING ARRAYS ARE NOT NEEDED OUTSIDE THIS MAIN PROGRAM.       TSN00210
      DIMENSION STMEST(5,25),NAMPRC(2),NAMESN(25),EQPEST(20,20),EPS(40),TSN00220
     *          SI(5,2),SO(5,2)                                        TSN00230
      EQUIVALENCE (EPS(1),SI(1,1)),(EPS(11),SO(1,1))                   TSN00240
      DATA IBLANK/4H    /                                              TSN00250
      WRITE(6,95)                                                      TSN00260
C  READ IN USERS SUBROUTINE NAME                                       TSN00270
      READ(5,96)NAMPRC(1),NAMPRC(2)                                    TSN00280
      WRITE(6,961) NAMPRC(1),NAMPRC(2)                                 TSN00290
C  TEST USER SUBROUTINE NAME TO SEE IF IT IS A LEGAL S E P S I M       TSN00300
C  NAME. PRINT WARNING IF IT IS NOT.                                   TSN00310
      DO 4 NDX=1,50                                                    TSN00320
      IF(NAMPRC(2).EQ.NAME(NDX))  GO TO 1                              TSN00330
  4   CONTINUE                                                         TSN00340
      GO TO 70                                                         TSN00350
  1   DO 2 I=1,50                                                      TSN00360
      IF(NAMPRC(1).EQ.NAME2(I)) GO TO 3                                TSN00370
  2   CONTINUE                                                         TSN00380
      GO TO 70                                                         TSN00390
  3   IF(I.EQ.NDX.OR.(I.EQ.33.AND.NDX.GT.32.AND.NDX.LT.43))GO TO 5     TSN00400
 70   NDX=50                                                           TSN00410
      WRITE(6,100)NAMPRC(1),NAMPRC(2)                                  TSN00420
C  SHOW CORRECT SUBROUTINE NAMES                                       TSN00430
      WRITE(6,120)(NAME2(I),NAME(I),I=1,50)                            TSN00440
C  READ IN CONTROL PARAMETERS                                          TSN00450
  5   READ (5,97)  NIN,NOUT,NSLMAX,KSETS                              TSN00460
      WRITE(6,971) NIN,NOUT,NSLMAX,KSETS                               TSN00470
C  SHOW CORRECT DOCUMENTATION THAT IS REQUIRED IN USER SUBROUTINES      TSN00480
      WRITE(6,101)                                                     TSN00490
C READ EN AND EQPEST VECTORS                                           TSN00500
C FIRST OBTAIN USABLE PARAMETER NAMES IF SUBROUTINE NAME WAS ILLEGAL   TSN00510
      IF(NDX.NE.50)GO TO 13                                            TSN00520
      WRITE(6,121)                                                     TSN00530
      DO 141 I=1,20                                                    TSN00540
 141  NAMEN(50,I)=IBLANK                                               TSN00550
 13   WRITE(6,122)                                                     TSN00560
```

