Optimal Design and Operation of Wastewater Treatment Plants

by

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cms (V,Q : Constant)

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ABSTRACT OF THE DISSERTATION

Optimal Design and Operation of

Wastewater Treatment Plants

by

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Traditional design procedures for wastewater treatment systems attempt to minimize total capital cost by considering steady state concepts for unit processes and design guidelines. Recent work has minimized capital as well as operation and maintenance costs using a single objective function and steady state models which are flawed because plant inputs vary as much as seven fold during a 24-hour period. Previous work using dynamic models for optimal design does not simultaneously consider both fixed and variable costs in a single objective function.

The objective of this dissertation was to develop a computer-based methodology which considers the dynamic interactions of unit processes and includes capital, operations and maintenance costs in a single objective function. This methodology can aid designers by selecting optimal design and operating parameters for the unit processes in order to produce the minimum, total discounted costs, while satisfying all design and operational constraints.

The treatment plant model includes primary clarification, aeration, secondary clarification, gravity thickening and anaerobic digestion. The dynamic model of a primary clarifier includes a non-steady state advection-diffusion equation which considers turbulence and deposit resuspension. From this an optimal depth to maximize efficiency was obtained. The activated sludge process model distinguishes between particulate and soluble substrates, and calculates oxygen requirements and sludge production from transient inputs and varying operating strategies. These form the basis of the variable operating costs.

The goal of the anaerobic digestion model was to predict gas flow rates and purities, volatile solids destruction, total and un-ionized volatile acids, and pH, for different solids retention times and organic loading rates. Methane gas production is based upon kinetics and stoichiometry which consider interspecies hydrogen transfer, the decomposition of propionate and butyrate to acetate, and aceticlastic methanogenesis. The revenues from methane production was subtracted from the variable operating costs.

The dynamic models of unit processes were interfaced with an optimization technique to determine optimal, independent design and operating parameters conforming to the EPA effluent quality standards. The models and optimization technique can be used to predict optimal design and operating parameters for future wastewater treatment plants, as well as minimizing the operating costs of existing plants.

It is concluded that the overall lifetime treatment plant cost is minimized if capital, operation, and maintenance costs are considered in a single objective function. It is demonstrated that this procedure produces a lower overall cost than stepwise procedures, which may provide a least-capital cost design, but

relies upon managers to minimize operational costs after plant construction. A sensitivity analysis of energy, labor, and sludge disposal costs was performed.

I. INTRODUCTION

The effect of pollution on society is recognized by most citizens and has resulted in a national commitment for the environmental clean-up. Public Law 92-500 was designed to "restore and maintain the chemical, physical and biological integrity of the nation's waters". This law changed the enforcement policy from stream standards to source standards (i.e. dischargers were required to limit their pollutants in accordance with EPA determined effluent limitations irrespective of the receiving body). Under this law, industries were required to employ the "best practicable technology" while municipalities were to provide a minimum of "secondary treatment" by 1977. Two thirds of all the municipalities in the nation needing to upgrade their treatment systems were unable to meet "secondary treatment" because of the magnitude of problems, and delays in Federal funding. Therefore a considerable amount of construction of new treatment plants and upgrading of the treatment facilities are expected in the near future. There is still ample opportunity to improve treatment plant design methodology to produce least cost designs.

The primary objective of wastewater treatment plant design is to provide treatment at a minimal cost while satisfying specific requirements. In least cost design studies, a total discounted cost is attained at the lowest possible level while satisfying a set of constraints. These constraints include (a) a specified effluent quality, and (b) various physical and biological constraints.

A recent trend in process research is to develop dynamic mathematical models which can be used to simulate treatment plant operation, and can lead to improved plant design and operation. Dynamic models are a useful tool for the calculation of predicted operating cost for computer controlled treatment

systems.

The main objective of this investigation is to develop a least cost design procedure for wastewater treatment systems, which satisfy a set of specified constraints, and minimize life time costs. Life time cost include capital, operation and maintenance costs. This work differs from the previous work in that the design and operation costs are considered in an integrated procedure. The specific objectives are:

1.   Model Development

    a.   develop and calibrate a dynamic mathematical model for primary clarifiers.

    b.   develop a dynamic mathematical model for activated sludge process including the dynamics of nitrification and solid liquid separation.

    c.   develop a dynamic mathematical model for the associated waste sludge treatment subsystem, anaerobic digestion, considering the new biological concepts of methanogenesis.

2.   Determine optimal least cost design and operation for a wastewater treatment system using the dynamic models coupled to a single economic objective function which includes capital cost, fixed and variable operation and maintenance cost. Figure 1.1 shows a typical treatment system.

For realistic model inputs, time series data were gathered and analyzed by Fourier transform analysis to obtain the deterministic components. Inputs to the model are constructed using the most significant Fourier coefficients, and
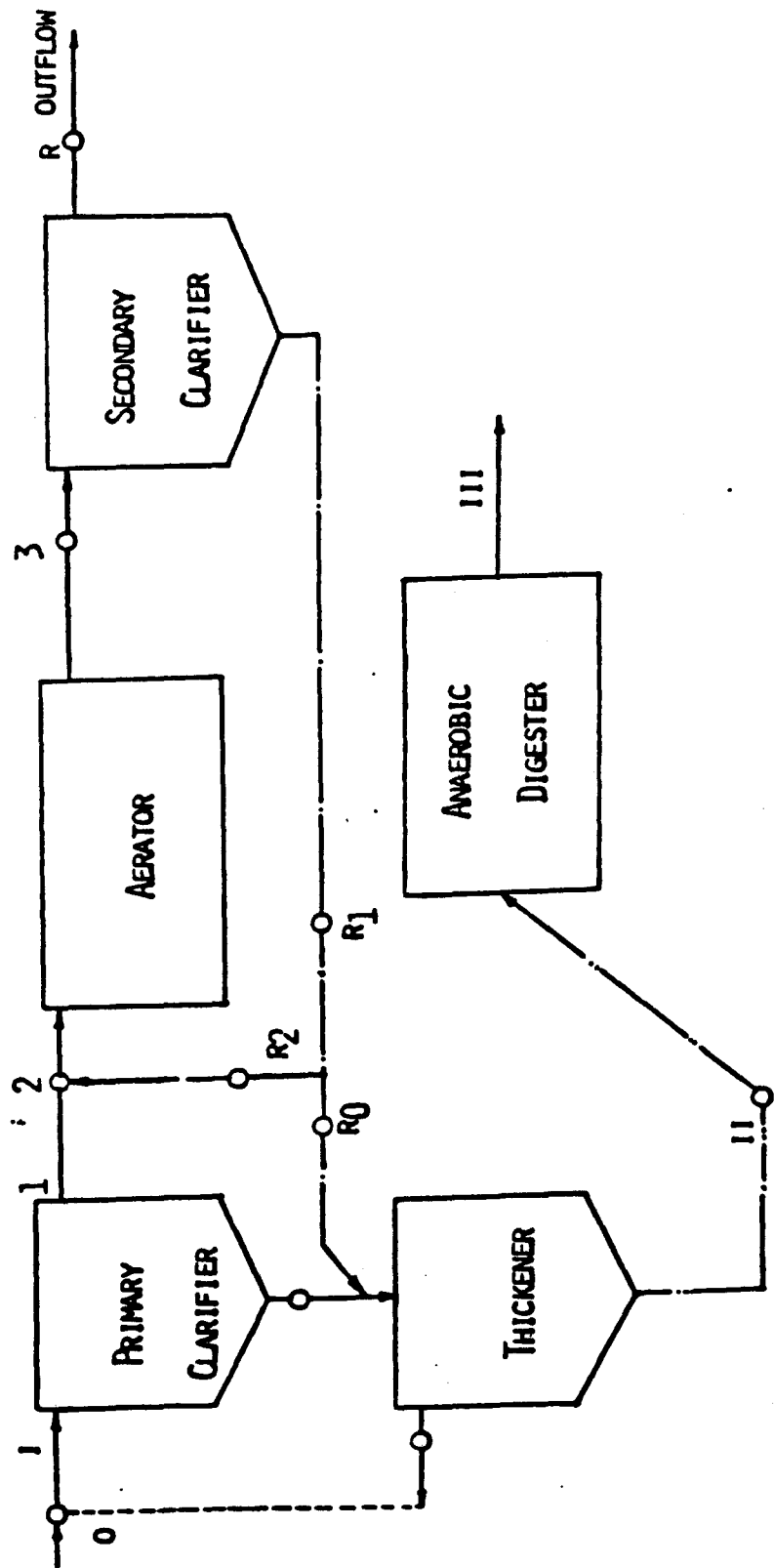
Fig. 1.1 Process System Diagram

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inputs perturbed with random noise are also considered to simulate realistic conditions.

The model of primary clarifier used herein is a modification of steady state model by Takamatsu et al. (1974) for non-steady state conditions. A non-steady state model is required for realistic input conditions, i.e. variable influent suspended solids concentration, BOD and flow rate. Turbulence and the effect of resuspension are also considered in the model.

The activated sludge process is a complex process mediated by a mixed population of organisms subject to varying physical and chemical characteristics of influent organic load and the variability of substrate concentration and flow rate. Conventional models for the process previously developed consider steady state conditions with assumptions of homogeneous substrates and organisms, and used zero-order, first-order or Monod (1942) kinetics for substrate removal. These methods are not capable of describing the rapid removal of substrates observed in case of the contact stabilization or step feed modifications of the activated sludge process. Storer and Gaudy (1969) have shown that the Monod (1942) model is not capable of predicting the lag in specific growth rate which occurs upon an increase in substrate concentration and influent flow rate.

The model of the activated sludge process used herein is a minor modification of the model proposed by Clift (1980) for carbonaceous substrate removal, combined with the nitrification model proposed by Poduska (1973). It is a structured model which overcomes the limitations of the zero order, first-order and Monod (1942) model. The carbonaceous model includes material balances of stored particulate mass, active, inert, stored, non-biodegradable mass and biodegradable and non-biodegradable soluble substrates. Material

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balances for ammonia, nitrite, nitrate and the nitrifying bacteria, *Nitrosomonas* and *Nitrobacter* are considered in the nitrification model. Material balances for oxygen utilization are also considered for both carbonaceous substrate removal and nitrification. The model for solid liquid separation is based upon solute flux theory as used by Dick (1970), and combines techniques used by other researchers (Bryant, 1972; Busby, 1973; Tracy, 1973, Stenstrom, 1976).

The sludge treatment subsystem considered includes gravity thickening and anaerobic digestion. The dynamic model of anaerobic digestion is developed considering new information, indicating that methanogens do not metabolize organic acids other than acetate and formate, with hydrogen production and utilization is a central position (Bryant, 1979). The dynamics of anaerobic digestion includes material balances for biodegradable solids, non-biodegradable solids, soluble organics, acids (propionic, n-butyric, and acetic) and hydrogen, biodegradable solid hydrolyzers, soluble substrate oxidizers, hydrogen consumers, and methane formers. The inhibition by un-ionized acids incorporated in Monod (1942) kinetics is considered in the model. The model also includes the carbonate material balance and theoretical calculation of pH.

In the past, the trend has been to design the most efficient unit processes, each at least cost and then combine the units to form an optimum wastewater treatment system. Erickson and Fan (1968), Naito et al. (1969), Fan et al. (1970, 1971), and McBeath and Eliassen (1966) conducted optimal design studies of the activated sludge subsystem (aeration tank and secondary clarifier). Parkin and Dague (1972) demonstrated that the most efficient individual units combined together may not produce an optimal system.

A large number of studies have been reported on the least cost design of treatment plants. Ecker and McNamara (1971), Shih and Krishnan (1969), and Shih and Defilippi (1970) used simple biological models for the optimal design of treatment plants, with the primary emphasis on the demonstration of a particular optimization technique, rather than working with a realistic problem. Parkin and Dague (1972), Middleton and Lawrence (1976), Berthouex (1975), and Fan et al. (1974) developed realistic biological models oriented towards practicing engineers, and used solution methods that can easily be applied to practice.

The original contribution of this dissertation is the development of a tool which can be used to produce an optimal treatment plant design, considering the time honored, traditional, design procedures, while simultaneously minimizing the capital and operating costs. A large fraction of the operating costs are calculated from the dynamic treatment plant models.

II. LITERATURE REVIEW

A. Primary Clarifier

Primary clarifiers in wastewater treatment plants are used to remove settleable solids from wastewater. Rich (1963) and Camp (1946) considered individual particle dynamics and demonstrated that settleable solids attain a terminal velocity with respect to carrier fluid, and proposed that this terminal velocity is a function of particle geometry and density and the fluid density and viscosity.

If all solids in wastewater are discrete particles of uniform size, shape and density and settle independently, i.e. no effect on the settling velocity of any other particles, then according to Camp (1946) and Rich (1963) the efficiency of sedimentation is only a function of terminal settling velocity. In the case of thickening, the particle concentration increases, causing a decrease in clarification rate. Camp (1953) developed an empirical equation using batch settling data to describe the performance and design of settling basins and proposed that the removal of suspended solids in sedimentation basins is mainly dependent on the surface area of the basin, and is unaffected by the depth of the tank, except through the influence of turbulence and scour at the bottom of the basin.

Solids in most wastewaters are not of such regular character, but heterogeneous in nature. Wastewater solids are flocculent, rather than discrete. Flocculation in sedimentation basin is due to the differences in settling velocities of particles and the velocity gradient in the liquid caused by the eddies, resulting from turbulence. As flocculent particles coalesce, the terminal velocity is

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increased, with an increasing efficiency as a function of detention time. (Camp, 1946; Fitch, 1957). The combined effect of flocculation and increasing solids concentration creates a difficult problem for the mathematical model. Therefore empirical analysis is frequently used for designing settling basins.

Hazen (1904) analyzed the settling of particles using the ideal basin concept. He assumed that (a) the direction of flow is horizontal uniform velocity throughout the settling zone, (b) the concentration of suspended particles is uniform over depth at the inlet of the settling zone, and (c) particles reaching the bottom remain discrete. His work demonstrated that the efficiency of sedimentation is governed by the surface area measured parallel to the direction of flow. Hazen (1904) and Camp (1953) concluded that the efficiency of primary sedimentation basin is independent of the basin depth but dependent on overflow rate. They have also proposed that for optimum efficiency, settling tanks should be long, narrow (minimize the effect of inlet and outlet disturbances, cross winds, density currents and longitudinal mixing) and relatively shallow. Hazen (1904) did not consider flocculation in his analysis.

The performance of settling basin is influenced by solids compaction rates, particle flocculation, solids settling characteristics, solids concentration, and inlet and outlet mixing patterns (Fitch, 1957; Wittwer, 1940). Babbit and Schlenz (1929) demonstrated that the hydraulic detention time, surface loading rate, and suspended solids concentration have marked influence in the efficiency of the sedimentation basin and removal efficiency increases with increase in retention time and solids concentration. Theroux and Betz (1959) conducted tests to determine the effect of surface loading rate, basin velocity, weir loading rates, and diurnal variation in influent flow rate and suspended

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solids concentration on the performance of primary sedimentation process. These data were used to develop an empirical equation to simulate suspended solids removal.

Villemónte et al. (1967) tested a prototype sedimentation basin characterizing the hydraulic flow regime and defined parameters such as short circuiting, stagnation, eddy diffusion, and recirculation eddy. Turbulent flow, currents induced by inertia of the incoming fluid, wind stress and density and temperature gradients, reduce efficiency. Short circuiting can be viewed as distorted plug flow, short detention time, increased overflow rate, with reduced efficiency. Villemonte et al. (1967) showed that real basins are neither plug flow nor complete mixing. The effects of short circuiting can be minimized by covering the basin (eliminates the effect of wind or heat induced currents), adding stream deflecting baffles, influent dividing mechanisms, and velocity dispersing feed walls. The effects of turbulence upon design and operational theory has been investigated by Dobbins(1944), Camp(1946), Goda(1956), and El-Baroudi(1969).

The empirical steady state model proposed by Smith (1969) predicts removal efficiency as an exponential function of overflow rate. function of a settler. Equation 2.1 is typical of empirical models used to describe primary clarifiers.

$$M_r = M_i \; f \, (Q_i, A, M_i)$$

(2.1)

where,

M	=	total concentration of settleable materials,
M_r	=	total concentration of settleable solids in the outflow of the settler,
M_i	=	total concentration in the inflow,

Q_i = inflow rate,
A = area of the settler.

Bryant (1972) developed a dynamic mathematical model considering both mixing and clarification. The hydraulic mixing regime is modeled as a series of complete mixing compartments, a technique commonly used in chemical engineering (Levenspiel, 1965; Himmelblau, 1968). Bryant (1972) approximated the mixing phenomena by considering five continuous stirred tank reactors in series, which leads to a mixing regime between a plug flow and complete mixing.

Settling basins are operated as continuous flow units and in order to deal with the time variation of flow rate and concentration, a dynamic model has to be developed. Takamatsu et al. (1974) developed a steady state mathematical model considering deposit scouring for the design of primary clarifier. Deposit scouring was treated by a diffusion type equation by introducing a parameter at the bottom boundary condition which described the rate of scouring and resuspension. The model developed later builds upon this concepts.

B. Activated Sludge Process

The activated sludge process oxidizes organic matter, both soluble and particulate in a semi-controlled environment with the presence of a mixed culture of organisms. The oxidation process removes nutrients and organics and returns the product of metabolism to the liquid.

Organics + nutrients + oxygen + Bacteria

----> New bacterial cells + residual organics

and inorganics + carbon-dioxide + water

+ energy

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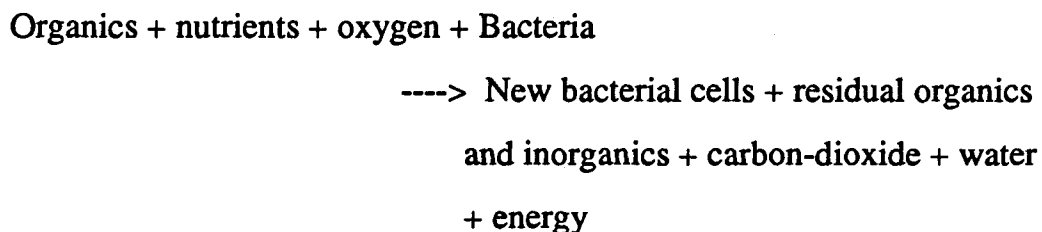
The actual oxidation is much more complex due to varying population of mixed culture and complex characteristics of organic matter.

The first mathematical model for continuous culture of micro-organisms was developed by Monod (1942). The purpose of the model is to describe the removal mechanism of a single substrate by a given bacterial population in a homogeneous medium. Monod kinetics, along with a first-order decay coefficient, adequately describes the steady state conventional activated sludge process over a limiting period.

Wastewater received by treatment plants contain a wide variety of substrates and operate with a heterogeneous mass, but the substrate and sludge mass have been considered homogeneous in the past. The Monod model does not predict the correct response with the process is subjected to time varying inputs. Reasons for this are the time lag in microbial growth and rapid uptake of exogenous substrate in the contact stabilization modification of the activated sludge process. More advanced models separate the microbial mass into different components such as stored reserves, active mass, particulate and inert mass.

Models used by Fan et al. (1974) and Kuo et al. (1974) include equations for dissolved and suspended components of substrates. Kinetics for growth upon suspended solids were considered as first-order, and dissolved substrate kinetics included an additional term in the denominator, proportional to suspended solids concentration, in order to reflect their masking effect.

The mathematical description of lag phase was first presented by Powell (1967). The incorporation of lag phase is essential for simulating the dynamic

response of an activated sludge process and one method for consideration of the lag period is to structure the microbial mass.

Most wastewater contains both soluble and particulate organic and inorganic matter. Heukelekian and Balmat (1959) proposed that domestic wastewater contains more organic carbon in colloidal and suspended form than the dissolved form. Hunter and Heukelekian (1965) found that particulate fraction is 66% to 83% organic and contributes 58% and 63% of volatile solids for domestic wastewater. The COD to volatile solids ratio for the particulate fraction is approximately 1.5 to 1.0 while for the soluble fraction varies from 0.6 to 0.8 to 1.0.