```
C I/O OF EQUIPMENT VECTORS PERMITTING A VECTOR TO BE STORED IN MORE THANTSN00570
C ONE ROW OF EN...  M IS THE WIDTH OF A ROW IN EN, N IS THE WIDTH OF A  TSN00580
C ROW OF DATA ON A CARD...  ASSUMED THAT M GT N.                         TSN00590
      M=20                                                              TSN00600
      N=8                                                               TSN00610
      WRITE(6,109)                                                      TSN00620
      READ(5,103) (EPS(I),I=1,N)                                        TSN00630
      RNE=EPS(1)                                                        TSN00640
      NE=IFIX(RNE)                                                      TSN00650
      RLN=EPS(2)                                                        TSN00660
      LN=IFIX(EPS(2))                                                   TSN00670
      NE1=NE                                                            TSN00680
      LN1=LN                                                            TSN00690
      DO 1102 I=1,N                                                     TSN00700
 1102 EN(NE,I)=EPS(I)                                                   TSN00710
      IF(LN.LT.M)M=LN                                                   TSN00720
      IF(LN.LE.N)GO TO 1103                                             TSN00730
      N=N+1                                                             TSN00740
      READ(5,103)(EN(NE,J),J=N,M)                                       TSN00750
 1103 WRITE(6,905)(J,NAMEN(NDX,J),EN(NE,J),J=1,M)                       TSN00760
      IF(LN.LE.M)GO TO 1149                                             TSN00770
      K=M+M                                                             TSN00780
 1104 NE=NE+1                                                           TSN00790
      IF(LN.LT.K)M=LN-K+M                                               TSN00800
      READ(5,103)(EN(NE,J),J=1,M)                                       TSN00810
      WRITE(6,9004)NE,(J,EN(NE,J),J=1,M)                                TSN00820
      IF(LN.LE.K)GO TO 1149                                             TSN00830
      K=K+M                                                             TSN00840
      GO TO 1104                                                        TSN00850
C NOW REPEAT FOR EQPEST                                                 TSN00860
 1149 M=20                                                              TSN00870
      N=8                                                               TSN00880
      WRITE(6,804)                                                      TSN00890
      NE=NE1                                                            TSN00900
      LN=LN1                                                            TSN00910
      IF(LN.LT.M)M=LN                                                   TSN00920
      READ(5,103)(EQPEST(NE,J),J=1,M)                                   TSN00930
      WRITE(6,905)(J,NAMEN(NDX,J),EQPEST(NE,J),J=1,M)                   TSN00940
      IF(LN.LE.M)GO TO 1249                                             TSN00950
      K=M+M                                                             TSN00960
 1204 NE=NE+1                                                           TSN00970
      IF(LN.LT.K)M=LN-K+M                                               TSN00980
      READ(5,103)(EQPEST(NE,J),J=1,M)                                   TSN00990
      WRITE(6,9004)NE,(J,EQPEST(NE,J),J=1,M)                            TSN01000
      IF(LN.LE.K)GO TO 1249                                             TSN01010
      K=K+M                                                             TSN01020
      GO TO 1204                                                        TSN01030
C CHECK EN AND EQPEST FOR NEGATIVE OR ZERO INITIAL VALUES               TSN01040
 1249 NE=NE1                                                            TSN01050
      M=20                                                              TSN01060
      IF(LN1.LT.M)M=LN1                                                 TSN01070
      K=0                                                               TSN01080
      N=3                                                               TSN01090
 1299 DO 1300 I=N,M                                                     TSN01100
      IF(EN(NE,I).LT.0.0)WRITE(6,50)NE,I                                TSN01110
      IF(EN(NE,I).EQ.0.0)WRITE(6,51)NE,I                                TSN01120
```