The composition of the sludge in the activated sludge process depends upon the characteristics of wastewater and design and operational characteristics of the process. Researchers have demonstrated that the potential activity of the sludge in the activated sludge process is only a small fraction of its total capacity. Garrett and Sawyer (1952) demonstrated that sludge in conventional plants react at only 4% of its maximum capability. Sludge consists of viable organisms, inert organic matter from death and lysis of cells, volatile solids and non-volatile solids from influent wastewater. The number of viable organisms and volatile solids in the sludge decreases as the sludge age increases, and the decrease is due to death of organisms, accumulation of inerts, depletion of particulate organic substrates and predator activity. Conventional and low rate sludges consists largely of non-viable solids. Weddle and Jenkins (1971) proposed that the viable heterotrophic organisms concentration in sludge is between 10% to 20%. Upadhyaya and Eckenfelder (1975) measured the biodegradable fraction of mixed liquor grown on skim milk to find the viable frac-

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tion. The biodegradable fraction of MLVSS at mean cell detention time of 12.1 days was found to be 0.67. Biodegradable fraction increases with an increase in F/M ratio but decreases with an increase in sludge age. Considering activated sludge with 85% volatile matter at mean residence time of 10 days, Adams and Asano (1978) estimated that approximately 60% of the total mass of sludge in a conventional plant can be considered biodegradable material, both cells and entrapped substrate. They have also suggested that the active fraction in sludge is between 0.2 to 0.3 at a sludge age of 10 days. Tench (1968) estimated the active fraction to vary from 0.2 to 0.37, and based his results on nitrogen content. Kountz and Fourney (1959) demonstrated that 23% of sludge is non-oxidizable and the accumulation of non-oxidizable sludge will be minimum only when there is sufficient nitrogen in the system.

The rate of transfer of substrate from the liquid is greater than the rate at which substrate is metabolized by floc. Ruchhoft and Butterfield (1939) presented data for rapid removal of substrate and proposed that substrates are stored as internal reserves, or as adsorbed material to floc surfaces by various metabolisms. These findings show little direct relationship between specific growth rate and concentration of substrate in the liquid, and suggests that the Monod model may not be directly applicable to the activated sludge process.

Eckenfelder (1963) used first-order kinetics for rapid removal of soluble substrates by activated sludge floc. Katz and Rohlich (1956) and Siddiqi et al. (1966) proposed that some saturation value of initial removal step must occur. Eckenfelder's model does not predict this result. Placak and Ruchhoft (1947) concluded that initial substrate removal is dependent on the specific substrate. Therefore, some soluble substrates follow rapid removal phenomena and others

may be metabolized directly from the liquid phase. Kuo et al. (1974) observed a lower rate of removal of dissolved substrates when particulate matter was present in the aeration tank, indicating the masking effect of active sites on the floc by particulate substrates.

The removal of particulate substrates by activated sludge is also very rapid, but degradation is very slow (Gujer, 1981). Mechanisms for removal are coagulation, entrainment, and adsorption (Weston and Eckenfelder, 1955). Adam and Asano (1978) proposed that the exopolymer component of activated sludge is a polyelectrolyte, effective in flocculation and removal of particulate matter involves adsorption and entrapment. Banerjee (1968) demonstrated that hydrolysis of colloidal substrates begins immediately upon contact with activated sludge floc. Weston and Eckenfelder (1955) showed that soluble substrate was initially removed until some initial BOD was reached, thereafter the removal rate was sharply decreased.

Jones (1971) hypothesized that removal mechanisms for soluble and particulate substrates are different. Mechanisms can be summarized as (a) adsorption and entrapment of particulate matter which can be approximated by first-order kinetics with a rate coefficient of the order of $10\ hr^{-1}$, (b) adsorption of soluble substrate by first-order kinetics with a rate coefficient of 0.1 to $0.20\ hr^{-1}$, and (c) hydrolysis of entrapped and adsorbed particles to soluble material which is then degraded as adsorbed soluble material. Gujer (1981) proposed that all particulate substrates do not degrade at a constant rate and degradation rates may vary from slow to fast for large to small particles to dissolved organic compounds. The degradation rate also depends on mean cell retention time of activated sludge process. Jacquart et al. (1973) proposed a

mathematical model considering substrates as dissolved and un-dissolved. The un-dissolved volatile matter is converted to reserves of un-dissolved origin by entrapment and reserves of dissolved and un-dissolved origins are transformed into active mass using Monod type saturation function but constants are different for different types of reserves. This model predicts both the rapid uptake mechanism and lag phases. Jacquart et al. (1973) did not consider the inert biological mass in their mathematical model. Takahasi et al. (1969) found that higher F/M ratio increases bacterial cells ability to store nutrients and use these stored materials when F/M ratio is low. They have also found that the addition of soluble substrates to an activated sludge previously in contact with only particulate matter renew the activity. This was due to new sludge which was formed rapidly upon addition of soluble substrates. Stabilized sludge has a very low concentration of storage products which will tend to accelerate the removal rate during contact with substrate.

A structured steady state model developed by Tench (1968) considered mass into three components; an adsorbed oxidizable, an active, and biologically inert. Blackwell (1971), Busby (1973) and Stenstrom (1975) developed the structured dynamic mathematical model for activated sludge. Busby (1973) modified Blackwell's equation by incorporating Monod type saturation function to account for the extracellular substrate concentration. Their models did not distinguish between soluble and particulate substrate, and assumed that all of the substrate passes through storage prior to metabolism.

Ekama and Marais (1979) studied the dynamic behavior of activated sludge and demonstrated that Blackwell's model provides significant improvement over unsaturated models for predicting transient responses. However,

they agreed that consideration should be given to extracellular substrate concentration. The modification of the model considering soluble and particulate substrates provided the best fit to their experimental data.

Nitrification is an important function of the activated sludge process. Nitrogenous compounds not only accelerate eutrophication, it also exert a significant oxygen demand. Nitrification can occur in the presence of carbonaceous oxygen demand if certain conditions exit. The necessary conditions are at least 0.5 to 1.0 mg/l of dissolved oxygen concentration and operation above the washout sludge age of nitrifiers.

Downing and Co-workers (1964) proposed the first model for nitrification. They used batch data and Monod kinetics to determine the kinetic coefficients. Poduska (1973) used Monod saturation kinetics and verified the model using the laboratory scale experimental data. He developed mass balances on ammonia, nitrite, nitrate and nitrifying species of the genera *Nitrosomonas* and *Nitrobacter*. Poduska's model is used here and discussed later. Poduska's work should be consulted for extensive literature review on nitrification.

C. Secondary Clarifier

Excellent removal of organic matter from municipal and industrial wastewater by activated sludge process is possible only by proper design and operation of secondary clarifiers. It has three distinct purposes (a) thickening of biological solids for recycle (b) clarification of effluent and (c) storage of biological mass in the settler. Coe and Clevenger (1916) were the first to provide a comprehensive description of thickening and design of secondary clarifier. The

steady state model was developed to predict solids handling capacity based on batch settling tests. Like Coe and Clevenger (1916), Kynch (1952) considered the upward propagation of zones of higher concentration with lower solids handling capacity, and presented a theoretical and more complicated interpretation of the batch settling process. Edde and Eckenfelder (1968) proposed an empirical, steady state model to relate the underflow concentration to the influent solids concentration and flux. Rex Chainbelt Incorporated (1972) developed a mathematical model to predict the solids concentration of both the underflow and overflow of a secondary clarifier, but their model failed to account for the effects of both influent flux and underflow rate on underflow solids concentration.

Bryant (1972) is the first to develop a dynamic model for continuous thickening process. By implementing Kynch's assumptions regarding the zone settling, Bryant (1972) derived a partial differential equation around a differential volume in a secondary clarifier.

$$\frac{\partial C}{\partial t} = -(U + \frac{\partial G_s}{\partial C}) \cdot \frac{\partial C}{\partial z}$$

$$(2.2)$$

where,

U   = underflow velocity, (L/T),

G_s = batch flux, $(M/L^2T) = C*V_s$

C   = suspended solids concentration, (M/L^3),

V_s = settling velocity, (L/T),

z   = vertical distance, (L),

t   = time, (T).

The above equation contains two unknowns, C and V_s. A second equation

describing settling velocity is required for the solution. Bryant solved this equation by lumping parameters to yield a set of ten elements defined by ordinary differential equations. Settling velocity in a secondary clarifier is a function of solids concentration, time, distance, depth, and perhaps partial derivative of concentration and velocity with respect to distance. The lumped parameter approximation can lead to erroneous results.

Tracy (1973) developed a dynamic continuous thickening model similar to that of Bryant's (1972). Tracy was one of the first to evaluate the limitations of the model by means of laboratory thickening experiments. For the solution of continuity equation using a computer, Tracy assumed that solids, upon entering the thick sludge blanket, are concentrated instantaneously to the limiting solids concentration. The limiting concentration was calculated by differentiating an empirical equation describing a solids flux curve. The results of this assumption is that the boundary condition for the surface of the thick sludge blanket is the limiting concentration. This resulted in a simulation error when limiting concentration is changed due the change in operational conditions. Tracy proposed that this simulation error is negligible. He observed the transient response of the thickener and proposed that layers of varying solids concentration tend to propagate through the sludge blanket as an distinct identity. Dennis (1976) developed a dynamic continuous thickening model with the assumption that limiting flux governs the transport of solids within the settler. Laboratory investigation showed that the flow of the displaced fluid through the sludge blanket is an important parameter in affecting the solids flux transmitted within the thickener. A liquid mass balance was incorporated in the model to take into account the effect of displaced fluid. A force balance, based on batch settling data, was considered in the model to accommodate the effect of

compressive stresses on subsidence rate of solids.

The second function of a secondary clarifier is clarification. The clarification efficiency of the secondary clarifier has great influence on treatment plant efficiency because particulate fraction contributes a major portion of effluent BOD. Pflantz (1969) conducted a study on secondary sedimentation and proposed that the effluent concentration is dependent on overflow rate, the concentration of feed solids to the settler, sludge settleability monitored by sludge volume index (SVI), wind, and temperature. Pflantz found that the concentration of suspended solids in mixed liquor is the most important factor for the clarity of the effluent. But he recommended that secondary clarifiers be designed on the basis of mixed liquor volatile suspended solids (MLVSS) concentration as well as hydraulic loading. For low MLVSS values, the required volume of the aeration basin is large, while for the secondary clarifier, it is small. For high MLVSS values, the situation is reversed. Direct relationship between MLVSS and effluent suspended solids concentration obtained from experiments by Tuntoolavest (1980) suggests that the low MLSS is the key to the optimal design of activated sludge process.

Chapman (1982) developed a regression equation using his pilot plant data which is a function of MLSS concentration, side water depth, and feed flow rate. The equation of effluent suspended solids concentration from the secondary clarifier is

$$XEFF = -180.6 + 40.3*MLSS + 133.24*Q_a/A$$

$$+ SWD (90.16 - 62.54*Q_a/A)$$

(2.3)

where,

XEFF = effluent suspended solids concentration, mg/l,

MLSS = mixed liquor suspended solids concentration, g/l,

Q_a/A = clarifier feed flow rate, m/h,
= $Q_i/A + Q_r/A$

Q_i/A = plant inflow per unit surface area, m/h,

Q_r/A = recycle flow per unit surface area, m/h,

A = surface area of the secondary clarifier, m^2,

SWD = side water depth, m.

Cashion (1981) proposed that effluent with low suspended solids concentration is possible for two operating conditions (a) SRT of about 2 days and HRT of about 12 hours, and (b) SRT of 8 days and HRT of about 4 hours. The overflow rate has very little effect on effluent suspended solids concentration.

A statistical analysis effluent data from 29 plants resulted the following relationship between BOD_5 and effluent suspended solids concentration:

$$BOD_5 = 8.8 + 0.61 * XEFF$$

(2.4)

where,

BOD_5 = 5 day biological oxygen demand, g/m^3,

XEFF = effluent suspended solids concentration, g/m^3.

Dick (1970) indicated that 1 mg of suspended solids is approximately 0.6 mg/l of BOD_5 where as Keffer's (1962) 20 years of data concluded a ratio of 0.55 mg of BOD_5/mg of suspended solids.

D. Anaerobic Digestion

The anaerobic digestion process degrades complex organic matter in the presence of a mixed culture of microbial mass under a controlled environment and forms carbon-dioxide and a useful end-product, methane gas. It is widely used for stabilizing municipal waste sludge, and there is an increasing interest in using this process for treating industrial waste which contains high concentrations of organics. There are significant advantages of anaerobic digestion over other processes used for this purpose, among these are a high degree of waste stabilization, low net microbial mass, low power requirements, formation of a usable product, methane gas and digested sludge which can be used as soil conditioner. But even with all these advantages, the process has not, in general, suffers because of its poor record of process stability.

Anaerobic digestion, a complex process hydrolyzes complex insoluble organic matter by extracellular enzymes; the hydrolysis products are fermented to volatile fatty acids by a group of facultative and anaerobic bacteria, known as 'acid formers', and finally the acids are converted to methane and CO_2 by obligate anaerobic bacteria and methanogens (Graef, 1972; Hill and Barth, 1977).

Recently Bryant et al. (1976, 1977, 1979), McInerney et al. (1979, 1980, 1981), Mah et al. (1977), Wolin (1976), and Boone and Smith (1978) proposed a new theory for anaerobic digestion. As before non-methanogenic bacteria degrade organic matter to form volatile fatty acids (acetic, propionic, n-butyric, valeric and caproic), H_2, and CO_2. Then fatty acids are converted to acetate and methane by syntrophic association with H_2-producing acetogenic bacteria and methanogens. This hypothesis is based on the work of Bryant et al. (1967) with *Methanobacillus omelianskii*, originally believed to be pure culture, that

degrades ethanol to acetate and methane in a symbiotic association of methanogens with H_2-producing bacteria.

D-1. Propionic and n-butyric acids

Obligate proton-reducing acetogenic bacteria are involved in oxidation of fatty acids of even and odd numbered carbons to acetate and H_2 and propionate, as shown in equations 2.5 and 2.6. Decarboxylation of propionate to acetate, CO_2, and H_2 is shown in equation 2.7.

$$CH_3CH_2CH_2COO^- + 2H_2O \longrightarrow 2CH_3COO^- + H^+ + 2H_2$$

$$\Delta G^o = + 11.5 \; K \; cal/reaction$$

$$(2.5)$$

$$CH_3CH_2CH_2CH_2COO^- + 2H_2O \longrightarrow CH_3COO^- + CH_3CH_2COO^-$$

$$+ H^+ + 2H_2$$

$$\Delta G^o = + 11.5 \; K \; cal/reaction$$

$$(2.6)$$

$$CH_3CH_2COO^- + 3H_2O \longrightarrow CH_3COO^- + HCO_3^- + H^+ + 3H_2$$

$$\Delta G^o = + 18.2 \; K \; cal/reaction$$

$$(2.7)$$
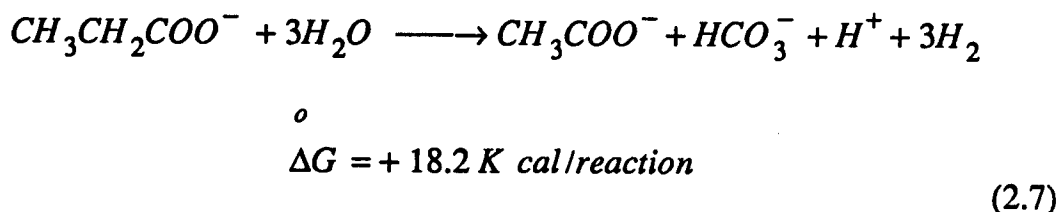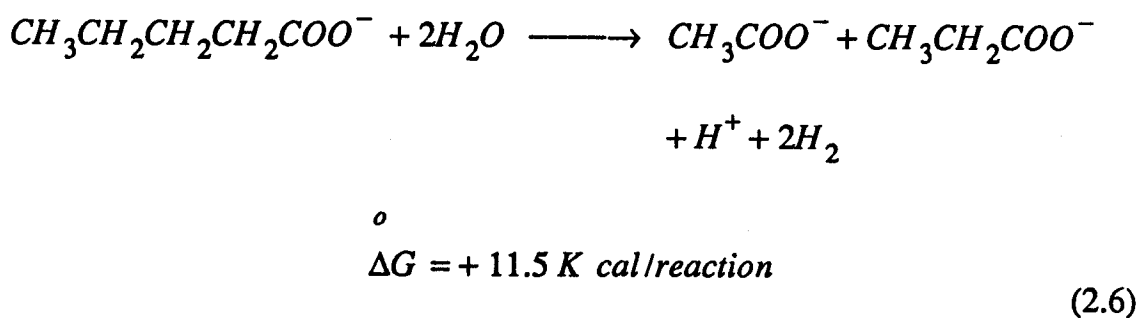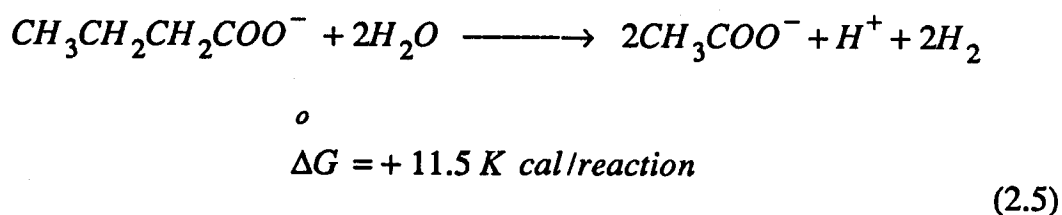
Sparging experiments developed by Boone and Smith (1978) demonstrated the ability of obligate proton reducers to produce H_2 from propionic and n-butyric acids, but not from acetic acid. They have also shown that propionate and butyrate enrichments utilize H_2 without a lag, and when they are vigorously sparged with CO_2, H_2 replaces methane as a product; this does not happen in acetate enrichments. Therefore, large amounts of H_2 can be produced during

dissimilation of propionate and butyrate, and large amounts of H_2 can be oxidized in the production of methane in these enrichments.

Short term exposure to H_2 strongly inhibits the degradation of propionate and butyrate but not acetate by enrichments (Boone and Smith, 1978) and in anaerobic digestion of domestic sludge (Kasper and Wuhrmann, 1978). So the oxidation of propionic and butyric acids is probably dependent on H_2 removal, which might be expected during interspecies H_2 transfer. Therefore, for thermodynamically favorable conditions of equations (2.5), (2.6), and (2.7) the partial pressure of H_2 should be maintained below 10^{-5} and 10^{-6} atmosphere for propionate and butyrate respectively (McInerney and Bryant, 1980).

The existence of obligate proton reducers was verified by the growth of the following co-cultures of two different organisms reported by Bryant and his co-workers for degradation of one of these substrates (Table 2.1).

The sulfate-reducing bacteria have implicated the propionate oxidation in anaerobic systems. A recent study by Boone and Bryant (1980), documented a species of bacteria (*Syntrophobacter wolinii*) which in co-culture with H_2-utilizing sulfate reducers (*Desulfovibrio Sp.*) degraded propionate and sulfate to acetate, sulfide, and CO_2. When *M. hungatei* was added to the culture with the absence of sulfate, the medium produced acetate, methane, and CO_2.

McInerney et al. (1979) isolated a species of anaerobic bacterium that degrades butyrate to acetate and H_2 in syntrophic association with either an H_2-utilizing methanogen or H_2-utilizing Desulfovibrio. This organism, called *Syntrophomonas wolfei*, oxidizes saturated fatty acids (butyrate through octanoate) to acetate or acetate and propionate with the proton serving as the

Table 2.1 Methanogenic Interspecies H_2 Transfer

Non-methanogens (H_2 producers)	Substrates	H_2 using bacterium	Mixed culture products	Reference
Syntrophobacter wolinii	Propionate and sulfate	*Desulfovibrio Sp.*	Acetate and H_2S	Boone and Bryant(1980)
	Propionate	*Desulfovibrio Sp.* and *Methanospirillum hungatei*	Acetate and CH_4	Boone and Bryant(1980)
Syntrophomonas wolfei	Butyrate	*Methanospirillum hungatei*	Acetate and CH_4	McInerney et al. (1979)
	Valerate	*Methanospirillum hungatei*	Acetate, CH_4 and Propionate	McInerney et al. (1981)

electron acceptor. But the degradation of butyrate is thermodynamically more favorable when it is coupled with H_2 utilization by a sulfate reducer rather than a methanogen because the reduction of sulfate to sulfide by H_2 is thermodynamically more favorable than reduction of CO_2 to methane by H_2 (Bryant et al. 1977; Thauer et al. 1977). By co-culturing *Syntrophomonas wolfei* with methanogens, McInerney et al. (1979,1981) showed that H_2 is the electron sink product and the methanogen present used only H_2 for growth and methanogenesis.