```
      IF(EQPEST(NE,I).LT.0.0)WRITE(6,52)NE,I                    TSN01130
      IF(EQPEST(NE,I).EQ.0.0)WRITE(6,53)NE,I                    TSN01140
 1300 CONTINUE                                                  TSN01150
      K=K+M                                                     TSN01160
      IF(LN1.LE.K)GO TO 1250                                    TSN01170
      NE=NE+1                                                   TSN01180
      IF(LN1.LT.K+M)M=LN1-K                                     TSN01190
      N=1                                                       TSN01200
      GO TO 1299                                                TSN01210
C I/O OF ADDITIONAL DATA AEN                                    TSN01220
 1250 READ(5,103) (EPS(I),I=1,8)                                TSN01230
      NE=IFIX(EPS(1))                                           TSN01240
      IF(NE.LE.0)GO TO 1271                                     TSN01250
      LN=IFIX(EPS(2))                                           TSN01260
      IF(LN.GT.8)READ(5,103)(EPS(I),I=9,LN)                     TSN01270
      WRITE(6,906)NE,LN,(I,EPS(I),I=3,LN)                       TSN01280
      DO 1252 I=3,LN                                            TSN01290
 1252 AEN(NE,I)=EPS(I)                                          TSN01300
      GO TO 1250                                                TSN01310
C  READ NAMES OF STREAM VECTOR PARAMETERS                       TSN01320
 1271 READ(5,99)(NAMESN(I),I=1,NSLMAX)                          TSN01330
      DO 220 I=1,NIN                                            TSN01340
      READ(5,103)(STRMI(I,J),J=1,NSLMAX)                        TSN01350
      SI(I,1)=STRMI(I,1)                                        TSN01360
 0220 SI(I,2)=STRMI(I,2)                                        TSN01370
      DO 221 I=1,NOUT                                           TSN01380
      READ (5,103) (STRMO(I,J),J=1,NSLMAX)                      TSN01390
      SO(I,1)=STRMO(I,1)                                        TSN01400
      SO(I,2)=STRMO(I,2)                                        TSN01410
 221  READ(5,103)(STMEST(I,J),J=1,NSLMAX)                       TSN01420
      WRITE(6,108)                                              TSN01430
      DO 1601 J=1,NSLMAX                                        TSN01440
 1601 WRITE (6,1101) NAMESN(J),(STRMI(I,J),I=1,NIN)             TSN01450
      WRITE(6,1081)                                             TSN01460
      DO 1602 J=1,NSLMAX                                        TSN01470
 1602 WRITE (6,1101) NAMESN(J),(STRMO(I,J),I=1,NOUT)            TSN01480
      WRITE(6,1082)                                             TSN01490
      DO 1603 J=1,NSLMAX                                        TSN01500
 1603 WRITE (6,1101) NAMESN(J),(STMEST(I,J),I=1,NOUT)           TSN01510
C  CHECK STRMI FOR NEGATIVE OR ZERO VALUES SUPPLIED IN DATA.    TSN01520
      DO 22 I=1,NIN                                             TSN01530
      DO 22 J=1,NSLMAX                                          TSN01540
      IF(STRMI(I,J)) 20,21,22                                   TSN01550
  20  WRITE(6,104)I,J                                           TSN01560
      GO TO 22                                                  TSN01570
  21  WRITE(6,105)I,J                                           TSN01580
  22  CONTINUE                                                  TSN01590
C  CHECK STMEST FOR NEGATIVE OR ZERO VALUES SUPPLIED AS DATA.   TSN01600
      DO 12 I=1,NOUT                                            TSN01610
      DO 12 J=1,NSLMAX                                          TSN01620
      IF(STMEST(I,J)) 30,31,12                                  TSN01630
  30  WRITE(6,106)I,J                                           TSN01640
      GO TO 12                                                  TSN01650
  31  WRITE(6,107)I,J                                           TSN01660
  12  CONTINUE                                                  TSN01670
C EXECUTE SUBROUTINE WITH GIVEN INITIAL VALUES                  TSN01680
```