The isolation of *Syntrophomonas wolfei* (McInerney et al. 1979, 1981) and *Syntrophobacter wolinii* (Boone and Bryant, 1980) via co-culture with H_2 using bacteria provided direct evidence for the existence of obligate proton reducing bacteria (Bryant, 1976) and for its role in the complete anaerobic degradation of organic matter to CO_2 and CH_4 (Zehnder, 1978; Kasper and Wuhrmann, 1978).

The continuous anaerobic digestion of wastes to CH_4 and CO_2 is dependent on the role of hydrogen on conversion of acetate to methane and CO_2. Smith and Mah (1978) and Zinder and Mah (1979) found that H_2 inhibits methane formation from acetate, resulting in an accumulation of acetate. Recently Boone (1982) experimentally showed that the acetate level in anaerobic digestion is higher, apparently due to increased H_2 and inhibition of acetate dissimilation.

D-2. Hydrogen Transfer Kinetics

Hydrogen is a major product of fermentation of organic matter in an anaerobic ecosystem, e.g. anaerobic digestion. Groups of bacteria present in anaerobic systems contain hydrogen-using micro-organisms (hydrogenotrophs) as well as hydrogen-producing microorganisms (hydrogenogens). Most methanogens (hydrogenotrophs) obtain energy for growth via reduction of CO_2 in the presence of H_2 to form methane.

$$4H_2 + HCO_3^- + H^+ \longrightarrow CH_4 + 3H_2O$$
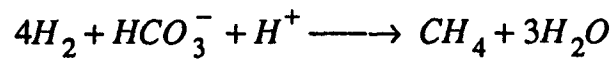
$$\Delta G^o = -32.4 \; k \; cal/reaction$$

(2.8)

In a mixed culture system (non-methanogenic and facultative anaerobes) in the presence of appropriate enzymes, H_2 is a major end product. Methanogens are completely dependent on non-methanogenic species for their supply of H_2 because the products (H_2 and CO_2) of the energy metabolism of hydrogenogens (non-methanogens) are the substrates for the growth of hydrogenotrophs (methanogens) (Table 2.2). H_2 formation is only thermodynamically favorable if the H_2 concentration is maintained at a very low level by removing it from the system; in the digester. THis is normally achieved by the methanogens. This phenomenon is known as 'Interspecies Hydrogen Transfer.' One explanation of this is illustrated by the following reactions.

1.   Propionate oxidizing acetogenic bacterium

$$CH_3CH_2COO^- + 3H_2O \longrightarrow CH_3COO^- + HCO_3^- + H^+ + 3H_2$$

Hydrogenogens only

ORGANIC SUBSTRATES

$\longrightarrow$ H_2 + CO_2

VOLATILE ORGANIC ACIDS

(e.g. Propionate, n-butyrate,
Caproate, Valerate etc.), and

NEUTRAL END PRODUCTS
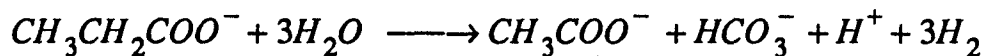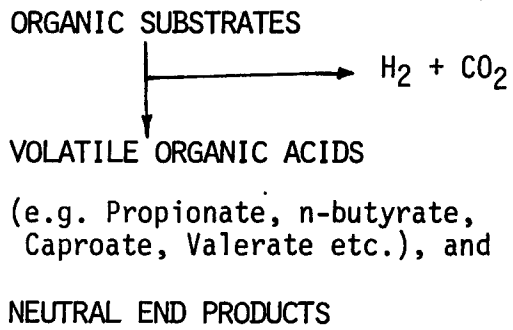
Hydrogenogens and Hydrogenotrophs

ORGANIC SUBSTRATES

(Hydrogenogens)

VOLATILE ORGANIC ACIDS $\longrightarrow$ H_2 + CO_2

(Hydrogenogens)

(Hydrogenotrophs)

ACETIC ACID CH_4 + CO_2

(Aceticlastic Methanogens)

CH_4 + CO_2
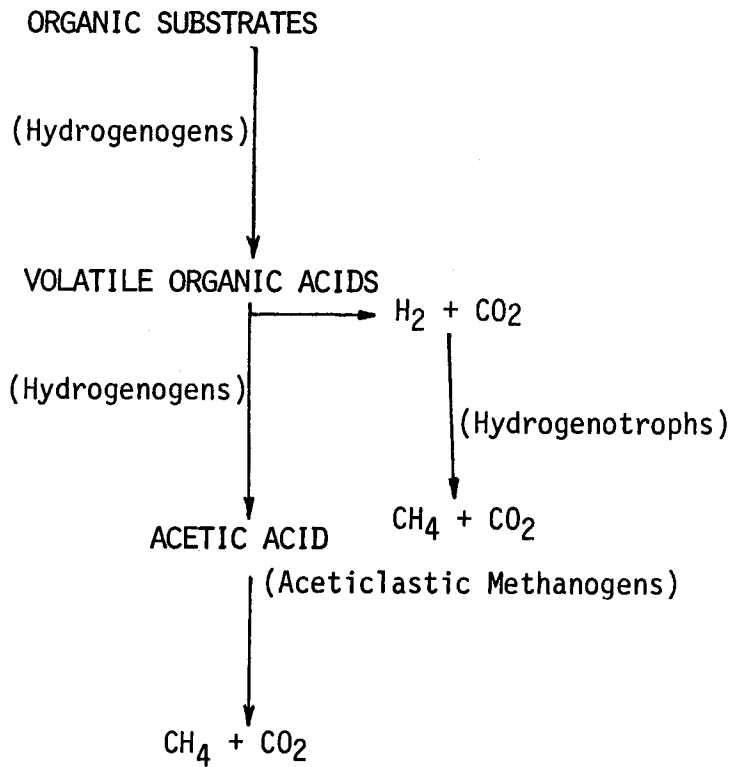
Table 2.2 Role of Methanogens on Interspecies H_2 Transfer

$$\overset{o}{\Delta G} = +18.2 \ k \ cal/reaction$$

<div align="right">(2.9)</div>

2.   Butyrate oxidizing acetogenic bacterium

$$CH_3CH_2CH_2COO^- + 2H_2O \longrightarrow 2CH_3COO^- + H^+ + 2H_2$$

$$\overset{o}{\Delta G} = 11.5 \ k \ cal/reaction$$

<div align="right">(2.10)</div>

3. H_2 utilizing methanogens

$$4H_2 + H^+ + HCO_3^- \longrightarrow CH_4 + 3H_2O$$
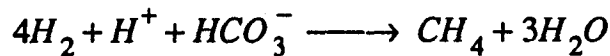
$$\overset{o}{\Delta G} = -32.4 \ kcal/reaction$$

<div align="right">(2.11)</div>

Add 1 and 3. Syntrophic Association

$$4CH_3CH_2COO^- + 3H_2O \longrightarrow 4CH_3COO^- + HCO_3^- + H^+ + 3CH_4$$
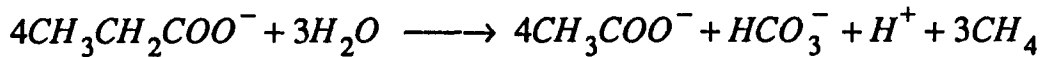
$$\overset{o}{\Delta G} = -24.4 \ k \ cal/reaction$$

<div align="right">(2.12)</div>

Add 2 and 3. Syntrophic Association

$$2CH_3CH_2CH_2COO^- + HCO_3^- + H_2O \longrightarrow 4CH_3COO^- + H^+ \ CH_4$$

$$\overset{o}{\Delta G} = -9.4 \ k \ cal/reaction$$

<div align="right">(2.13)</div>
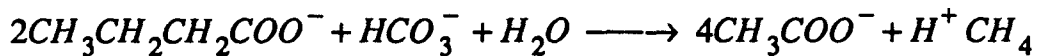
where

$$\overset{o}{\Delta G} = \text{change in free energy (Thauer et al., 1977).}$$

According to Hungate (1967) the partial pressure of H_2 is low for an active methane formation in an anaerobic environment and the reported partial pressure of H_2 is about $3 \ x \ 10^{-4}$ atmosphere for the bovine rumen ecosystem.

A large negative change in free energy in the equilibrium of the reaction, equation (2.8) demonstrates that the reduction of CO_2 favors the use of H_2 and formation of CH_4. The rapid use of H_2 by methanogens maintains a very low partial pressure of H_2, even though a large amount of H_2 is produced. According to Smith and Mah (1966), Mah et al. (1977), methanogens degrade acetate according to the following equation in the absence of exogenous electron acceptors (O_2, NO_3^-, SO_4^{-2}).

$$CH_3COO^- + H_2O \longrightarrow CH_4 + HCO_3^-$$

$$\Delta G^o = -7.4\ k\ cal/reaction$$

(2.14)

In case of anaerobic municipal waste digestion, acetate is the main precursor of methane (Jeris and McCarty, 1965; Smith and Mah 1966) where the acetate is directly converted to methane and CO_2 by aceticlastic bacteria.

D-3. Inhibition

Inhibition is the impeding property of a reaction caused by a higher concentration of some troublesome substances. It has been observed in anaerobic digestion by many investigators, among them are Andrews (1969), McCarty (1964), and Buswell (1936). McCarty (1964) proposed that volatile acids are inhibitory to methane bacteria through a reduction in pH and this inhibition is relieved by maintaining the pH near neutrality. But Buswell (1936) mentioned that volatile acids concentration greater than 2000 to 3000 gm/m^3 is inhibitory regardless of pH and this inhibition can be relieved by reducing organic loading or diluting the reactor content. Data from the bench scale study by Andrews (1969) resolved the 'volatile acids controversy' by considering inhibition due to

greater concentration of un-ionized volatile acids ($> 0.007\ gm/m^3$). Since the un-ionized acids concentration is a function of pH and total acids concentration, both are important. Pure culture studies by Levine and Fellers (1940) and Rahn and Conn (1944) led to the conclusion that the un-ionized form of a substrate is inhibitory to microorganisms. Andrews (1969) proposed that un-ionized volatile acids are rate limiting at low concentrations and inhibitory at high concentrations and formulated an inhibition function which is analogous to enzyme inhibition equation (Dixon and Webb, 1964).

$$\mu = \mu^*/(1.+(K_s/HS)+(HS/KI))$$

(2.15)

where,

μ = specific growth rate, 1/days,

μ^* = maximum specific growth rate, 1/days,

KI = inhibition constant, moles/liter,

HS = un-ionized substrate concentration, moles/liter,

K_s = saturation constant, moles/liter.

Fermentation of organic waste forms acetic, propionic and butyric acids and H_2 as intermediates, and CO_2 and CH_4 as end products. Boone and Smith's (1981) experiment showed large amounts of hydrogen production during dissimilation of propionate and butyrate, and large amounts of H_2 oxidation in the production of methane. McInerney et al. (1981) demonstrated that an initial partial pressure 0.8 atm. of H_2 completely inhibits butyrate degradation by the *Syntrophomonas wolfei* in co-culture with *M. hungatei*. Acetate dissimila-

tion is slightly inhibited by molecular hydrogen, while propionate and butyrate degradation is completely stopped (Boone and Bryant, 1980). They have also showed that higher sulfide concentration inhibits propionate degradation by repressing the growth of the co-culture of *Syntrophobacter wolinii Desulfovibrio Sp.*, with the main effect on *Syntrophobacter wolinii.* Zinder and Mah (1979), and Boone (1982) proposed that hydrogen inhibits methane formation from acetate. Therefore, in the presence of increased H_2 concentration methanogenesis will be repressed, and acetic, propionic, and butyric acid concentrations will accumulate with a drop in pH. So the maintenance of very low hydrogen concentration is essential for the dissimilation of volatile acids.

D-4. Process Design and Process Modeling

Kinetic failure of anaerobic digestion results from the continuous reduction of solids retention time until limiting solids retention time exceeds the inverse of maximum specific growth rate causing a washout microbial mass. Failure is due to an increased concentration of short and long chain fatty acids, evidenced by the near cessation of CH_4 production and decreased stabilization rate. McCarty (1966) and O'Rourke's (1968) research on digestion of primary domestic waste sludge indicated that the fermentation of short and long chain fatty acids to methane and CO_2 is the rate limiting step. Ghosh et al. (1975), Kasper and Wuhrmann (1978), Pretorius (1969), Bryant (1976), and Boone (1982) proposed that the rate-limiting step in anaerobic digestion of organic matter is the methanogenic reactions involving reduction of CO_2 with H_2 and degradation of acetate. Conversion of acetate to methane and CO_2 is more rate-limiting than reduction of CO_2 with H_2 to methane (Kasper and Wuhrmann, 1978).

Lawrence (1971) studied the application of process kinetics on the design of anaerobic processes with the consideration of three main volatile acids, acetic, propionic, and butyric acids formed as intermediates in the fermentation of organic matter to CH_4 and CO_2. These three main acids were chosen because (a) acetic acid is the precursor of about 70% of methane formation in anaerobic digestion of domestic waste sludge (Smith and Mah, 1966; McCarty, 1964), (b) acetic and propionic acids together are the precursor of 85% of the methane formation (McCarty, 1964), and (c) butyric acid is the precursor of an additional 8% of the methane formed (Smith et al. 1970). The stoichiometry of fermentation of these volatile fatty acids used by Lawrence (1971) is shown in the following equations.

Acetic Acid:

$$CH_3COO^- + H_2O \longrightarrow CH_4 + HCO_3^-$$

(2.16)

Propionic Acid:

$$CH_3CH_2COO^- + \frac{1}{2}H_2O \longrightarrow CH_3COO^- + \frac{3}{4}CH_4 + \frac{1}{4}CO_2$$

(2.17)

Butyric Acid

$$CH_3CH_2CH_2COO^- + HCO_3^- \longrightarrow 2CH_3COO^- + \frac{1}{2}CH_4 + \frac{1}{2}CO_2$$

(2.18)
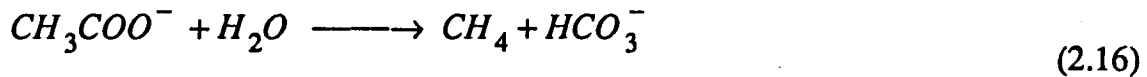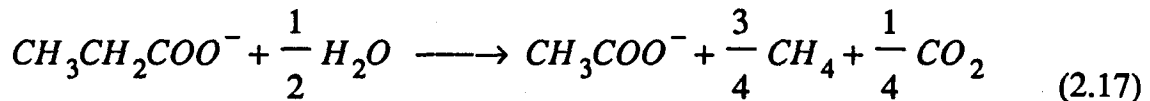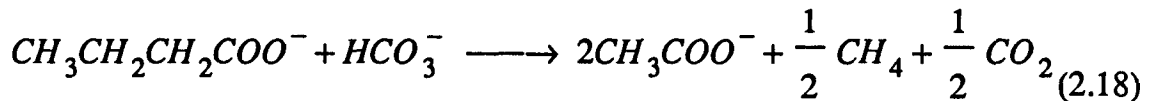
Lawrence and McCarty (1969) determined kinetic coefficients for the stabilization of acetic acid to methane and dissimilation of propionic and butyric acid. Values of growth coefficients were computed on the basis of mg of biological solids per mg of substrate COD converted for energy, i.e. to methane. Values of decay coefficients were considered constant.

Most mathematical models used for the design and operation of anaerobic digestion, even today are steady state models. These models include acid formation and removal, as well as methane formation. Monod kinetics have been used and shown to be satisfactory for steady state design and operation (Andrews and Graef, 1971; Lawrence and McCarty, 1969; Fan et al, 1973). Modeling of conventional anaerobic digestion is based on the assumption that the stoichiometry of volatile acids concentration is approximated by the stoichiometry for acetic acid conversion (Andrews and Graef, 1971).

Steady state mathematical models cannot be used for the prediction of performance during start up operation or under transient conditions resulting from the change in inputs. The reputation of anaerobic digestion as an unstable system encouraged the development of dynamic mathematical models to obtain better control procedures for preventing process failure and for optimizing process performances. Dynamic models should also be used for improved process design (decreased need for oversizing) because it would allow the comparison of different versions of process in terms of process stability.

Graef (1972) developed a dynamic mathematical model of anaerobic digestion to investigate control strategies and process stability. The dynamic model considered (a) an inhibition function for specific growth of methanogens, (b) un-ionized fractions of volatile acids are rate limiting at low concentration and inhibitory at high concentration, (c) un-ionized acids concentration is a function of both the total concentration of acids and pH, and (d) interaction in and between the liquid, gas and biological phases of digestion. This interaction permits to predict the dynamic response of pH, volatile acids concentrations, alkalinity, gas flow rate, and gas composition.

Hill and Barth (1977) developed a dynamic mathematical model for the simulation of animal waste digestion which involved influent with more organic matter and extremely high nitrogen content. The model developed attempted to include the breakdown of waste and acid formation, production of gas and carbonate equilibria with the addition of nitrogen and cation balances. Finally the mathematical model was verified with the data collected from the pilot scale digesters. According to Hill and Barth (1977), the problem of animal waste digestion is process instability because this waste can inhibit itself either by high ammonia concentration or high organic acids.

Simulation and mathematical modeling help us to understand the process mechanisms as well as save time and money. Moreover, knowledge from simulation is useful for modifying the mathematical model and developing laboratory experiments, but simulation primarily offers qualitative answers rather than quantitative.

E. Optimization

Two main objectives of wastewater treatment plants are to maximize the efficiency and minimize the cost. As these two objectives are conflicting, research must be conducted by accessing a specified requirement that restricts the size of the process units to maximum efficiency or minimize cost. The most frequently observed objective is to minimize cost with a specified insured efficiency.

In the past, engineers had the tendency to optimize the individual system not the overall. The trend had been to design the most efficient unit processes, each at least cost and then combine the units to form an optimum wastewater

treatment system. If only aeration tanks are optimized in an activated sludge plant, it will be found that the least cost alternatives will be the one with the lowest possible detention time with minimum possible solids concentration. This will lead to an increased loading in the stabilization stage of the system, resulting in an increased cost for that phase. So for an optimal overall system, the individual units cannot be minimized separately, must be considered as a part of the total system. There was neither an effort to maximize the efficiency without considering cost, nor an attempt to arrive at a minimum cost without considering the efficiency. The accuracy of the optimum solution depends upon the accuracy of the mathematical model describing treatment plant operation, cost functions, and accuracy of the optimizing algorithm.

Two principal trends in the optimization of wastewater treatment systems have been encountered in the literature (a) Simplified mathematical model with elaborate and advanced optimization technique (b) Advanced and elaborate mathematical model with simplified optimization technique.

The literature on the performance of unit processes is voluminous, but techniques to find the optimal performance is limited. Smith (1969) was the first researcher to calculate the performance and cost of the system as a whole, based on the relationship developed for the individual unit processes.

E-1. Simplified Mathematical Models:

Shih and Krishnan (1969) developed an optimum wastewater treatment system using dynamic programming. Ecker and McNamara (1971) demonstrated the use of geometric programming in the optimal design of wastewater treatment systems by reworking the example problem solved by Shih and

Krishnan. According to Ecker and McNamara (1971) decision variables are BOD_5 removal efficiencies at each of unit process.

$$\eta_j = \frac{BOD_{5_{out_j}}}{BOD_{5_{in_j}}}$$

(2.19)

where,

η_j = *efficiency of the unit j.*

Optimum combinations and efficiencies of various unit processes were identified but no wastewater component except BOD_5 appeared in the model. The cost associated with the unit process considered was

$$C_j = a_j \cdot \eta_j^{b_j}$$

(2.20)

where,

C_j = total annual cost,

a_j, b_j = constants for process j.