```
      WRITE (6,951)                                                    TSN01690
      NE=NE1                                                           TSN01700
      CALL TSTING                                                      TSN01710
      WRITE (6,95)                                                     TSN01720
      WRITE (6,952)                                                    TSN01730
C  PRINT OUT RESULTS OF OUTPUT STREAM VECTOR CALCULATED IN THE USER    TSN01740
C  WRITTEN SUBROUTINE.                                                TSN01750
      WRITE(6,110)                                                     TSN01760
      DO 1600 J=1,NSLMAX                                               TSN01770
 1600 WRITE (6,1101) NAMESN(J),(STRMO(I,J),I=1,NOUT)                   TSN01780
C CHECK FOR CHANGES IN FIRST TWO ELEMENTS OF VECTORS                   TSN01790
      DO 1311 J=1,2                                                    TSN01800
      DO 1310 I=1,NIN                                                  TSN01810
      IF(STRMI(I,J).NE.SI(I,J))WRITE(6,56)I,J                          TSN01820
 1310 CONTINUE                                                         TSN01830
      DO 1311 I=1,NOUT                                                 TSN01840
      IF(STRMO(I,J).NE.SO(I,J))WRITE(6,57)I,J                          TSN01850
 1311 CONTINUE                                                         TSN01860
C  CHECK FOR NEGATIVE OR ZERO VALUES IN STRMO FROM USER                TSN01870
C  WRITTEN SUBROUTINE.                                                TSN01880
      DO 14 I=1,NOUT                                                   TSN01890
      DO 14 J=3,NSLMAX                                                 TSN01900
      IF(STRMO(I,J)) 40,41,14                                          TSN01910
  40  WRITE(6,111)I,J,STRMO(I,J)                                       TSN01920
      GO TO 14                                                         TSN01930
  41  WRITE(6,112)I,J                                                  TSN01940
  14  CONTINUE                                                         TSN01950
C  COMPARE USER CALCULATED RESULTS IN STRMO TO ESTIMATED RESULTS       TSN01960
C  IN STMEST.                                                         TSN01970
      NCOUNT=0                                                         TSN01980
      DO 15 I=1,NOUT                                                   TSN01990
      DO 15 J=3,NSLMAX                                                 TSN02000
      A=STMEST(I,J)                                                    TSN02010
      B=STRMO(I,J)                                                     TSN02020
      C=ABS(A-B)                                                       TSN02030
      IF(A.GE.C.AND.B.GE.C)  GO TO 15                                  TSN02040
      WRITE (6,113)I,J                                                 TSN02050
      NCOUNT=1                                                         TSN02060
  15  CONTINUE                                                         TSN02070
C  IF RESULTS ARE IN DISAGREEMENT WITH ESTIMATES ,                     TSN02080
C  PRINT OUT A CHECK LIST.                                            TSN02090
      IF (NCOUNT)60,60,61                                              TSN02100
 61   WRITE(6,114)                                                     TSN02110
C PRINT OUT VALUES OF EN VECTOR AS POSSIBLY MODIFIED BY SUBROUTINE     TSN02120
      WRITE(6,59)                                                      TSN02130
      NE=NE1                                                           TSN02140
      LN=LN1                                                           TSN02150
      M=20                                                             TSN02160
      IF(LN.LT.M)M=LN                                                  TSN02170
      WRITE(6,905)(J,NAMEN(NDX,J),EN(NE,J),J=1,M)                      TSN02180
      IF(LN.LE.M)GO TO 1500                                            TSN02190
      K=M+M                                                            TSN02200
   16 NE=NE+1                                                          TSN02210
      IF(LN.LT.K)M=LN-K+M                                              TSN02220
      WRITE(6,9004)NE,(J,EN(NE,J),J=1,M)                               TSN02230
      IF(LN.LE.K)GO TO 1500                                            TSN02240
```

```
      K=K+M                                                              TSN02250
      GO TO 16                                                           TSN02260
 1500 IF(EN(NE1,1).NE.RNE)WRITE(6,54)NE1                                 TSN02270
      IF(EN(NE1,2).NE.RLN )WRITE(6,55)NE1                                TSN02280
C COMPARE EN AFTER SUBROUTINE CALCULATIONS TO ESTIMATED VALUES           TSN02290
      NE=NE1                                                             TSN02300
      M=20                                                               TSN02310
      IF(LN1.LT.M)M=LN1                                                  TSN02320
      K=0                                                                TSN02330
      N=3                                                                TSN02340
      NCOUNT=0                                                           TSN02350
 1320 DO 1350 I=N,M                                                      TSN02360
      IF(EN(NE,I).LT.0.0)WRITE(6,50)NE,I                                 TSN02370
      IF(EN(NE,I).EQ.0.0)WRITE(6,51)NE,I                                 TSN02380
      A=EQPEST(NE,I)                                                     TSN02390
      B=EN(NE,I)                                                         TSN02400
      C=ABS(A-B)                                                         TSN02410
      IF(A.GE.C.AND.B.GE.C)GO TO 1350                                    TSN02420
      WRITE(6,58)NE,I                                                    TSN02430
      NCOUNT=1                                                           TSN02440
 1350 CONTINUE                                                           TSN02450
      K=K+M                                                              TSN02460
      IF(LN1.LE.K)GO TO 1400                                             TSN02470
      NE=NE+1                                                            TSN02480
      IF(LN1.LT.K+M)M=LN1-K                                              TSN02480
      N=1                                                                TSN02500
      GO TO 1320                                                         TSN02510
 1400 IF(NCOUNT.EQ.1)WRITE(6,114)                                        TSN02520
C  SET STRMI AND STRMO TO ZERO.                                          TSN02530
   60 DO 200 I=1,NIN                                                     TSN02540
      DO 200 J=3,NSLMAX                                                  TSN02550
  200 STRMI(I,J)=0.                                                      TSN02560
     *(,I2,1H,,I2,2H).)                                                  TSN02760
 0058 FORMAT(45H0ESTIMATED AND CALCULATED FINAL VALUES OF EN(,I2,1H,,I2,TSN02770
     *11H) DIFFER BY/47H MORE THAN 100 PER CENT OF THE SMALLER OF THE 2)TSN02780
 0059 FORMAT(30H0EQUIPMENT VECTOR FINAL VALUES/)                         TSN02790
   95 FORMAT(14H1TESTER OUTPUT )                                         TSN02800
   96 FORMAT(2A3)                                                        TSN02810
 0097 FORMAT(4I10)                                                       TSN02820
   99 FORMAT (8(A4,6X))                                                  TSN02830
  100 FORMAT(' ',5X,'SUBROUTINE NAME ',2A3,' IS ILLEGAL',/,'     PROPER TSN02840
     *NAMES ARE  ')                                                      TSN02850
  101 FORMAT(1H0,    ' COMMENTS AT START OF USER WRITTEN SUBROUTINE MUST TSN02860
     *INCLUDE '/                                                         TSN02870
     *       '0      SOURCE OF MODEL'/'       MODIFICATION OF MODEL'/'  TSN02880
     *     TYPE OF PROGRAM'/'       PROGRAM DESCRIPTION'/'       DEFINITSN02890
     *ION OF PARAMETERS'/'       AUTHOR NAMES AND ADDRESSES'/'       COMTSN02900
     *MENTS DESCRIBING EACH OPERATION IN YOUR PROGRAM')                   TSN02910
  103 FORMAT(8F10.3)                                                     TSN02920
  104 FORMAT('0',5X,' WARNING.. STRMI(',2I3,')HAS NEGATIVE VALUE')       TSN02930
  105 FORMAT('0',5X,' WARNING.. STRMI(',2I3,') HAS VALUE OF ZERO')       TSN02940
  106 FORMAT('0',5X,'WARNING...STMEST(',2I3,') HAS NEGATIVE VALUE')      TSN02950
  107 FORMAT('0',5X,' WARNING...STMEST(',2I3,') HAS VALUE OF ZERO')      TSN02960
  108 FORMAT( 35H0GIVEN THE FOLLOWING STREAM VECTORS/20H0PROCESS INPUT STSN02970
     *TRMI/)                                                             TSN02980
  109 FORMAT(37H0GIVEN THE FOLLOWING EQUIPMENT VECTOR/)                  TSN02990
```