The above equation implies that removal efficiencies are independent of influent concentration and the position of the plant i.e., each unit is capable of removing any BOD_5 load from zero to removal approaching 100% with the constraint of non-negativity of the constant b_j.

Shih and Defilippi (1970) demonstrated the application of dynamic programming in optimal design of wastewater systems and considered BOD_5 removal in primary sedimentation tank as a function of overflow rate and influent BOD_5 and load for other units with certain restrictions.

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Optimal design of wastewater treatment plants considered above, were more concerned with the demonstration of a particular optimization technique rather than working with a realistic model.

E-2. Advanced Mathematical Model

The models developed by Parkin and Dague (1972), Berthouex and Polkowski (1970), Middleton and Lawrence (1976), Fan et al. (1974), and Tyteca and Smeers (1981) are complex and complete with fewer process units but optimization techniques used are much simpler than preceding cases. These models are more oriented towards practicing design engineers with the type of problem encountered in the field and solution methods that can easily be adapted in practice.

Parkin and Dague (1972) applied an enumeration technique in the optimal design of a wastewater treatment system and showed that the least efficient primary sedimentation tank, in terms of suspended solids removal, i.e. smallest primary sedimentation tank is desirable, high mixed liquor suspended solids in the aeration tank is economical, and anaerobic digestion is less expensive than aerobic digestion of excess sludge stabilization. This concludes that the most efficient individual units combined together may not lead to the optimal system. Enumeration technique is simple and easily be applied in practice by design engineers.

Middleton and Lawrence (1976) proposed an enumerative graphic technique for cost optimization of wastewater treatment using steady state mathematical model, and showed that unit sizes and capacities are functions of activated sludge solids retention time, mixed liquor volatile suspended solids,

recycle ratio, thickener underflow suspended solids concentration, suspended solids removal efficiency of primary settling tank and digester solid retention time. The minimum cost was determined graphically for constant and variable solid retention time of each subsystem.

Berthouex and Polkowski (1970) used Hookes and Jeeves pattern search technique, considering the parameter of uncertainty in the design of wastewater treatment systems. Their study was more realistic and permitted relative reliability of each unit process along with cost and treatment capabilities in obtaining the optimal design.

In all the above cases, the objective function appeared is given below,

$$Minimize \ \ TC = \sum_{i=1}^{n} C_i(\eta_i) + \sum_{i=1}^{n} \sum_{t=1}^{\Gamma} \frac{1}{(1+\alpha)^t} C_{it}(\eta_i) \qquad (2.21)$$

where,

Γ = discount rate,

t = number of periods in planned horizon,

η_i = design variables,

$C_i(\eta_i)$ = capital cost,

$C_{it}(\eta_i)$ = operating cost,

i=1,...,n denotes the unit process.

The cost functions used are in the form,

$$C = \sum_{i=1}^{n} A_i \ (f_i(\eta_i))^{B_i} \qquad (2.22)$$

where,

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C	=	capital or operating costs,
A_i and B_i	=	estimate constants,
η_i	=	process design parameters,
$f_i(\eta_i)$	=	a simple function of η, generally η or e^{η}.

Middleton and Lawrence (1976) also showed that the combination of independently optimized process units will not lead to a global optimal system which confirms Parkin and Dague (1972) and Narbaitz and Adams' (1980) conclusion. Fan et al. (1974) used a modified simplex pattern search technique for the treatment systems with objective function on capital costs only.

McBeath and Eliassen's (1966) sensitivity analysis showed that the variables which have more influence on the total cost are the global efficiency, influent flow rate, and mixed liquor suspended solids concentration in the aerator and influent BOD_5 load. They have also showed that the accuracy of cost parameters have much greater influence on total cost than the performance variables. Middleton and Lawrence (1976) proposed the selection of an optimal design 'region' rather than pinpoint to take into account the inaccuracy of parameters and decision variables and to provide greater flexibility in applying optimal values to the system design.

Tyteca and Smeers (1981) developed an advanced mathematical model of steady state activated sludge wastewater treatment systems and optimized the system using geometric programming. They considered capital and operation and maintenance costs in their objective function and O & M costs were considered constant. They recommended that the discount factor should be replaced by a continuous function for variable O & M costs.

Lynn et al. (1962) used linear programming for optimal design of waste-water treatment systems. The problem formulated is equivalent to the trans-shipment problem and be solved by network algorithm. One advantage of this technique is that it can handle problems which involve a system of non-serial nature. The algorithm and computational procedure developed are elaborate and cost and performance relationships are simplified, similar to Ecker and McNamara (1971).

All studies mentioned above have undertaken system optimization with BOD_5 reduction only. With the introduction of performance constraints such as suspended solids, COD and nutrient removal, the current procedure will be very complex. Optimal solution of BOD_5 removal may not lead to optimality by others. Network model (with splitting nodes) is capable of handling multiple constraint parameters, such as BOD_5, suspended solids, COD and nutrient removal which overcomes the difficulties encountered by mathematical programming formulations in this direction. Thus cost minimization may be achieved with respect to multiple water quality parameters. Adams and Panagiotakopoulos (1977) presented a network algorithm which was used to solve the industrial wastewater treatment problem formulated by Shih and Krishnan (1969) and the approach was suggested for use in solving the multiparameter effluent quality optimization problem. They proposed that the network algorithm is capable of handling both convex and non-linear cost transformation function of the non-decreasing type.

III. MODEL DEVELOPMENT

Modeling is the art of approximating a system for the purpose of learning its characteristics without interacting the system itself. Modeling by its nature is revolutionary, provides a test ground for studying the effects of various changes that it can have on real world systems. One of the objectives of this research is to develop a dynamic mathematical model for the activated sludge process describing process oxygen requirement, the solid production rate, and oxygen demand of treated effluent during transient loading. Plants which are designed for carbonaceous substrates removal may achieve nitrification when sludge age is high. In such a case, the oxygen utilization will be different since nitrification exerts a significant portion of oxygen demand and for this reason the dynamics of nitrification is considered herein. The dynamic model considered also includes anaerobic digestion. In order to use a model for design and operation, it must be capable of predicting process oxygen requirements, solid production rates, and oxygen demand of the treated effluent during transient loadings. Influent suspended solids and refractory substances are also incorporated in the model because these will change the design and operational parameters.

A. Model Inputs

Wastewater flow rates and pollutant concentrations vary constantly. They are influenced by diurnal, weekly, yearly seasonal, and random forces. The mean values of the diurnally varying parameters are commonly used as an input for steady state analysis, whereas time series analysis is used for dynamic analysis, to determine periodic or deterministic components of the input. Box and Jenkins (1970) have developed the time series analysis and Goel and

LaGrega (1974), Berthouex and Co-workers (1975, 1978) used this technique to predict wastewater flow rates and pollutant concentrations.

An alternative time series analysis, Fourier Transform Analysis, is used in this investigation. The time series analysis by Box and Jenkins (1970) is considered more powerful, but with the limited data available, the use of Fourier Transform Analysis was more applicable.

Influent BOD_5, total suspended solids and volatile suspended solids data are obtained from the City of Atlanta treatment plant. Figures 3.1 and 3.2 show the original BOD_5 data and Fourier Transform reconstruction using five components. Harmonic spectrum diagram indicates the fluctuations and seventh and fourteenth (Figure 3.2) correspond to daily and twice daily fluctuations.

Another problem with input parameters is the relationship between various oxygen demand measurements. The exact relationships between BOD_5, BOD_U, COD, and TOD are not possible because it depends on the composition and levels of treatment of wastewater and others. The relationships used by Busby (1973) are used for the purpose of this investigation. Relationships between different pollutant concentrations used by Stenstrom (1975) with the modification of soluble non-biodegradable substrate shown in Figure 3.3 are used in this investigation.

B. Primary Clarifier

The primary clarifier is the principal process used in wastewater treatment plant to remove settleable solids from wastewater before entering the biological treatment process. This also results in a reduction in BOD and the 'masking effect', the phenomenon of reduction in activities of biological sludge
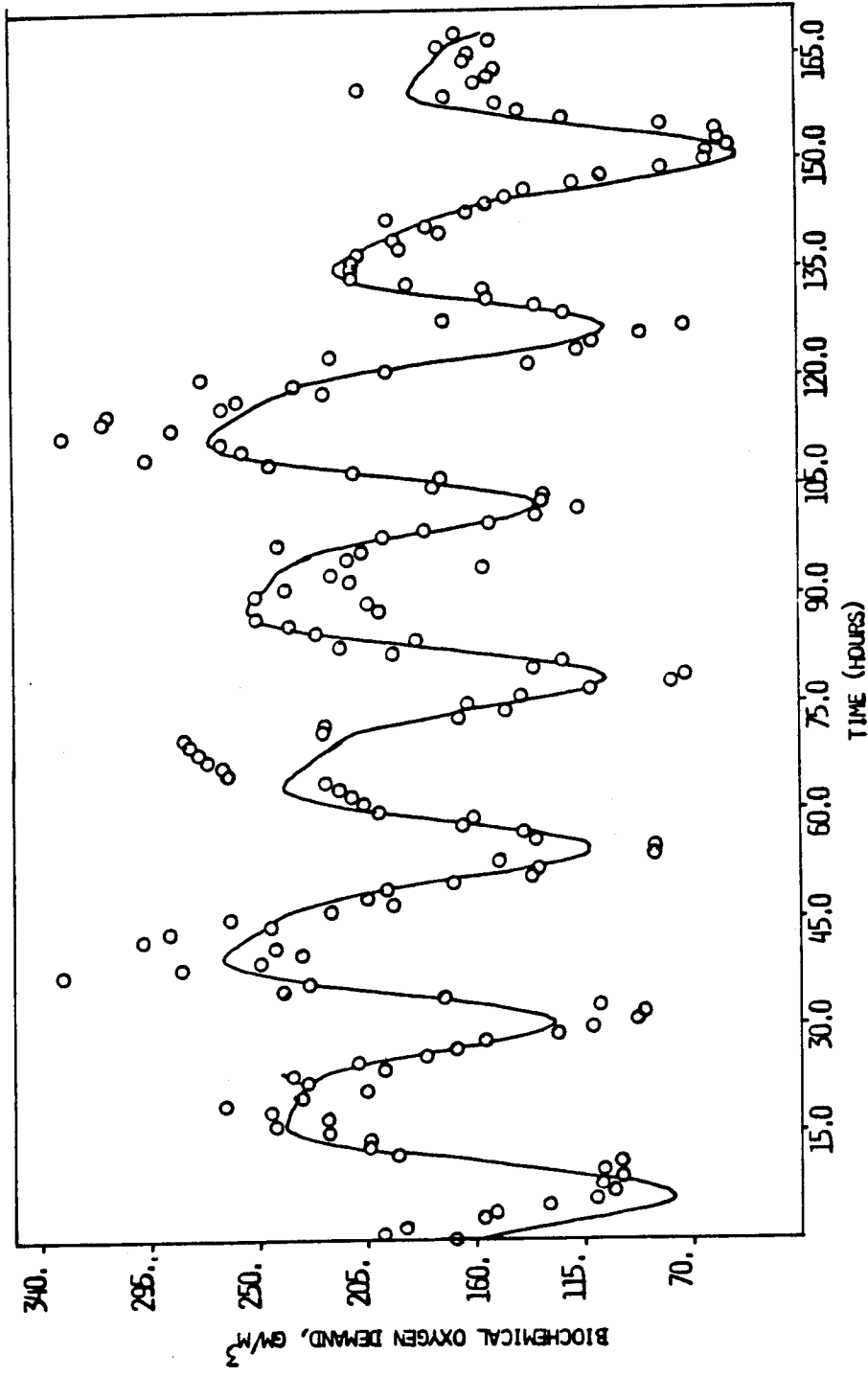
Fig. 3.1 Actual and Reconstructed Biochemical Oxygen Demand, gm/m^3

43
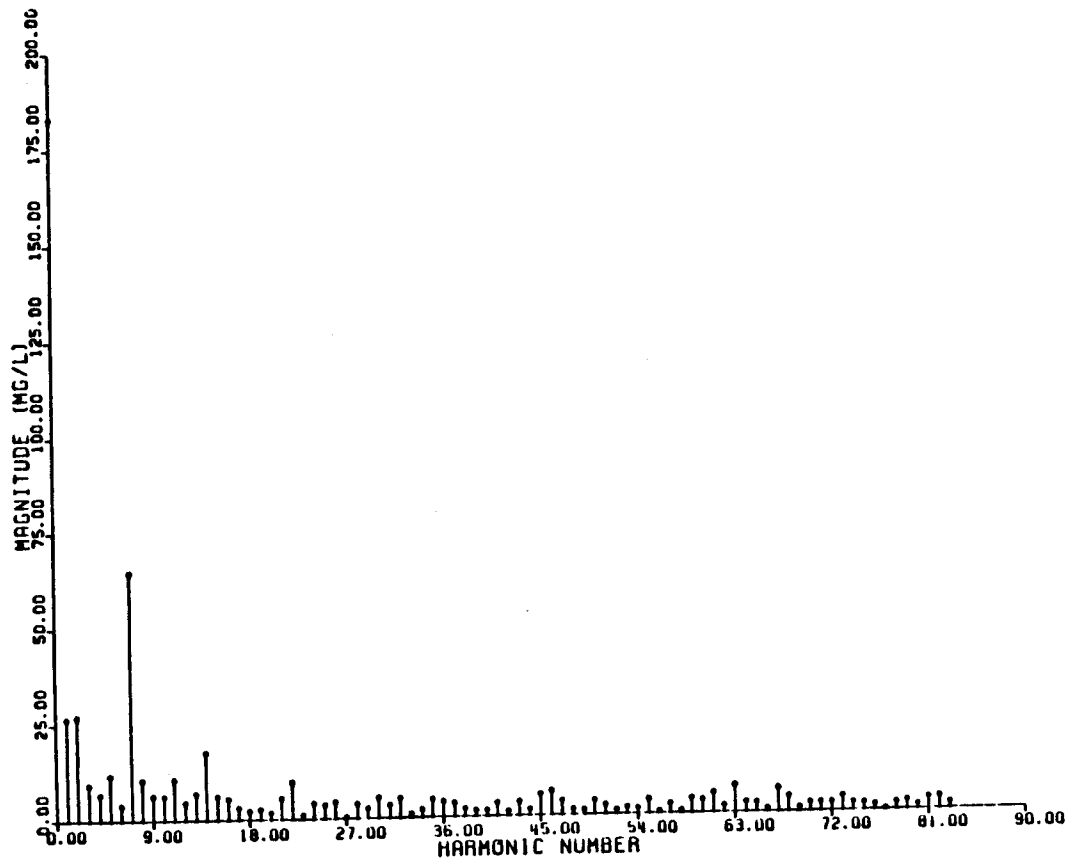
Fig. 3.2 Magnitude Spectrum for Biochemical Oxygen Demand, gm/m^3

SOLUBLE

TOD
1.0
→ 0.80 →
COD
0.80
→ 0.85 →
BOD$_U$
0.68
→ 0.63 →
BOD$_5$
0.43

0.20

PARTICULATE

TSS
1.0
→ 0.79 →
VSS
0.79
→ 0.7 →
VSS
BIO-DEGRADABLE
0.553
→ 1.5 →
BOD$_U$
0.83

0.21
SS
NON-VOLATILE
0.21

0.3
VSS
NON-BIODEGRADABLE
0.237
→ 1.5 →
TOD
NON-BIODEGRADABLE
0.356
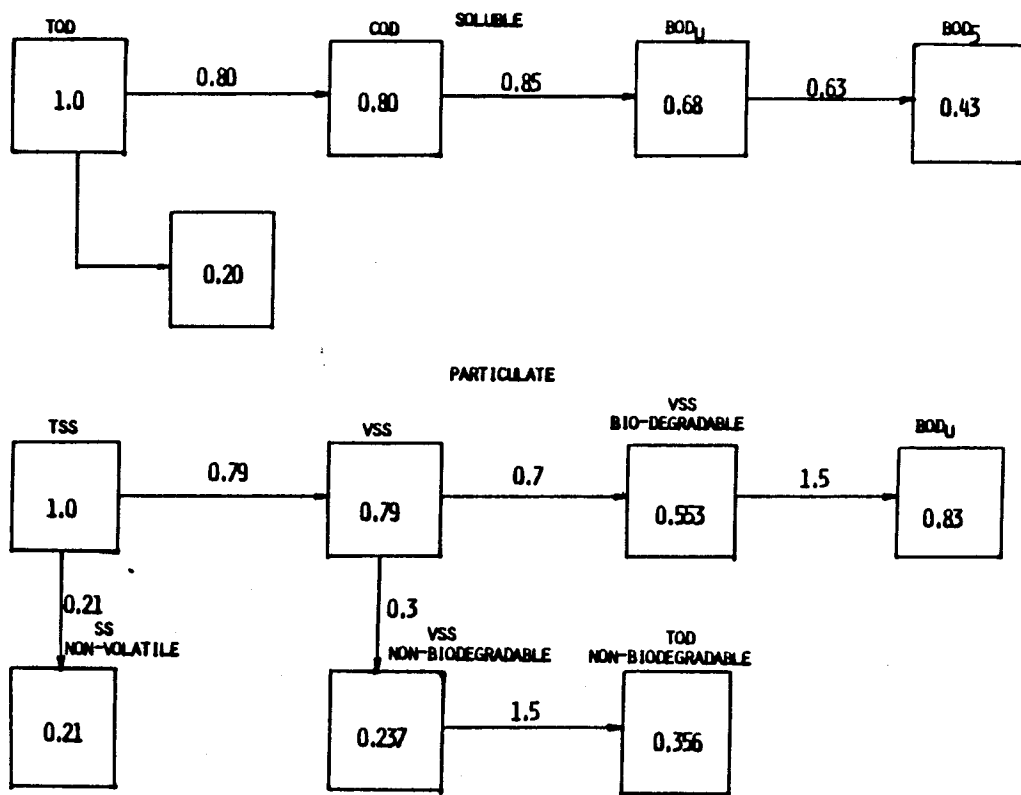
Fig. 3.3   Relationship Between Pollutant Concentrations

due to adsorption of suspended solids (Kuo et al. 1974) and a substantial damping of shock loads.

Design and modeling of primary clarifiers are difficult due to variable influent suspended solids and flow rate. The design of a primary clarifier is also affected by the distribution of settling velocities caused by the variation in size, shape, and density of suspended particles in influent wastewater. Density and temperature fluctuations are also important.

Hazen (1904) used the ideal basin concept and demonstrated that clarification is a function of surface area and independent of basin depth. However, Hazen did not consider flocculation in his analysis. Flocculent particles can coalesce increasing the terminal settling velocity. Bryant (1972) proposed a dynamic mathematical model considering both mixing and clarification. The mixing phenomena was approximated by considering five continuous flow stirred tank reactors (CFSTR) in series. The use of five continuous flow stirred tank reactors leads to a mixing regime which is neither plug flow nor complete mixing. Levenspiel (1967) has shown that this concept is useful for approximating a non-ideal mixing regime.

Hazen's ideal settling basin model has been gradually changed to turbulent mixing models proposed by later investigators, including Dobbins (1944), Camp (1946) and Shiba (1979). Takamatsu et al. (1974) developed a steady state parabolic partial differential equation to find the effect of resuspension on removal efficiency and to predict the optimal depth of sedimentation basin. The scouring problem was treated as a boundary value problem of the second order PDE with specific boundary condition including scouring parameter. The same concept with the modification of non-steady state is used in this

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research.