```
  110  FORMAT( 77H0YOUR SUBROUTINE CALCULATED THE FOLLOWING PROCESS OUTPUTSN03000
     *T STREAM VECTORS STRMO/)                                            TSN03010
  111  FORMAT('0',5X,'STRMO(',2I3,') HAS VALUE',F10.3,' CHECK TO SEE' /  TSN03020
     *' IF THIS NEGATIVE VALUE IS CORRECT')                               TSN03030
  112  FORMAT('0',5X,' STRMO(',2I3,') HAS VALUE ZERO.' / '     CHECK TO STSN03040
     *EE IF THIS IS CORRECT')                                             TSN03050
  113  FORMAT(42H0ESTIMATED AND CALCULATED VALUES OF STRMO(,I2,1H,,I2,    TSN03060
     *11H) DIFFER BY/47H MORE THAN 100 PER CENT OF THE SMALLER OF THE 2)TSN03070
  114  FORMAT('0',5X,'CHECK THE FOLLOWING  ' / '    POOR ESTIMATES' /    TSN03080
     *'     ARE PARAMETERS IN CORRECT POSITIONS IN VECTORS ' / '    CHECKTSN03090
     * ARITHMETIC STATEMENTS FOR BRACKETS,WRONG SEQUENCE ETC' /          TSN03100
     *'     TRY WRITING EQUATIONS FROM FORTRAN STATEMENTS AND CHECK' /   TSN03110
     *'     CHECK INPUT DATA')                                          TSN03120
  115  FORMAT('0            STREAM VECTORS HAVE BEEN SET TO ZERO AND '/  TSN03130
     *' PROGRAM WILL BE RE-EXECUTED.  IF EXECUTION HALTS BEFORE NEXT'/   TSN03140
     *' TESTER OUTPUT, YOU HAVE NOT PROTECTED YOUR PROGRAN AGAINST'/     TSN03150
     *' DIVISION BY ZERO-VALUED STREAM VECTOR COMPONENTS.')              TSN03160
  120  FORMAT('0',5X,2A3,5X,2A3,5X,2A3,5X,2A3,5X,2A3)                     TSN03170
  121  FORMAT( 89H0EQUIPMENT PARAMETER NAMES CANNOT BE PRINTED SINCE SUBRTSN03180
     -OUTINE NAME SUPPLIED IS NOT LEGAL. /)                              TSN03190
  122  FORMAT( 71H0IF TESTER STOPS HERE DUE TO NAMEN BEING UNDEFINED, THETSN03200
     -N THE BLOCK DATA/54H SUBPROGRAM SUPPLIED WITH THE SUBROUTINE IS INTSN03210
     *CORRECT./)                                                         TSN03220
 0804  FORMAT(63H0GIVEN THE FOLLOWING ESTIMATES OF EQUIPMENT VECTOR FINALTSN03230
     * VALUES/)                                                          TSN03240
  805  FORMAT(1H /(1H ,7X,3(3X,I2,1X,A4,1H=,F10.3)))                      TSN03250
  906  FORMAT(1H0,10X,26HADDITIONAL INPUT DATA AFN(,I1,3H,3-,I2,1H)/      TSN03260
     *      (1H ,8X,5(1X,I2,1X,1PE10.3)))                               TSN03270
  951  FORMAT(57H0YOUR SUBROUTINE WILL NOW BE EXECUTED WITH THE ABOVE DATTSN03280
     *A)                                                                 TSN03290
  952  FORMAT(79H YOUR SUBROUTINE HAS NOW BEEN EXECUTED - ANY PRINTOUT FRTSN03300
     *OM IT, ABOVE, SHOULD BE /80H AS EXPECTED WITH THE GIVEN VALUE OF KTSN03310
     *SETS.  FOR EXAMPLE, PRINTOUT OF STRMI(1,3) /80H FOR DEBUGGING MAY TSN03320
     *BE COMMANDED WITH THE DATA KSETS=1 IF THE SUBROUTINE CONTAINS /    TSN03330
     *27H THE FOLLOWING STATEMENTS../41H0      IF(KSETS.EQ.1)WRITE(6,1)STSN03340
     *TRMI(1,3)/36H  0001 FORMAT(12H STRMI(1,3)=,10E.3)/)                TSN03350
  961  FORMAT(26H GIVEN SUBROUTINE NAME IS ,2A3)                          TSN03360
  971  FORMAT(41H0GIVEN NUMBER OF INPUT STREAMS IS        ,I3/          TSN03370
     *       41H GIVEN NUMBER OF OUTPUT STREAMS IS       ,I3/          TSN03380
     *       41H GIVEN LENGTH OF STREAM VECTOR IS        ,I3/          TSN03390
     *       41H GIVEN SUBROUTINE ACTION SIGNAL KSETS IS ,I3)          TSN03400
 1081  FORMAT(1H0/36H PROCESS OUTPUT STRMO INITIAL VALUES/)               TSN03410
 1082  FORMAT(1H0/29H ESTIMATED STRMO FINAL VALUES/)                      TSN03420
 1101  FORMAT(1H ,A4,6X,5F10.3)                                           TSN03430
 2005  FORMAT(79H YOUR SUBROUTINE HAS BEEN SUCCESSFULLY RE-EXECUTED WITH TSN03440
     *INITIAL VALUES OF ZERO./27H THIS IS THE END OF TESTER.)            TSN03450
 9004  FORMAT(1H ,10X,19HADDITIONAL ROW, NE=,I3/                          TSN03460
     *      (1H ,8X,5(1X,I2,1X,1PE10.3)))                               TSN03470
       STOP                                                             TSN03480
       END                                                              TSN03490
       BLOCK DATA                                                       TSN03500
C                                                                       TSN03510
C  THIS SUBPROGRAM INITIALIZES VARIABLES IN COMMON BLOCK                TSN03520
       COMMON/NITNAM/ NAME2(50),NAME(50)                                TSN03530
C  FOR SUBROUTINE NAMES USED AS A STANDARD BY THE MAIN PROGRAM.         TSN03540
C                                                                       TSN03550
```

```
      DATA NAME2 /                    3HMIX,3HPRI,3HTRF,3HACS,3HACS,3HDIG,TSN03560
     *3H CH,3HSEC,3HBFL,3H VA,3HMEC,3H DR,3H TH,3H WA,3H XF,3H HI,3H  C,TSN03570
     *3H XF,3HPHC,3HADS,3H DI,3H ST,3H XC,3H  X,3HXTR,3HDST,3H FL,3HXTR,TSN03580
     *3H CR,3H BL,3H CO,3HREA,3HUNA,3HUNA,3HUNA,3HUNA,3HUNA,3HUNA,3HUNA,TSN03590
     *3HUNA,3HUNA,3HUNA,3H    ,3H    ,3H    ,3H    ,3H    ,3H    ,3H    ,3H DU/TSN03600
      DATA NAME /                     3HER3,3HSTL,3HLTR,3HLD1,3HLD2,3HSTR,TSN03610
     *3HLOR,3HSET,3HTER,3HCFL,3HFIL,3HYER,3HICK,3HSHR,3HLOT,3HOXP,3HOAG,TSN03620
     *3HLOC,3HONT,3HORP,3HALS,3HRIP,3HHAN,3HCIN,3HANS,3HIL1,3HASH,3HAC2,TSN03630
     *3HYST,3HOW2,3HOL4,3HCT1,3HME0,3HME1,3HME2,3HME3,3HME4,3HME5,3HME6,TSN03640
     *3HME7,3HME8,3HME9,3H    ,3H    ,3H    ,3H    ,3H    ,3H    ,3H    ,3HMMY/TSN03650
C                                                                       TSN03660
      END                                                               TSN03670
```

B.5 Sample Output

The following page illustrates the output with the standard version. With the WATFIV version the output is the same except there is no reference to estimated equipment vector final values or to the Block Data subprogram.

```
TESTER OUTPUT
GIVEN SUBROUTINE NAME IS MIXER3

GIVEN NUMBER OF INPUT STREAMS IS          2
GIVEN NUMBER OF OUTPUT STREAMS IS         2
GIVEN LENGTH OF STREAM VECTOR IS          3
GIVEN SUBROUTINE ACTION SIGNAL KSETS IS   4

 COMMENTS AT START OF USER WRITTEN SUBROUTINE MUST INCLUDE

      SOURCE OF MODEL
      MODIFICATION OF MODEL
      TYPE OF PROGRAM
      PROGRAM DESCRIPTION
      DEFINITION OF PARAMETERS
      AUTHOR NAMES AND ADDRESSES
      COMMENTS DESCRIBING EACH OPERATION IN YOUR PROGRAM

IF TESTER STOPS HERE DUE TO NAMEN BEING UNDEFINED, THEN THE BLOCK DATA
SUBPROGRAM SUPPLIED WITH THE SUBROUTINE IS INCORRECT.