The two dimensional non-steady state dispersion model for the rectangular basin is represented by

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} - w_p \frac{\partial C}{\partial z} = E_x \frac{\partial^2 C}{\partial x^2} + E_z \frac{\partial^2 C}{\partial z^2} \qquad (3.1)$$

The boundary conditions are:

$$C = C_0 \ at \ x = 0 \qquad (3.2)$$

$$\frac{\partial C}{\partial x} = 0 \ at \ x = L \qquad (3.3)$$

$$E_z \frac{\partial C}{\partial z} + k \, w_p \, C = 0 \ ; \quad at \ z = 0 \qquad (3.4)$$

$$E_z \frac{\partial C}{\partial z} + w_p \, C = 0 \ ; \quad at \ z = H \qquad (3.5)$$

where,

x	=	flow direction (L)
z	=	upward direction (L)
C_0	=	concentration of suspended solids at the inlet (M/L^3),
C	=	concentration of suspended solids (M/L^3),
u	=	longitudinal mean velocity of the flow (L/T),
w_p	=	settling velocity of suspended solids (L/T),
E_x	=	longitudinal dispersion coefficient (L^2/T),
E_z	=	vertical dispersion coefficient (L^2/T),
k	=	scouring parameter.

u, w_p, E_x, E_z and k considered constant throughout the basin. The physical interpretation of the scouring parameter are given by Goda (1956) as follows: k > 1, tendency of scouring; k=1 balance of deposition and scouring; 0 < k < 1, tendency to deposit; and k=0, deposition only. In a case of normal operation the rate of deposition exceeds the rate of scouring. Therefore, the value of k is usually between zero and one. Equation (3.4) indicates that some of the sediments at the bottom will come back again to the main body of the flow. Equation (3.5) means that there is no transport of particles across the free surface.

Scouring parameter is an important index for the design and operation of settling basins. It depends on both the characteristics of basin hydraulic properties (e.g. flow rate, mixing intensity, and flow pattern) and settling properties of sediments (e.g. density, shape, and particle diameter distribution).

The dispersion coefficient (E_x) can be measured experimentally using tracer studies. Takamatsu et al. (1974) formulated an equation which describes his experimental results, which are used here for estimating E_x. The mathematical equation formulated is given by

$$E_x = 3.59 \, exp \, (58.5*F)$$

(3.6)

where,

$$F = Froude \ number \ = u / \sqrt{g} \, H$$

(3.7)

C. Biological Reactor Model

The purpose of biological treatment of wastewater is to coagulate and remove non-settleable colloidal solids and to stabilize organic matter in the presence of microbial mass under a controlled environment. The first model for

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continuous growth system was developed by Monod (1942) using pure culture and a single soluble substrate. Monod (1942) proposed that the growth rate is a function of limiting substrate concentration as shown in equation (3.8)

$$\mu = \frac{\mu^* S}{K_s + S}$$ (3.8)

where,

μ^* = maximum specific growth rate (T^{-1}),

S = limiting substrate concentration (M/L^3),

K_s = saturation concentration (M/L^3).

Many other formulations exist for growth rate coefficient, but Monod's model is widely used.

Net organism production considering Monod's model can be written as follows:

$$r_x = (\mu - K_d)^* X$$ (3.9)

where,

r_x = net organism production (M/L^3),

K_d = decay coefficient (T^{-1}).

The applicability of equation (3.8) to wastewater treatment can be criticized because it is developed for a single soluble and homogeneous substrate. Siddiqi et al. (1966) proposed that domestic wastewater contains 60% to 70% particulate matter. Equation (3.9) does not consider the lag phase and it is non-specific with respect to microbial mass. Actually growth rate should be proportional to active mass, not the entire MLVSS. Moreover, the Monod model cannot be

used for time varying organic loading and influent flow rate.

Structured models were developed to correct the limitations of Monod and other distributed models. The structured model developed by Tench (1968) for the treatment of domestic wastewater considered sludge mass into three components: an adsorbed oxidizable fraction, active portion and biologically inert portion. Westberg (1967) considered biological solids into living and dead cells and also accounted for non-biodegradable suspended matter in the influent wastewater. The structured model schematic used in this investigation is shown in Figure 3.4.

The particulate and complex organic matters are adsorbed on activated sludge floc and the energy is stored. Porges et al. (1956) concluded from their experiments that substrates can be stored on organisms and the rate of storage can exceed the rate of stored substrate utilization by up to 2.6 times. Direct evidence of adsorption and storage phenomenon can be found in the case of contact stabilization.

The removal and transport of soluble substrate to stored substrate developed by Blackwell (1971) was modified by Ekama and Marais (1979) to account for the direct metabolism of soluble substrate by active organism. The net rate of removal of biodegradable substrate is expressed as:

$$r_{SD} = KT * XA * SD * (f_s^* - f_s) - RSD * XA * SD$$

(3.10)

where,

r_{SD} = removal rate of biodegradable soluble substrate, $(M/L^3 T)$,

SD = biodegradable soluble substrate

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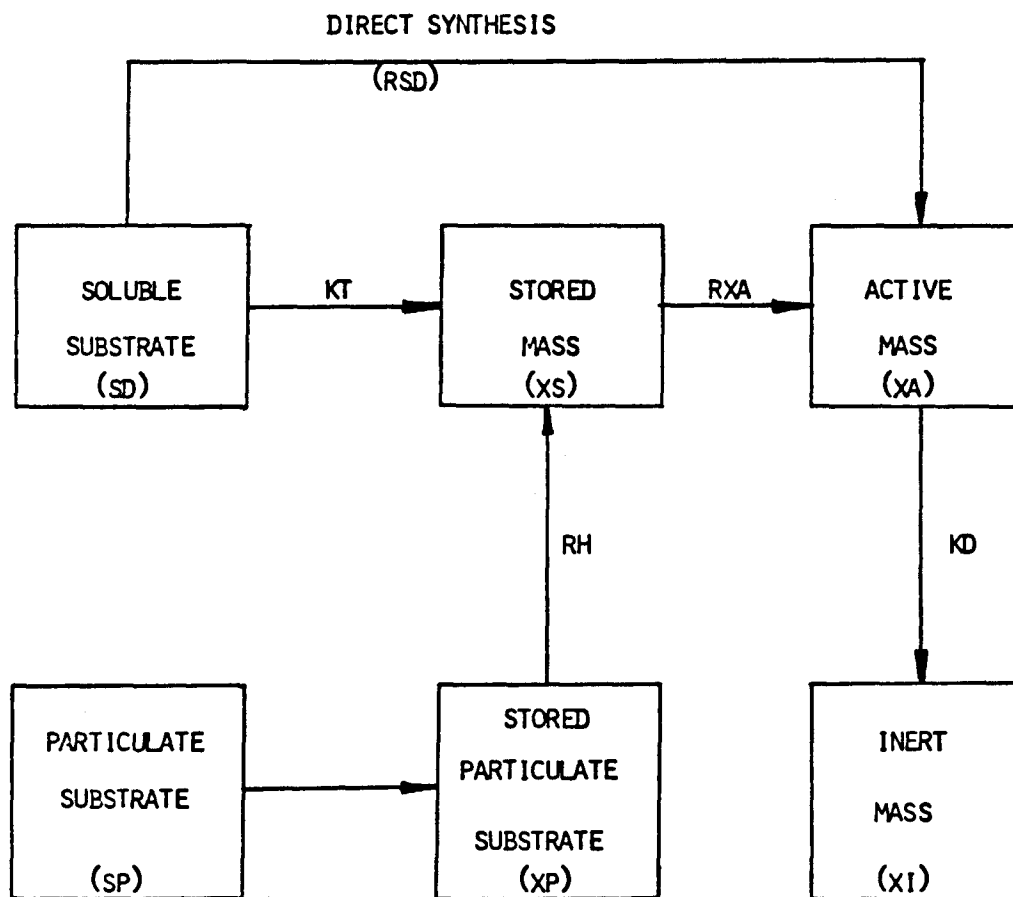
Fig. 3.4 Schematic Structured Model

concentration, (M/L^3),

KT $\quad = \quad$ transport rate coefficient $(L^3/M\ T)$,

f_s^* $\quad = \quad$ maximum fraction of stored mass,

f_s $\quad = \quad$ fraction of stored mass, XS/(XS+XA),

RSD $\quad = \quad$ direct growth rate coefficient $(L^3/M\ T)$.

XA $\quad = \quad$ active mass concentration (M/L^3)

XS $\quad = \quad$ stored mass concentration (M/L^3).

The removal of particulate matter from the liquid phase by the activated sludge is much faster than removal of soluble substrates. A transport expression of particulate matter is not required because it is removed immediately upon contact with flocs. The biodegradable stored particulate fraction undergoes hydrolysis and transforms to stored mass.

Clift (1980) proposed the rate of stored particulate hydrolysis in terms of Monod type saturation function which is represented by the equation below:

$$r_{XP} = -RH* (fp/(K_{sp} + fp))*XA*Y_3$$

(3.11)

where,

r_{XP} $\quad = \quad$ rate of stored particulate substrate hydrolysis $(M/L^3 T)$,

RH $\quad = \quad$ hydrolysis rate coefficient (T^{-1}),

fp $\quad = \quad$ fraction of stored particulate substrate, (XP/(XP+XA))

K_{sp} $\quad = \quad$ saturation coefficient,

Y_3 $\quad = \quad$ conversion factor, gm of XS or SD/gm of XA,

XP $\quad = \quad$ stored particulate substrate (M/L^3).

Active mass is synthesized from stored mass as well as extracellular soluble substrate. The equation proposed by Clift (1980) for the production of active mass from stored mass and direct metabolism of extracellular soluble substrate is expressed as:

$$r_{XA} = RXA*XA*f_s + Y_1*RSD*XA*SD$$

(3.12)

where,

r_{XA} = the net rate of production from stored mass and soluble substrate (M/L^3T),

RXA = storage growth rate coefficient, (T^{-1}),

Y_1 = mass of XA produced per unit mass of XS or SD utilized.

A residual non-biodegradable particulate fraction is formed during the decay of active organisms. The production of inert mass is expressed as follows:

$$r_{XI} = Y_2*K_D*XA$$

(3.13)

r_{XI} = rate of production of inert mass (M/L^3T),

Y_2 = mass of XI produced per unit mass of XA,

K_D = decay rate coefficient (T^{-1}).

Stored mass is obtained from soluble substrate and hydrolysis of stored particulates. It is assumed that no oxygen is required for the hydrolysis of stored particulate substrate and transport of soluble substrate to stored mass.

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$$r_{XS} = KT*XA*SD*(f_s^* - f_s) + RH*XA*(f_p/(K_{sp} + f_p))$$

(3.14)

r_{XS} = stored mass production rate (M/L^3T).

The non-biodegradable soluble organics and non-volatile solids are included in the model because non-biodegradable soluble organics exert an oxygen demand when measured by COD or TOD. Non-volatile solids strongly influence on sludge production.

C-1. Nitrification

The use of Monod growth rate function in wastewater treatment systems has been criticized previously mainly for it's incapability in predicting the time lag in the growth phase. However, many researchers (Hofman and Lees, 1953; Lees and Simpson, 1957) have demonstrated that Monod kinetics can be used in case of nitrification because there is no significant time lag due to change in substrate concentration on the growth rate response to the nitrifying bacteria.

Nitrification is a process in which oxidation of ammonium to nitrite and nitrite to nitrate is carried out by autotrophic bacteria, *Nitrosomonas* and *Nitrobacter*. The growth rate of *Nitrosomonas* can be expressed as follows:

$$r_{XNS} = (\mu_{NS} - K_{DNS})*XNS$$

(3.15)

where,

r_{XNS}	=	net growth rate of *Nitrosomonas* (M/L^3T),
μ_{NS}	=	specific growth rate of *Nitrosomonas* (T^{-1}),
K_{DNS}	=	*Nitrosomonas* decay coefficient (T^{-1}).

The rate of removal of ammonium nitrogen by *Nitrosomonas* can be expressed

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as:

$$r_{NH_4^+} = -\mu_{NS} * \frac{XNS}{Y_{NS}}$$
(3.16)

where,

$r_{NH_4^+}$ = rate of removal of ammonium nitrogen due to nitrification (M/L^3T),

Y_{NS} = yield coefficient, mass of *Nitrosomonas* formed per unit mass of ammonium nitrogen oxidized.

Ammonium nitrogen is also consumed by heterotrophic bacteria. Ammonia is released to the solution as a result of breakdown of nitrogeneous matter and autolysis of cells, and it is removed from the solution as a result of the synthesis of new cells. In the case of domestic wastewater without nitrification, the concentration of ammonium nitrogen in the effluent is close to that in the influent wastewater, but the concentration of the organic residual nitrogen in the effluent is much less than in the influent wastewater. This difference satisfies the net nitrogen requirement during synthesis of new cells. It is assumed that ammonium nitrogen is produced during organism decay as a result of lysis. The rate of ammonium nitrogen removal by heterotrophs is considered proportional to the net rate of active mass formation as follows:

$$r_{HNH_4^+} = -(Y_{NS} * XA * (RXA * f_s + Y_1 * RSD * SD) - Y_{ND} * K_D * XA)$$
(3.17)

where,

$r_{HNH_4^+}$ = net rate of ammonium nitrogen removal by heterotrophic organism ($M-NH_4^+ -N/L^3T$),

Y_{NS} = mass of ammonium nitrogen utilized per unit active mass produced during synthesis,

Y_{ND} = mass of ammonium nitrogen produced per unit active mass destroyed.

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Hoover and Porges (1952) have shown that the composition of activated sludge approximately correspond to the empirical formula $C_5H_7NO_2$. Thus for each gram increase in sludge mass 0.124 grams of ammonium nitrogen is required. The overall rate of ammonium nitrogen removal is the sum of the equation (3.16) and (3.17).

The growth rate expression of *Nitrobacter* is similar to *Nitrosomonas*.

$$r_{XNB} = (\mu_{NB} - K_{DNB})*XNB$$

(3.18)

where,

r_{XNB} =   net growth rate of *Nitrobacter* (M/L^3T),

μ_{NB} =   specific growth rate of *Nitrobacter* (T^{-1}),

K_{DNB} =   *Nitrobacter* decay coefficient (T^{-1})

The expression for nitrite nitrogen contains two terms for growth rate , a positive term for conversion of ammonium nitrogen to nitrite by *Nitrosomonas* and a negative term for the oxidation of nitrite to nitrate by *Nitrobacter*.

$$r_{NO_2^-} = \frac{\mu_{NS}*XNS}{Y_{NS}} - \frac{\mu_{NB}*XNB}{Y_{NB}}$$

(3.19)

where,

$r_{NO_2^-}$ =   nitrite nitrogen production rate $(M-NO_2^- -N/L^3T)$,

Y_{NB} =   yield coefficient, mass of *Nitrobacter* formed per unit mass of nitrite nitrogen oxidized.

The rate of production of nitrate nitrogen by *Nitrobacter* is represented as follows:

$$r_{NO_3^-} = \frac{\mu_{NB} * XNB}{Y_{NB}}$$

(3.20)

where,

$r_{NO_3^-}$ = nitrate nitrogen production rate, $(M-NO_3^--N/L^3T)$.

For a more detailed analysis Poduska's (1973) work should be consulted.

C.2. Oxygen Utilization

Dissolved oxygen in activated sludge is utilized in two ways (a) utilization of oxygen by heterotrophic bacteria for the destruction of carbonaceous matter, and (b) utilization of oxygen by autotrophic bacteria for the synthesis of active mass from stored mass and extracellular substrates and decay of organisms. There is an oxygen requirement for the hydrolysis of particulate substrate but it is considered negligible for this research.

The oxygen utilization by heterotrophic bacteria is represented as follows:

$$r_{OH} = (\frac{1-Y_1}{Y_1})*XA* (RXA*f_s+Y_1*RSD*SD) + (1-Y_2)*K_D*XA$$

(3.21)

where,

r_{OH} = net oxygen uptake rate by heterotrophic bacteria, (M/L^3T).

The term $(1-Y_1)$ represents the oxygen equivalent used for respiration. The first term in equation (3.21) represents the oxygen requirements for synthesis of stored mass and extracellular substrate and the last term is for endogeneous respiration.

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The concentration of ammonium, nitrite and nitrate nitrogen is expressed as elemental nitrogen. The theoretical oxygen demand for conversion of ammonium to nitrite and nitrite to nitrate can be calculated from the oxidation equations.

$$2NH_4^+ + 3O_2 \longrightarrow 2NO_2^- + 2H_2O + 4H^+$$
(3.22)

$$2NO_2^- + O_2 \longrightarrow 2NO_3^-$$
(3.23)
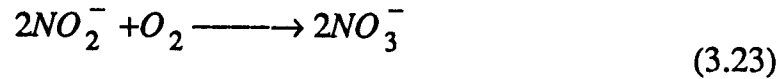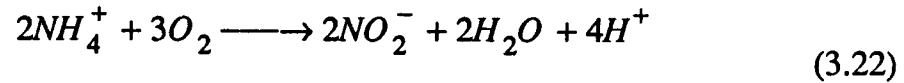
3.42 grams of nitrogen is required for the oxidation of 1 gram of ammonium nitrogen to nitrite nitrogen. An additional 1.142 grams of oxygen is required for the oxidation of 1 gram of nitrite to nitrate. The amount of nitrogen used for synthesis is considered negligible compared to the amount oxidized to obtain energy.

The rate of nitrogeneous oxygen demand by nitrifiers can be expressed as follows:

$$r_{ON} = 3.42 \frac{\mu_{NS} * XNS}{Y_{NS}} + 1.142 \frac{\mu_{NB} * XNB}{Y_{NB}}$$
(3.24)

where,

r_{ON} = oxygen uptake rate by nitrifiers (M/L^3T).

The transfer of oxygen from gas phase to liquid phase is proportional to the saturation concentration of dissolved oxygen and the actual concentration. Therefore,

$$r_{DO} = K_{LA}(DO_s - DO)$$
(3.25)

where,

r_{DO} =   oxygen transfer rate ($M/L^3 T$),

$$K_{LA} = \text{oxygen mass transfer coefficient } (T^{-1}),$$

$$DO_s = \text{saturation dissolved oxygen concentration} = K_H*P$$

$$K_H = \text{Henry's law constant, M/L atm.,}$$
$$P = \text{partial pressure of oxygen at gas phase, atm.}$$

The net dissolved oxygen consumption is represented as follows:

$$r_{OT} = -\left(\frac{1-Y_1}{Y_1}\right)*XA*(RXA*f_s + Y_1*RSD*SD)$$

$$-(1-Y_2)*K_D*XA - 3.42\frac{\mu_{NS}*XNS}{Y_{NS}} - 1.142\frac{\mu_{NB}*XNB}{Y_{NB}}$$

$$+ K_{LA}(DO_s - DO)$$

$$(3.26)$$

The summary of the mathematical model and the information flow is shown in Figure 3.5.

D. Secondary Clarifier Model

The dynamic analysis of activated sludge will be incomplete without the settler dynamics. The process performance of activated sludge is directly dependent on the secondary clarifier because the recycle organisms concentration is primarily a function of thickening capabilities of the clarifiers. Steady state models were considered useful for the design and the process evaluation in the past but they are inadequate for process control because they fail to predict the time dependent responses to the transient inputs.

Many researchers (Bryant, 1972; Busby, 1973; Tracy, 1973) have proposed dynamic mathematical models for the solid liquid separator. All these models used some constraints to predict the result consistent with the solids flux

Top inputs (arrows down):

KT, RH, RS

f_s^*, f_s, RXA

K_D, Y_1, Y_2

μ_{NS}, μ_{NB}, K_{DNS}

Y_{NS}, Y_{NB}, K_{DNB}

V_j, $K_L A_j$, DO_S

Left inputs:

S_0, SR

SN_0, SNR

XP_0, XPR

XS_0, XSR

XA_0, XAR

XI_0, XIR

XN_0, XNR

NH_{40}, NH_{43}

NO_{20}, NO_{23}

NO_{30}, NO_{33}

XNS_0, XNSR

XNB_0, XNBR

DO_0, DOR

Q_1, QR

Middle column:

S_j

SN_j

XP_j

XS_j

XA_j

XI_j

XN_j

NH_{4j}

NO_{2j}

NO_{3j}

XNS_j

XNB_j

DO_j

$= I.A_j - E.A_e$

Right equations:

$- KT \cdot XA_j \cdot S_j (f_s^* - f_{s_j}) - RS \cdot XA_j \cdot S_j$

$- RH \cdot XA_j \left(f_P / K_{SP} + f_P \right)$

$- KT \cdot XA_j \cdot S_j (f_s^* - f_{s_j}) - RH \cdot XA_j - RXA \cdot XA_j \cdot f_{s_j} / Y_1$

$- RXA \cdot XA_j \cdot f_{s_j} - Y_1 \cdot RS \cdot XA_j \cdot S_j - K_D \cdot XA_j$

$- Y_2 \cdot K_D \cdot XA_j$

$- \mu_{NS} \cdot XNS / Y_{NS}$

$(\mu_{NS} \cdot XNS_j / Y_{NS}) - (\mu_{NB} \cdot XNB_j / Y_{NB})$

$\mu_{NB} \cdot XNB_j / Y_{NB}$

$XNS_j (\mu_{NS} - K_{DNS})$

$XNB_j (\mu_{NB} - K_{DNB})$

$- \dfrac{(1. - Y_1)}{Y_1} \cdot XA_j (RXA \cdot XA_j + Y_1 \cdot RSD \cdot S_j)$

$- (1 - Y_2) \cdot K_D \cdot XA_j - 3.42 \, \mu_{NS} - 1 \cdot 142 \, \mu_{NB} + K_L A_j (DO_s - DO_j)$

Right outputs:

S_3

SN_3

XP_3

XS_3

XP_3

XA_3

XI_3

NH_{43}

NO_{23}

NO_{33}

XNS_3

XNB_3

DO_3

Fig. 3.5 Summary of Mathematical Model and Information Flow Diagram

theory (Dick, 1970). The constraints were imposed upon the model to keep the concentration at all points above the compression zone less than the limiting concentration. Stenstrom's (1975) approach is used here which is essentially same as Bryant's (1972), except that the flux limitation used between layers in the separator, rather than a constant based upon the steady state flux curve.

The non-steady state one dimensional continuity equation for a separator is formulated using a material balance which is represented as:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}(D\,\frac{\partial C}{\partial z}) - \frac{(\partial V_s C)}{\partial z} - Reaction \qquad (3.27)$$

where,

$$
\begin{aligned}
C &= \text{concentration } (M/L^3), \\
t &= \text{time } (T), \\
D &= \text{dispersion coefficient } (L^2/T), \\
V_s &= \text{velocity } (L/T), \\
z &= \text{distance } (L).
\end{aligned}
$$

Assumptions are (a) zero dispersion (plug flow, D=0), (b) no biological reaction in the reactor, and (c) uniform solids concentration in the horizontal plane, the continuity equation becomes:

$$\frac{\partial C}{\partial t} = -(V_s + U)\frac{\partial C}{\partial z} - C\,\frac{\partial V_s}{\partial z} \qquad (3.28)$$

where,

C = slurry concentration (M/L^3),

V_s = settling velocity of slurry concentration relative to fluid (L/T),

U = downward fluid velocity (L/T),

z = vertical distance in the solid liquid separator (L),
t = time (T).

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The settling velocity is determined by measuring the initial subsidence of a slurry in a large cylinder. By using different concentrations, a set of data which defines the settling velocity function is obtained. The batch flux is obtained by multiplying settling velocity by concentration as shown in Figure 3.6. The bulk flux is obtained by multiplying underflow concentration with solids concentration and the addition of bulk flux and batch flux results in total flux shown in Figure 3.6.

The concentration at the minimum of the total flux curve is known as limiting concentration which is useful for the determination of loading condition of the solid liquid separator. The solids concentration in the sludge blanket may be predicted for critical loading, unloading and overloading conditions using flux theory as shown in Figure 3.7. A settler becomes overloaded when the limiting layer rises up and reaches the feed point.

Tanks in the series method is used for the solution of the transport equation in which number of differential elements is a function of dispersion coefficient. The modified continuity equation is solved by $CSMP_3$.

The material balance around the ith differential element produces the following equation:

$$\frac{\partial C}{\partial t} = \frac{U(C_{i-1} - C_i)}{\Delta z} + \frac{Min(GS_{i-1}, GS_i) - Min(GS_i, GS_{i+1})}{\Delta z} \qquad (3.29)$$

Equation (3.29) is modified to include boundary conditions for the top and the bottom element. The equation for the top element becomes;
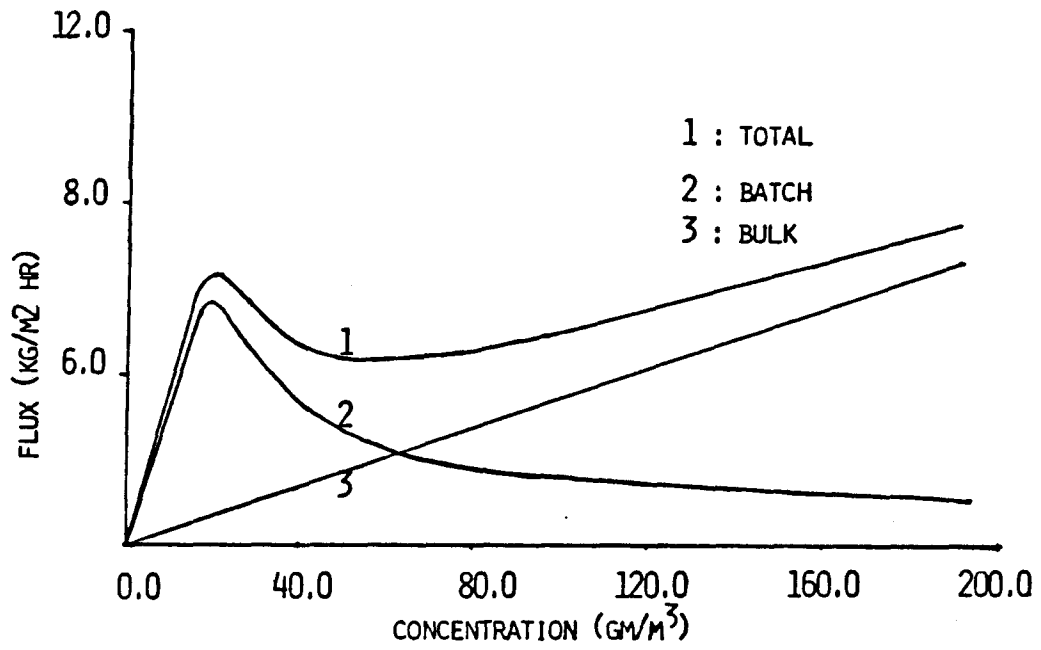
Fig. 3.6 Flux Curves.
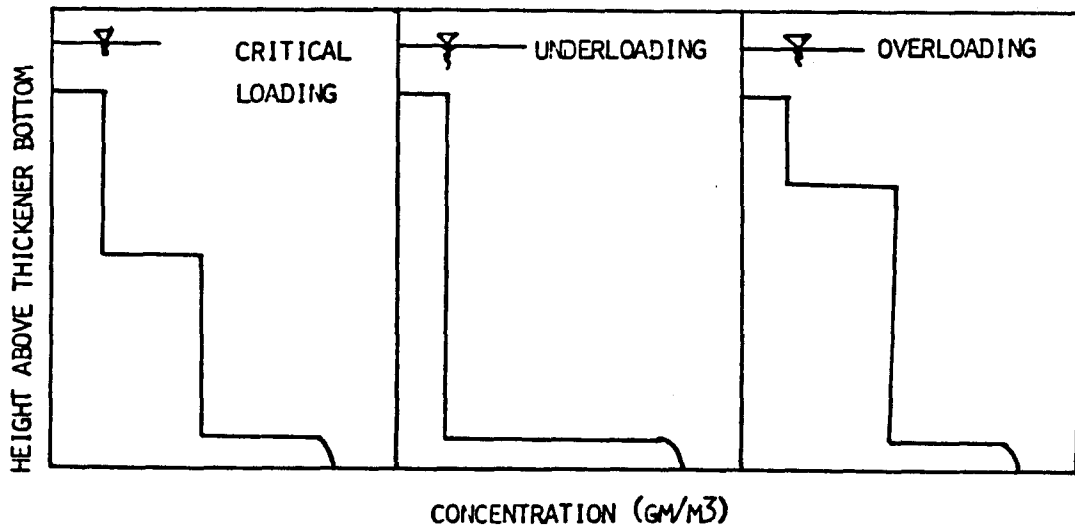
Fig. 3.7 Solids Concentration Profiles

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$$\frac{\partial C_1}{\partial t} = \frac{FLUXIN - U.C_1 - Min\,(GS_i, GS_{i+1})}{\Delta z}$$

(3.30)

where,

FLUXIN = net flux into the settler (M/L^3T),
= $(Q_3{*}MLSS - (Q_3{-}QR_1){*}XEFF)/A$,

Q_3 = flow rate to the clarifier (including recycle),(L^3/T),

QR_1 = flow rate of return sludge (including flow rate of waste sludge),(L^3/T),

MLSS = mixed liquor suspended solids concentration, (M/L^3),

XEFF = effluent suspended solids concentration, (M/L^3),

A = area of the solid liquid separator (L^2).

Zero settling flux at the bottom of the clarifier simplifies the equation (3.29) to:

$$\frac{\partial C_n}{\partial t} = \frac{U.(C_{n-1} - C_n) + GS_n}{\Delta z}$$

(3.31)

where,

n = subscript of the bottom element.

The effluent suspended solids concentration is calculated using second order regression model of Cashion (1981). The second order model is represented as follows:

$$XEFF = B_0 + B_1{*}SRT + B_2{*}HRT + B_3{*}ORA + B_{11}{*}SRT^2$$

$$+ B_{22}{*}\ HRT^2 + B_{33}{*}ORA^2 + B_{12}{*}SRT{*}HRT$$

$$+ B_{13}{*}\ SRT{*}ORA + B_{23}{*}HRT{*}ORA$$

(3.32)

where,

| B | = | statistical parameters, |
| SRT | = | $$\frac{VA*MLSS+VC*MLSSM}{(Q_1-QR_0)*XEFF+QR_0*MLSSR}$$ (3.33) |

VA = volume of the aeration basin, L^3,

MLSS = mixed liquor suspended solids concentration, M/L^3,

VC = volume of the clarifier, L^3,

MLSSM = mean solids concentration in the clarifier, M/L^3,

Q_1 = influent flow rate, L^3/T,

QR_0 = waste flow rate, L^3/T,

XEFF = effluent suspended solids concentration, M/L^3,

MLSSR = underflow solids concentration, M/L^3,

HRT = hydraulic retention time, T,
= VA/Q_1,

ORA = clarifier overflow rate, L^3/L^2T,
= QR/A

QR = clarifier effluent flow rate, L^3/T,

A = surface area of the clarifier, L^2/T.

The above equation for the effluent suspended solids concentration is valid only in the case of a steady state condition. This equation is used here only because there does not exit any relationship which predicts effluent concentration more accurately than Cashion's (1981). The overall system information flow, excluding anaerobic digestion is shown in Figure 3.8.

E. Anaerobic Digestion

Anaerobic digestion is a biological process used in waste treatment for the controlled destruction of biodegradable organic matter. This process is currently applied at most major municipal waste treatment plants. Despite the

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PRIMARY SEDIMENTATION BASIN

Q_i TSS NH_4 BOD

v_p

u

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial X} - v_p E_x \frac{\partial^2 C}{\partial X^2} + E_z \frac{\partial^2 C}{\partial Z^2}$$

$$C = C_0 \quad \text{at} \quad X = 0$$

$$\frac{\partial C}{\partial X} = 0 \quad \text{at} \quad X = L$$

$$E_z \frac{\partial C}{\partial Z} + k \cdot v_p \cdot C = 0 \quad \text{at} \quad Z = 0$$

$$E_z \frac{\partial C}{\partial Z} + k \cdot v_p \cdot C = 0 \quad \text{at} \quad Z = H$$

QI

Q_1 SO SNO XAO XPO XSO XNO XIO

AERATION BASIN

PARAM

XSR
XPR
XIR
XNR
QR_2
S_3

DO_3 Q_3 S_3 SN_3 XA_3 XS_3

XP_3 XN_3 XI_3 NH_{43} NO_{23} NO_{33}

PARAM SOLID LIQUID SEPARATOR

QR XEFF S_3 SN_3
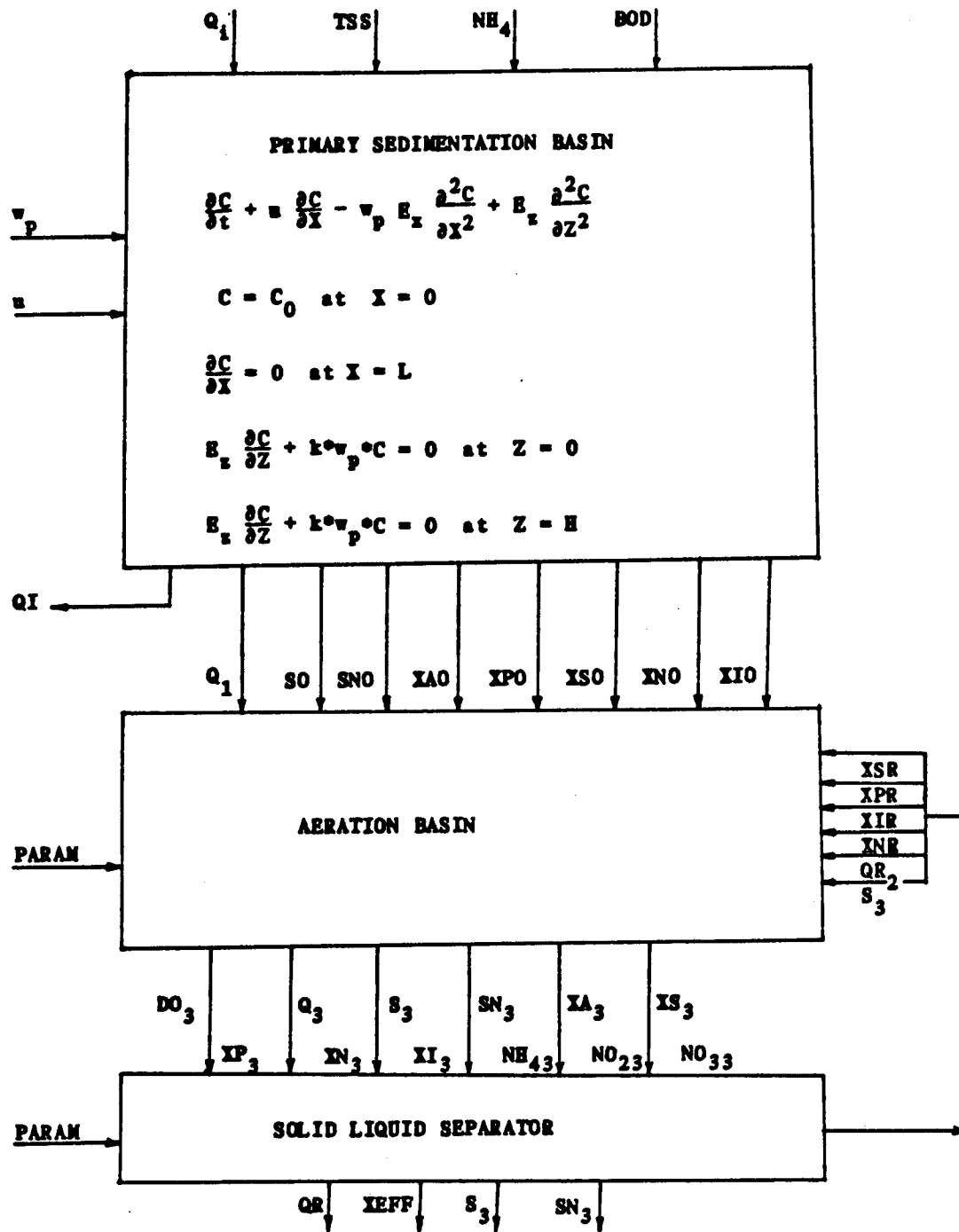
Fig. 3.8 System Information Flow Diagram

widespread application of anaerobic digestion, the development of process control parameters are empirical due to the complexities of the system. One of the objectives of digestion research is the understanding of the complex ecosystem and development of more scientific and reliable means of process design and control.

Early researchers concluded that anaerobic digestion is a process in which solid organic matter is hydrolyzed by external enzymes to form short chain fatty acids. The short chain fatty acids are consequently converted to methane and carbon dioxide as shown in Figure 3.9.

Jeris and McCarty (1976) observed that both acetic acid conversion and carbon dioxide reduction were involved in methane formation. They proposed that about 75% of the methane formed was from acetic acid conversion.

Recent research strongly suggests that the only organic acids which methanogens metabolize are acetate and formate, and emphasize the central position of hydrogen production and utilization in acetate and formate fermentation (Bryant (1976), and Mah et al. (1977)). The new model shows the process for carbohydrate metabolism which is most consistent with the current information on anaerobic digestion (Figure 3.10). In the old concept, as before, fermentative bacteria hydrolyze organic matter and form organic acids, hydrogen, and carbon dioxide. Hydrogen producing acetogenic bacteria obtain energy for growth by producing acetate, hydrogen, and sometimes carbon dioxide from organic acids produced by fermentative bacteria. Methanogens utilize acetate, carbon dioxide, and hydrogen and produce methane and carbon dioxide as final products (Bryant, 1979). The new concept with the consideration of different acids (acetic, propionic, and n-butyric) are chosen for the