GIVEN THE FOLLOWING EQUIPMENT VECTOR

          EQVE=     5.000      LNTH=     4.000      MAG =     1.000
           DIV=     0.500

GIVEN THE FOLLOWING ESTIMATES OF EQUIPMENT VECTOR FINAL VALUES

          EQVE=     5.000      LNTH=     4.000      MAG =     1.000
           DIV=     0.500

GIVEN THE FOLLOWING STREAM VECTORS

PROCESS INPUT STRM1

STNO          1.000     2.000
VLN           3.000     3.000
FLOW          4.000     5.000


PROCESS OUTPUT STRM0 INITIAL VALUES

STNO          1.000     2.000
VLN           3.000     0.000
FLOW          0.000     0.000
```

```
ESTIMATED STRMO FINAL VALUES

STNO            1.000       2.000
VLN             0.000       0.000
FLOW            0.000       0.000

      WARNING...STMEST(  1   2) HAS VALUE OF ZERO

      WARNING...STMEST(  1   3) HAS VALUE OF ZERO

      WARNING...STMEST(  2   2) HAS VALUE OF ZERO

      WARNING...STMEST(  2   3) HAS VALUE OF ZERO


YOUR SUBROUTINE WILL NOW BE EXECUTED WITH THE ABOVE DATA


TESTER OUTPUT
YOUR SUBROUTINE HAS NOW BEEN EXECUTED - ANY PRINTOUT FROM IT, ABOVE, SHOULD BE
AS EXPECTED WITH THE GIVEN VALUE OF KSETS.  FOR EXAMPLE, PRINTOUT OF STRMI(1,3)
FOR DEBUGGING MAY BE COMMANDED WITH THE DATA KSETS=1 IF THE SUBROUTINE CONTAINS
THE FOLLOWING STATEMENTS..

      IF(KSETS.EQ.1)WRITE(6,1)STRMI(1,3)
 0001 FORMAT(12H STRMI(1,3)=,10E.3)


YOUR SUBROUTINE CALCULATED THE FOLLOWING PROCESS OUTPUT STREAM VECTORS STRMO

STNO            1.000       2.000
VLN             3.000       0.000
FLOW            5.000       5.000

ESTIMATED AND CALCULATED VALUES OF STRMO( 1, 3) DIFFER BY
MORE THAN 100 PER CENT OF THE SMALLER OF THE 2

ESTIMATED AND CALCULATED VALUES OF STRMO( 2, 3) DIFFER BY
MORE THAN 100 PER CENT OF THE SMALLER OF THE 2

     CHECK THE FOLLOWING
   POOR ESTIMATES
   ARE PARAMETERS IN CORRECT POSITIONS IN VECTORS
   CHECK ARITHMETIC STATEMENTS FOR BRACKETS,WRONG SEQUENCE ETC
   TRY WRITING EQUATIONS FROM FORTRAN STATEMENTS AND CHECK
   CHECK INPUT DATA

EQUIPMENT VECTOR FINAL VALUES


          EQVE=     5.000       LNTH=     4.000       MAG =     1.000
           DIV=     0.500

           STREAM VECTORS HAVE BEEN SET TO ZERO AND
PROGRAM WILL BE RE-EXECUTED.  IF EXECUTION HALTS BEFORE NEXT
TESTER OUTPUT, YOU HAVE NOT PROTECTED YOUR PROGRAM AGAINST
DIVISION BY ZERO-VALUED STREAM VECTOR COMPONENTS.


TESTER OUTPUT
YOUR SUBROUTINE HAS BEEN SUCCESSFULLY RE-EXECUTED WITH INITIAL VALUES OF ZERO.
THIS IS THE END OF TESTER.
```

B.6 Background Information

The TESTER program was originally developed by Mr. Ken Birkett and Dr. P.L. Silveston of B & P Silveston, Engineers, 550 Glasgow Street, Kitchener, Ontario, for the simulation workshop conducted under the auspices of EPS at the Canada Centre for Inland Waters, January, 1974. The latest version, by Mr. F. James Allan of B & P Silveston, Engineers, incorporates improvements suggested by experience at that workshop.

Additional information and copies of the TESTER program may be obtained from B & P Silveston, Engineers. There will be a nominal charge to cover costs of materials, preparation and mailing.