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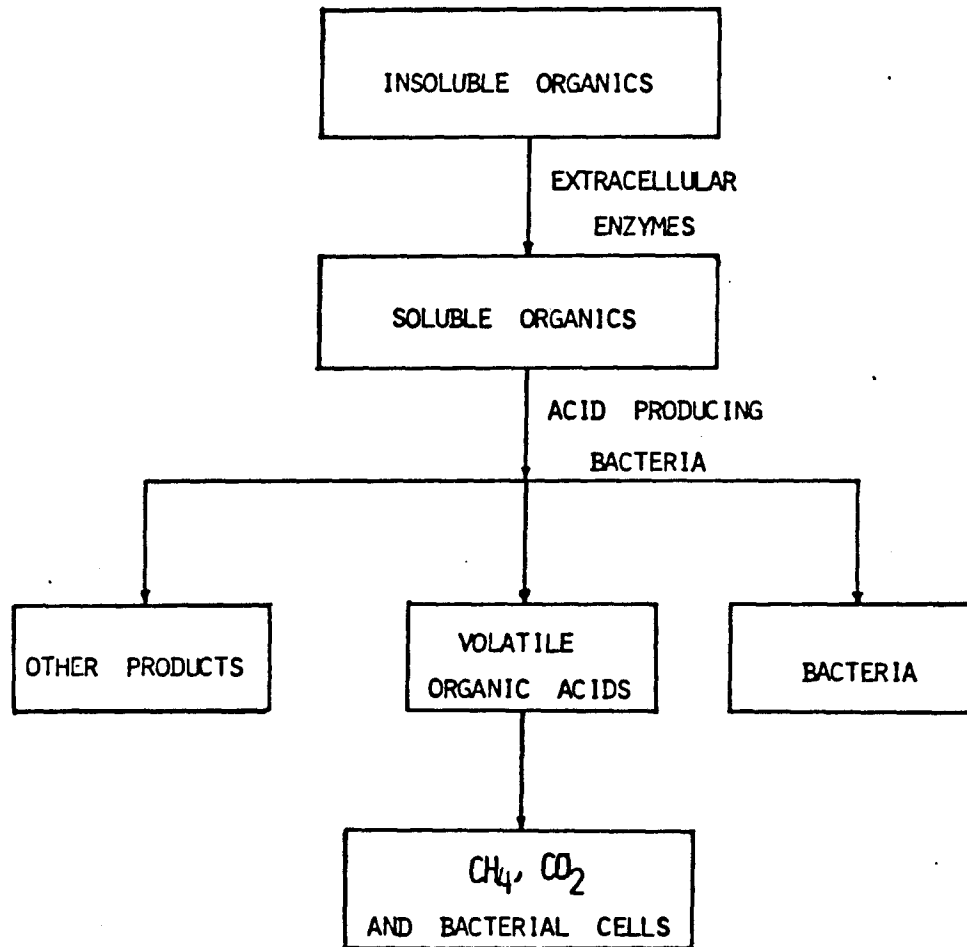
Fig. 3.9 Anaerobic Digestion of Organic Wastes (Old Concept)
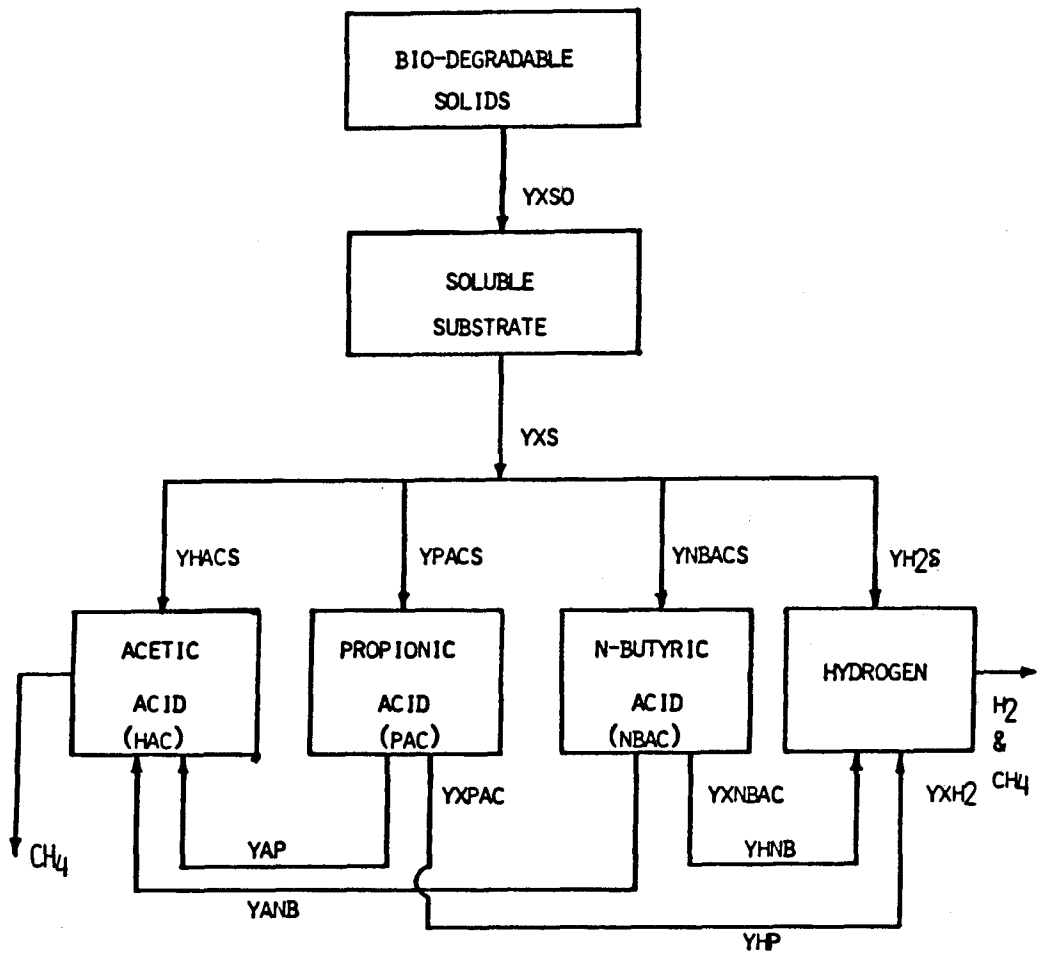
Fig. 3.10 Anaerobic Digestion of Organic Wastes (New Concept)

mathematical model because;

a. acetic acid has been shown to be precursor of approximately 70% of the methane formed in the treatment of domestic waste,

b. propionic and n-butyric acid together are the precursor of 80% of total acetic acid formed,

c. propionate $+3H_2O \longrightarrow$ acetate $+3H_2 + HCO_3^- + H^+$

d. butyrate $\longrightarrow$ 2 acetate $+ 2H_2$

McCarty (1971) showed that protein and carbohydrate fermenting bacteria grow rapidly, fermenting substrates at a retention time of less than one day. However, fatty acids fermenting bacteria grow more slowly and active fermentation is possible only for retention times greater than 5 days.

Most current steady state models of anaerobic digestion process are based upon Monod's (1942) saturation kinetics. Lawrence (1971) used a steady state mathematical model for the design of the anaerobic digestion. Graef (1972) proposed a dynamic mathematical model for various control strategies that can be applied to prevent digester failure. The dynamic mathematical model developed by Hill and Barth (1977) on animal waste digestion was to interface the fundamental characteristics of the process and to understand the overall operation. Andrews (1969) proposed that un-ionized volatile acids are growth limiting and inhibitory to methane bacteria. He presented experimental evidence and evidence from microbiological literature to support this hypothesis and computer simulations showed that inhibition by unionized volatile acids predicts results similar to those observed in the field. Graef (1972)

and Hill and Barth (1977) considered the old concept in their mathematical model of anaerobic digestion.

One of the objectives of this research is to develop a dynamic mathematical model of anaerobic digestion of domestic wastewater using the new concept.

E-1. Mathematical Development

The dynamic mathematical model of anaerobic digestion is developed by material balance equations of different variables and species. Starting point for material balance on anaerobic digestion is biodegradable solids and the concentration at any time can be obtained by integrating the material balance equation.

$$(dBD/dt)=(QII/VD)*(BDO - BD)-(\mu_{BD}*XBD/Y_{XSO}*CF)$$
(3.34)

where,

$$BDO = C_{11}*((MLSSR1+CONBD*PCC)/MLSSR2)$$
(3.35)

$$MLSSR1 = XAR+XPR+XSR+XNBR+XNSR$$
(3.36)

$$MLSSR2=MLSSR1+XIR+PCC+XNR$$
(3.37)

C_{11} = settleable solids concentration, M/L^3,

QII = influent flow rate, L/T^3,

VD = volume of the digester, L^3,

PCC = concentration of sludge from primary clarifier, M/L^3,

CONBD = biodegradability of the sludge from the primary clarifier,

XAR = active mass concentration of recycle sludge, M/L^3,

XSR	=	stored mass concentration of recycle sludge, M/L^3,
XPR	=	particulate mass concentration of recycle sludge, M/L^3,
XNBR	=	concentration of *Nitrobacter* of recycle sludge, M/L^3,
XNSR	=	concentration of *Nitrosomonas* of recycle sludge, M/L^3,
XNVR	=	non-volatile solids concentration of recycle sludge, M/L^3,
XIR	=	inert mass concentration of recycle sludge, M/L^3,
XNR	=	non-biodegradable solids concentrations of recycle sludge, M/L^3,
μ_{BD}	=	specific growth of the biodegradable solids hydrolyzers, T^{-1},
XBD	=	concentration of the biodegradable solids hydrolyzers, M/L^3,
Y_{XSO}	=	soluble organic yield coefficient, mg of organism/mg of soluble substrate,
CF	=	conversion factor, 1 mg soluble substrate per mg of biodegradable solids.

The reaction term in equation (3.34) represents the conversion of insoluble biodegradable solids to soluble organics.

The material balance of non-biodegradable solids is represented by:

$$(dNNB/dt) = (QII/VD)*(NNBO - NNB)$$

(3.38)

where,

NNBO = influent non-biodegradable solids concentration, M/L^3,

$$= C_{11}*((XIR+CONNBD*PCC)/MLSSR2)$$

(3.39)

CONNBD = non-biodegradability of the sludge from the primary clarifier.

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The material balance of soluble organics is given by:

$$(dS/dt) = (QII/VD)*(SO - S) - (\mu*XS/Y_{XS})$$

$$+ (\mu_{BD}*XBD/Y_{XSO}*CF)*(1.-Y_{XSO}-Y_{CO_{21}}) \tag{3.40}$$

where,

SO $\quad = \quad$ influent concentration of soluble organics, M/L^3,

$Y_{XS} \quad = \quad$ yield coefficient for acid formers, mg of organisms/mg of soluble substrate,

$\mu \quad = \quad$ soluble substrate specific growth rate, T^{-1},

XS $\quad = \quad$ microbial concentration of soluble substrate oxidizers, M/L^3,

XP $\quad = \quad$ microbial concentration of propionic acid oxidizers, M/L^3,

XB $\quad = \quad$ microbial concentration of n-butyric acid oxidizers, M/L^3,

$Y_{CO_{21}} \quad = \quad$ yield coefficient of CO_2 from biodegradable solids, gm of CO_2/gm of organism.

Second and last terms in equation (3.40) represent the utilization of soluble organics by acid formers in their metabolism and production of soluble organics from biodegradable solids respectively.

The material balances on propionic, n-butyric, acetic acid and hydrogen can be written as:

$$(dPT/dt) = (QII/VD)*(PTIN - PT) - (\mu_P*XPT/Y_{XPAC})$$

$$+ (\mu*XS/Y_{XS})*(1.-Y_{XS}-Y_{CO_{22}})*Y_{PACS} \tag{3.41}$$

$$(dNBT/dt) = (QII/VD)*(NBTIN-NBT)-(\mu_B*XBT/Y_{XNBAC})$$

$$+ (\mu*XS/Y_{XS})*(1.-Y_{XS}-Y_{CO_{22}})*Y_{NBACS} \qquad (3.42)$$

$$(dHT/dt) = (QII/VD)*(HTIN-HT)-(\mu_M*XM/Y_{XA})$$

$$+ (\mu_P*XPT/Y_{XPAC})*(1.-Y_{XPAC})*Y_{AP}$$

$$+ (\mu_B*XBT/Y_{XNBAC})*(1.-Y_{XNBAC})*Y_{ANB}$$

$$+ (\mu*XS/Y_{XS})*(1.-Y_{XS}-Y_{CO_{22}})*Y_{HCS} \qquad (3.43)$$

$$(dH_2/dt) = (QII/VD)*(H_2IN-H_2)-(\mu_H*XH_2/Y_{XH_2})$$

$$+ (\mu_P*XPT/Y_{XPAC})*(1.-Y_{XNPAC})*Y_{HP}$$

$$+ (\mu B*XBT/Y_{XNBAC})*(1.-Y_{XNBAC})*Y_{HNB}$$

$$+ (\mu*XS/Y_{XS})*(1.-Y_{XS}-Y_{CO_{22}})*Y_{H_{2s}} + (dH_2/dt) \qquad (3.44)$$

where,

PTIN	=	influent concentration of propionic acid, M/L^3,
NTIN	=	influent concentration of n-butyric acid, M/L^3,
HTIN	=	influent concentration of acetic acid, M/L^3,
H_2IN	=	influent concentration of hydrogen, M/L^3,
Y_{PACS}	=	yield coefficient of propionic acid, moles of propionic acid/ moles of soluble substrate,
Y_{NBACS}	=	yield coefficient of n-butyric acid, moles of n-butyric acid/ moles of soluble substrate,
Y_{HACS}	=	yield coefficient of acetic acid, moles of acetic acid/ moles of soluble substrate,
$Y_{H_{2s}}$	=	yield coefficient of hydrogen, moles of

hydrogen/moles of soluble substrate,

Y_{XPAC} = yield coefficient, moles of organism /moles of propionic acid,

Y_{XNBAC} = yield coefficient, moles of organism/moles of n-butyric acid,

Y_{XA} = yield coefficient of methane, moles of organism/ moles of acetic acid,

Y_{XH_2} = yield coefficient, moles of organism/ moles of hydrogen,

Y_{AP} = yield of acetic acid from propionic acid, moles of acetic acid/moles of propionic acid,

Y_{ANB} = yield of acetic acid from n-butyric acid, moles of acetic acid/moles of n-butyric acid,

Y_{HP} = yield of hydrogen from propionic acid, moles of hydrogen/ moles of propionic acid,

Y_{HNB} = yield of hydrogen from n-butyric acid, moles of hydrogen/ moles of n-butyric acid,

Y_{CO_2} = yield coefficient of CO_2 form soluble substrate, gm of CO_2/ gm of organism,

(dH_2/dt) = net rate of hydrogen transfer between gas and liquid phase.

Second terms in equations (3.41) and (3.42) represent the conversion of that acid to acetic acid and second terms in equations (3.43) and (3.44) represent conversion of acetic acid and hydrogen to methane gas. The third and forth terms in equations (3.43) and (3.44) are the conversion of propionic and n-butyric acid to acetic acid and hydrogen. Last terms in equations (3.41) and (3.42) are inputs of propionic and n-butyric acids from soluble organics. Last terms in equations (3.43) and (3.44) are acetic acid and hydrogen from soluble organics. There are few unknowns in equations (3.41), (3.42), (3.43), and (3.44) which we need to find out for the determination of total propionic, n-butyric, acetic acid, and hydrogen concentration.

The material balances for biodegradable solids hydrolyzers, acids oxidizers (propionic and n-butyric), soluble substrate oxidizers, hydrogen consumers, and methane formers can be represented as:

$$(dXBD/dt) = (QII/VD)^* (XBDO - XBD) + (\mu_{BD} - K_{DBD})^* XBD \tag{3.45}$$

$$(dXPT/dt) = (QII/VD)^* (XPTO - XPT) + (\mu_P - K_{DP})^* XPT \tag{3.46}$$

$$(dXBT/dt) = (QII/VD)^* (XBTO - XBT) + (\mu_B - K_{DB})^* XBT \tag{3.47}$$

$$(dXS/dt) = (QII/VD)^* (XSO - XS) + (\mu - K_{DS})^* XS \tag{3.48}$$

$$(dXH_2/dt) = (QII/VD)^* (XH_2O - XH_2) + (\mu_H - K_{DH_2})^* XH_2 \tag{3.49}$$

$$(dXM/dt) = (QII/VD)^* (XMO - XM) + (\mu_M - K_{DM})^* XM \tag{3.50}$$

where,

K_{DBD}, K_{DP}, K_{DB}, K_{DS}, K_{DH_2}, and K_{DM} are the decay coefficients for biodegradable solids hydrolyzers, propionic and n-butyric acids and soluble substrate oxidizers, hydrogen consumers, and methane formers respectively.

μ_{BD}, μ_P, μ_B, μ, μ_{H_2}, and μ_M are the growth rates for biodegradable solids hydrolyzers, propionic, n-butyric acid, and soluble substrate oxidizers, hydrogen consumers, and methane formers, respectively.

Andrews (1969) considered un-ionized volatile acids as an inhibitory agent. This is because concentrations of un-ionized acids are functions of pH and total acids concentration. His model showed that inhibition can be relieved by maintaining pH near neutrality and/or reducing the organic loading. There is some evidence that hydrogen pressure of the order of 10^{-2} atmosphere are toxic

to the organisms mediating the turnover of propionate and will retard the fermentation of acetate to methane (Shea et al. 1968). Because of this evidence hydrogen inhibition is included in propionic, n-butyric, and acetic acid growth rate equations.

The inhibition by un-ionized acids have been incorporated into the Monod growth kinetics as follows:

$$\mu_P = \mu_P^*/(1 + K_{SP}/PA + DMU + H_2 K_{H_2 I})$$

$$(3.51)$$

$$\mu_B = \mu_B^*/(1 + K_{SB}/NBA + DMU + H_2/K_{H_2 I})$$

$$(3.52)$$

$$\mu_H = \mu_H^*/(1 + K_{H_2}/H_2 + DMU)$$

$$(3.53)$$

$$\mu_M = \mu_M^*/(1 + K_{TA}/TA + DMU + H_2/K_{H_2 I})$$

$$(3.54)$$

$$\mu_{BD} = \mu_{BD}^*/(1 + K_{SBD}/BD)$$

$$(3.55)$$

$$\mu = \mu^*/(1 + K_S/S + TACID/K_{SI})$$

$$(3.56)$$

where,

TA = total un-ionized acids concentration, M/L^3, = PA+NBA+HA

TACID= total acids concentration, M/L^3,

$$DMU = \frac{PA}{K_{1P}} + \frac{NBA}{K_{1B}} + \frac{HA}{K_{1A}}$$

$K_{SP}, K_{SB}, KH_2, K_{TA}, K_{SBD}$, and K_S are saturation coefficients for propionic, n-butyric acids,

hydrogen, total un-ionized acid, biodegradable solids, and soluble organics, respectively.

K_{1P}, K_{1B}, K_{1A}, K_{H_2I}, and K_{SI} are inhibition coefficients for propionic, n-butyric, and acetic acid,

hydrogen, and soluble substrate respectively.

HA = un-ionized acetic acid concentration, M/L^3,

PA = un-ionized propionic acid concentration, M/L^3,

NA = un-ionized n-butyric acid concentration , M/L^3.

The un-ionized acids concentration can be calculated using the equilibria for acids.

$$HA = (H^+)(HA^-)/(K_{HAC})$$

(3.57)

$$PA = (H^+)(PA^-)/(K_{PAC})$$

(3.58)

$$NBA = (H^+)(NA^-)/(K_{NBAC})$$

(3.59)

$$HTA = HA + HA^-$$

(3.60)

$$PTA = PA + PA^-$$

(3.61)

$$NTA = NBA + NA^-$$

(3.62)

where,

HTA	=	total acetic acid concentration, M/L^3,
PTA	=	total propionic acid concentration, M/L^3,
NTA	=	total n-butyric acid concentration, M/L^3,
K_{HAC}	=	ionization constant of acetic acid, $1.738x10^{-5}$ at 25° C
K_{PAC}	=	ionization constant of propionic acid, $1.349x10^{-5}$ at 25° C

$$K_{NBAC} = \text{ionization constant of n-butyric acid,}$$
$$1.479 x\, 10^{-5}\ at\ 25^o C$$

The above equations can be solved only by proper analysis of carbonate system.

E.2. Carbonate System and pH

The detailed description of carbonate material balances and calculation of pH is presented in Hill and Barth (1977) and Graef (1972). The formulation is presented here with some modification.

The carbonic acid equilibrium is given by:

$$CO_2 + H_2O \underset{\longleftarrow}{\overset{\longrightarrow}{}} HCO_3^- + H^+ \qquad (3.63)$$

$$K_1 = (H^+)(HCO_3^-)/(CO_2) \qquad (3.64)$$

where,

$(CO_2)_D$ = dissolved CO_2 concentration, M/L^3,

K_1 = ionization constant for CO_2, $3.98\,X\,10^{-7}\ at\ 25^o C$.

The net rate of mass transfer between the gas and liquid phase can be expressed by two film theory.

$$(dCO_2/dt)_T = K_L A\,(CO_2 S - CO_2) \qquad (3.65)$$

At equilibrium, the CO_2 concentration in the liquid phase is proportional to the partial pressure of CO_2 in the gas phase. Therefore,

$$CO_2 S = KCO_2 * PCO_2 \qquad (3.66)$$

where,

$CO_2 S$ = saturation concentration of CO_2, M/L^3,

$K_L A$ = gas transfer coefficient, T^{-1},

$$K_{CO_2} \quad = \quad \text{Henry's law constant,}$$
$$3.23x\,10^{-5}, \text{ moles/mm Hg.l at } 25^{\circ}C,$$

$$PCO_2 \quad = \quad \text{partial pressure of } CO_2 \text{ in gas phase, mm Hg.}$$

The PCO_2 material balance equation is:

$$(dPCO_2/dt) = -(TP)*D*(VD/VG)(dCO_2/dt)-(PCO_2/VG)*Q \tag{3.67}$$

where,

$$Q \quad = \quad QCH_4 + QCO_2 + QH_2 \tag{3.68}$$

$$QCO_2 \quad = \quad CO_2 \text{ gas production, } L^3/T,$$

$$QCH_4 \quad = \quad CH_4 \text{ gas production, } L^3/T,$$

TP $\quad = \quad$ total pressure of CO_2 and CH_4 in gas storage unit, assumed 730 mm Hg,

D $\quad = \quad$ conversion factor for changing moles of gas to liters at ambient temperature and pressure,

VG $\quad = \quad$ gas storage volume, L^3,

VD $\quad = \quad$ volume of the digester, L^3.

$$QH_2 = -(dH_2/dt)*VD*D \tag{3.69}$$

Similarly, the net hydrogen transfer between the gas and liquid phase can be expressed as;

$$d(H_2/dt) = K_L A_1*(H_2S - H_2) \tag{3.70}$$

where,

$$H_2S \quad = \quad \text{saturation concentration of hydrogen, } M/L^3,$$
$$= \quad K_{HH_2}*PH_2*MH_2$$

$$K_L A_1 \quad = \quad \text{gas transfer coefficient, } T^{-1},$$

$$MH_2 \quad = \quad \text{molecular weight of hydrogen,}$$

$$PH_2 \quad = \quad \text{partial pressure of hydrogen in gas phase, mm Hg.}$$

$$K_{HH_2} \quad = \quad \text{Henry's law constant of hydrogen, moles/mm Hg.l}$$

The PH_2 material balance is expressed as,

$$(dPH_2/dt) = -(TP*D)*(VD/VG)*(dH_2/dt) - (PH_2/VG)*Q \tag{3.71}$$

The rate of methane formation is given by:

$$RCH_4 = Y_{CH_4X}*\mu_M*XM \tag{3.72}$$

where,

$$Y_{CH_4X} = \text{yield coefficient of methanogens.}$$

Rate of methane entering the gas phase is equal to the rate at which methane is produced because methane is almost insoluble. Therefore,

$$QCH_4 = (Y_{CH_4X}*\mu_M*XM/XMW + (\mu_H*XH_2/Y_{XH_2})*Y_{MH}/CH_4M))*D*VD \tag{3.73}$$

The rate of biological production of CO_2 is given by:

$$RCO_2 = Y_{CO_2X}*\mu_M*XM \tag{3.74}$$

where,

$$Y_{CO_2X} = \text{carbon dioxide yield coefficient,}$$
moles of CO_2/moles of organism.

The rate of CO_2 escaping into the gas phase is represented by:

$$QCO_2 = (dCO_2/dt)_T*VD*D \tag{3.75}$$

The rate of CO_2 formation by methane formers is written as:

$$(dCO_2/dt)_M = (\mu_M*XM*Y_{CO_2X})/XMW \tag{3.76}$$

where

CH_4M =   molecular weight of methane,

XMW   =   molecular weight of microbial mass.

The rate of production of CO_2 form HCO_3^- by acids (propionic, n-butyric, and acetic acid) formers (chemical) is represented as:

$$(dCO_2/dt)_{PT} = dPT/dt$$

(3.77)

$$(dCO_2/dt)_{NT} = dNT/dt$$

(3.78)

$$(dCO_2/dt)_{HT} = dHT/dt$$

(3.79)

where,

(dPT/dt), (dNT/dt), and (dHT/dt) are material balances of propionic, n-butyric and acetic acids, M/L^3T.

The rate of CO_2 production from HCO_3^- by cation formation can be written as:

$$(dCO_2/dt)_C = dZ^+/dt$$

(3.80)

where,

$$(dZ^+/dt) = (QII/VD)*(ZI - Z^{+)}$$

(3.81)

Z^+ = net cation concentration, except H^+, eq/L^3.

The rate of CO_2 production (biological) is written as:

$$(dCO_2/dt)_{BDC} = (\mu_{BD}*XBD/Y_{XSO})*Y_{CO_{21}} + (\mu*XS/Y_{XS})*Y_{CO_{22}}$$

(3.82)

The charge balance requires the following differential:

$$(dCO_2/dt)_{NH_4^+} = (dNH_4^+/dt)$$

(3.83)

where,

$$dNH_4^+/dt \quad = \quad (QII/VD)*(NH_4IN-NH_4^+) + \mu*XS*Y_{NH_4}$$

$$Y_{NH_4} \quad = \quad \text{yield coefficient of ammonia from raw waste, mg } NH_4^+/mg \text{ of organism,}$$

$$NH_4^+IN \quad = \quad \text{influent ammonia concentration, } M/L^3,$$

$$NH_4^+ \quad = \quad \text{effluent ammonia concentration, } M/L^3.$$

(HCO_3^-) concentration is required before the carbonate equilibria is established to calculate pH. The balance between cations and anions are required in order to find the (HCO_3^-) concentration. The charge can be written as:

$$(NH_4^+)+(H^+)+(C^+) = (HCO_3^-)+2(CO_2^-)+(HA^-)+(PA^-)+(NA^-)$$
$$+(OH^-)+(A^-) \tag{3.85}$$

For pH in the range of 5 to 8, the above equation becomes:

$$(NH_4^+)+(C^+)-(A^-) = (HCO_3^-)+(HA^-)+(PA^-)+(NA^-) \tag{3.86}$$

$$(HCO_3^-)=(Z^+)+(NH_4^+)-(HA^-)-(PA^-)-(NA^-) \tag{3.87}$$

Therefore, the material balance of carbon dioxide used is:

$$(dCO_2/dt) = (QII/VD)*(CO_2IN-CO_2)+(dCO_2/dt)_M + (QII/VD)$$
$$*(HCO_3^-IN-HCO_3^-)+(dCO_2/dt)_T+(dCO_2/dt)_{HT}$$
$$+(dCO_2/dt)_{PT}+(dCO_2/dt)_{NT}-(dCO_2/dt)_C+(dCO_2/dt)_{NH_4}$$
$$+(dCO_2/dt)_{BDC} \tag{3.88}$$

where,

$$CO_2IN \quad = \quad \text{influent dissolved } CO_2 \text{ concentration, } M/L^3,$$

$$CO_2 \quad = \quad \text{effluent dissolved } CO_2 \text{ concentration, } M/L^3,$$

$$HCO_3^-IN \quad = \quad \text{influent } HCO_3^- \text{ concentration, } M/L^3,$$

$$HCO_3^- \quad = \quad \text{effluent } HCO_3^- \text{ concentration}, M/L^3.$$

The summary of the mathematical model and information flow indicating the interaction between the three phases in the system is given in Figure 3.11.

F. Optimization Description

Optimization of the treatment plant is accomplished through a minimization of the objective function, formulated as a weighted sum of capital and operation and maintenance (fixed and variable) costs. The objective function is;

$$TC = \sum_{k1=1}^{N} (CCOST_{k1}/\Gamma) + \sum_{k1=1}^{N} (OM_{k1} + VOPC_{k1}) \qquad (3.89)$$

where,

TC $\quad$ = $\quad$ the total discounted cost,

$CCOST_{k1}$ $\quad$ = $\quad$ capital cost of unit k1,

OM_{k1} $\quad$ = $\quad$ operation and maintenance cost of unit k1,

N $\quad$ = $\quad$ total number of cost functions considered,

Γ $\quad$ = $\quad$ a discount factor, defined as a function of discount rate, i, and number of years, n_1, in the planned horizon.

$$= \quad \sum_{j=1}^{n_1} (1./(1.+i)^{-j}) = (1.-(1.+i)^{-n_1})/i \qquad (3.90)$$

VOPC $\quad$ = $\quad$ variable operating cost.

For the dynamic operations of a plant, process energy costs are not constant. For this reason the variable operating cost has been included in the objective function.

GAS PHASE

$$\dot{PCO_2} = -(TP \cdot D) \cdot (VD/VG) \cdot (\dot{CO_2})_T - (PCO_2/VG) \cdot Q$$

$$\dot{PH_2} = -(TP \cdot D) \cdot (VD/VG) \cdot (\dot{H_2})_T - (PH_2/VG) \cdot Q$$

$$Q = QCH_4 + QCO_2 + QH_2$$

$$QCO_2 = -(\dot{CO_2})_T \cdot D \cdot VD \qquad QH_2 = -(\dot{H_2})_T \cdot D \cdot VD$$

Inputs (left): VD, VG ; TP, D

Outputs (right): Q, PCO_2, PH_2

Middle flows: PCO_2 | PH_2 | QCH_4 | $(\dot{CO_2})_T$ | $(\dot{H_2})_T$

LIQUID PHASE

$$\dot{PT} = CON - RXN11 + RXN21 \cdot Y_{PACS}$$

$$\dot{NBT} = CON - RXN31 + RXN21 \cdot Y_{NBACS}$$

$$\dot{HT} = CON - (\mu_M \cdot XM/Y_{XA}) + RXN11 \cdot (1 - Y_{XPAC}) \cdot Y_{AP}$$
$$\qquad + RXN31 \cdot (1 - Y_{XNBAC}) \cdot Y_{ANB} + RXN21 \cdot Y_{HCS}$$

$$\dot{H_2} = CON - (\mu_H \cdot XH_2/Y_{XH_2}) + RXN11 \cdot (1 - Y_{XPAC}) \cdot Y_{HP}$$
$$\qquad + RXN31 \cdot (1 - Y_{XNBAC}) \cdot Y_{HNB} + RXN21 \cdot Y_{H_2S} + (\dot{H_2})_T$$

$$RXN21 = (\mu \cdot XS/Y_{XS}) \cdot (1 - Y_{XS} - Y_{CO_{22}})$$

$$RXN11 = (\mu_p \cdot XPT/Y_{XPAC}) \qquad RXN31 = (\mu_B \cdot XBT/Y_{XNBAC})$$

$$(\dot{CO_2})_T = K_{LA} \cdot (CO_{2S} - CO_2) \qquad HA = (H^+)(H\bar{A})/K_{HAC}$$

$$CO_{2S} = K_{CO_2} \cdot PCO_2 \qquad PA = (H^+)(PA^-)/K_{PAC}$$

$$(\dot{H_2})_T = K_{LA1} \cdot (H_{2S} - H_2) \qquad NA = (H^+)(NA^-)/K_{NBAC}$$

$$H_{2S} = K_{HH_2} \cdot PH_2 \qquad (H^+) = K_1 \cdot CO_2/HCO_3^-$$

$$(CO_2) = CON + (QII/VD) \cdot (HCO_3 IN - HCO_3^-) + (\dot{CO_2})_M + (\dot{CO_2})_T$$
$$\qquad + (\dot{CO_2})_{PT} + (\dot{CO_2})_{NBT} + (\dot{CO_2})_{HT} + (\dot{CO_2})_{NH_4} - (\dot{CO_2})_C$$
$$\qquad + (\dot{CO_2})_{BDC}$$

$$(\dot{CO_2})_{PT} = PT \qquad (\dot{CO_2})_{NBT} = NBT \qquad (\dot{CO_2})_{HT} = HT$$

$$(\dot{CO_2})_{BDC} = (\mu_{BD} \cdot XBD/Y_{XSO}) \cdot Y_{CO_{21}} + (\mu \cdot XS/Y_{XS}) \cdot Y_{CO_{22}}$$

$$(HCO_3^-) = Z^+ + NH_4^+ - HA^- - PA^- - NBA^-$$

Inputs (left): QII, D ; NH_4IN ; ZI, VD ; K_LA ; K_LA_1 ; CO_2IN ; HCO_3IN ; K_{HH_2} ; K_{HAC} ; K_{PAC} ; K_{NBAC} ; Y_{PACS} ; Y_{NBACS} ; Y_{XPAC} ; Y_{XNBAC} ; $Y_{CO_{22}}$; K_1

Outputs (right): Z^+ ; NH_4 ; (CO_2) ; PAC ; NBAC ; HAC ; H^+ ; HCO_3^-

Bottom flows:

μ_P μ_B μ	XPT XBT XS	QCH_4 XM	μ_{BD} μ_H μ_M	TA TACID H_2	PA NBA HA

contd.

BIOLOGICAL PHASE

Inputs (top): μ_P, μ_B, μ | XPT, XBT, XS | QCH$_4$, XM | μ_{BD}, μ_H, μ_M | TA, TACID, H$_2$ | PA, NBA, HA

Outputs (right): BD, S, XBD, XBT, XPT, XS, XH$_2$, XM

$$\dot{BD} = CON - (\mu_{BD} \cdot XBD/Y_{XSO} \cdot CF)$$

$$\dot{S} = CON - (\mu \cdot XS/Y_{XS}) + (\mu_{BD} \cdot XBD/Y_{XSO} \cdot CF) \cdot OMY_{S1}$$

$$\dot{XBD} = CON + (\mu_{BD} - K_{DBD}) \cdot XBD$$

$$\dot{XPT} = CON + (\mu_P - K_{DB}) \cdot XPT$$

$$\dot{XBT} = CON + (\mu_B - K_{DB}) \cdot XBT$$

$$\dot{XS} = CON + (\mu - K_{DS}) \cdot XS$$

$$\dot{XH_2} = CON + (\mu_H - K_{DH_2}) \cdot XH_2$$

$$\dot{XM} = CON + (\mu_M - K_{DM}) \cdot XM$$

$$\mu_{BD} = \dot{\mu}_{BD}/(1 + (K_{SBD}/BD))$$

$$\mu = \mu^*/(1 + (K_S/S) + TACID/K_{SI})$$

$$\mu_P = \mu_P^*/(1 + (K_{SP}/PA) + DMU + H_2/K_{H_2I})$$

$$\mu_B = \mu_B^*/(1 + (K_{SB}/NBA) + DMU + H_2/K_{H_2I})$$

$$\mu_M = \mu_M^*/(1 + (K_{TA}/TA) + DMU + H_2/K_{H_2I})$$

$$\mu_H = \mu_H^*/(1 + (K_{H_2}/H_2) + DMU)$$

$$DMU = (PA/K_{1P}) + (NBA/K_{1B}) + (HA/K_{1A})$$

$$QCH_4 = ((\mu_M \cdot XM/Y_{CH_4X}) + (\mu_H \cdot XH_2/Y_{XH_2}) \cdot Y_{MH}) \cdot D \cdot VD$$

$$CON = (QIL/VD) \cdot (IN - OUT)$$

$$OMY_{S1} = (1 - Y_{XSO} - Y_{CO_21})$$

Fig. 3.11 Summary of Mathematical Model and Information Flow

To obtain a realistic optimum, constraints are required on many process variables. Constraints are required because regulations or physically realizable conditions through limits on linear or nonlinear functions of those variables. Constraints considered in this study are the following:

a. Constraint on the effluent suspended solid concentration.

$$XEFF \leq 30 \ gm/m^3$$

(3.91)

b. Constraints for secondary clarifier:

(1) For thickening:

$$Operating \ flux \leq G_L$$

(3.92)

(2) For Clarification:

$$OVEL \geq OVEL_{min}$$

(3.93)

where,

G_L = limiting solid flux of secondary clarifier, $Kg/m^3/day$,

$OVEL_{min}$ = minimum overflow rate, $m^3/m^2/day$,

$OVEL$ = overflow rate, $m^3/m^2/day$.

c. Constraint for anaerobic digestion:

(1) Constraint on sludge retention time:

$$\Theta_d > \Theta_{dmin}$$

(3.94))

(2) Constraint on the maximum permissible loading:

$$LF_d \leq LF_d^m$$

<div align="right">(3.95)</div>

where,

Θ_d = sludge retention time, days,

Θ_{dmin} = minimum solids retention time, days,

LF_d^m = maximum permissible loading rate, Kg VSS/m^3 day,

LF_d = loading rate, Kg VSS/m^3 day.

Cost functions (capital costs and O&M costs (excluding process energy costs)) in terms of design variables for different unit processes are developed using the data available in Patterson and Banker (1971), and Smith (1973). Cost functions are to be updated to use in the present year.

Various indices are available for updating costs. For this research, the most frequently used ENR Construction Cost Index (CCI) is used. Data available for energy and labor of different unit processes are in KWH/yr and hrs/yr, respectively. So the updating using Construction Cost Index (CCI) is required for only capital and maintenance costs.

The influence coefficient algorithm developed by Becker and Yeh (1972, 1973) is combined here with the minimum criteria to obtain a linear programming formulation. Influence coefficient is used to cope with the nonlinearities involved in the cost functions of the unit processes of treatment plant. The algorithm requires the initial estimates of the parameters in the feasible region. The error in the parameters are then optimized i.e., parameters are optimized to minimize the objective function. The information flow diagram including the optimization is shown in the Figure 3.12. The algorithm applied to the optimal design and operation of treatment plant is outlined below:
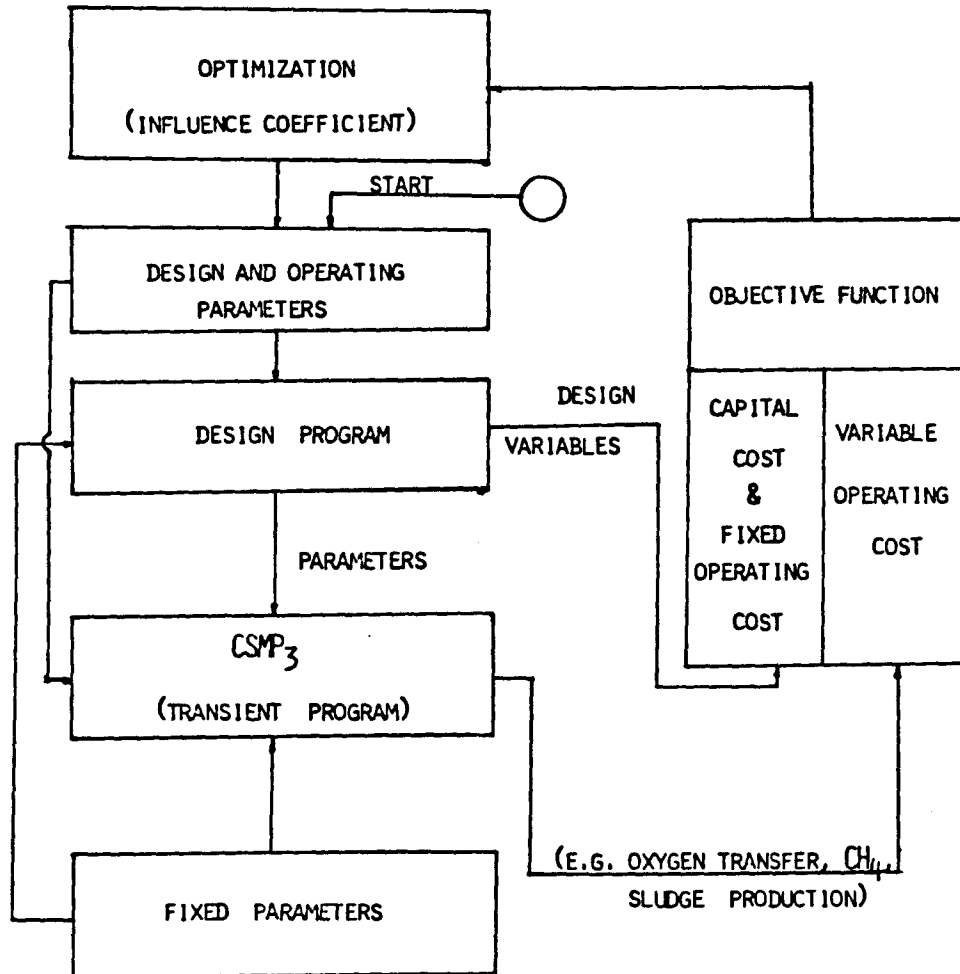
Fig. 3.12 Information Flow Diagram for the Least Cost Design and
Operation

1. Initial estimates of the parameters in the feasible region are used for the solution of the steady state model. The output obtained from the steady state model is design variables. Each function of capital cost and operating and maintenance cost (fixed) for each unit process are functions of design variables. Dynamic mathematical model solved by CSMP III. calculates dynamic oxygen requirement, sludge production, and gas production from anaerobic digestion. Variable operating costs are process energy cost, sludge disposal cost, and the revenue by selling methane gas. Values of each of the cost functions are calculated using design parameters obtained from the steady state model. The error a_{ik1} and b_{ik1} are:

a_{ik1} = [(Capital Costs Using Perturbed Parameters) -(Cost Using Parameter Estimates)] / Changes in Parameters)

b_{ik1} = (Fixed O&M Costs Using Perturbed Parameters) -(Fixed O&M Costs Using initial Parameter Estimates)] / (Changes in Parameters)

where,

k1 = 1,......,N

i = 1,......,M

N = number of cost functions,

M = number of parameters.

2. Mathematically, the objective function is;

$$\min\left[\sum_{k1=1}^{N} CCOST_{k1}/\Gamma + \sum_{k1=1}^{N} OM_{k1} + VOPC \right] \qquad (3.96)$$

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3. Each parameters are perturbed independently in turn and the following influence coefficient matrix is calculated;

$$CCOST1,............,CCOSTN \quad OM1,.................,OMN$$

η_P a11 a12 a13,......,a1N b11 b12 b13,......,b1N

SRT a21 a22 a23,......,a2N b21 b22 b23,......,b2N

Θ_d a31 a32 a33,......,a3N b31 b32 b33,......,b3N

OLR a41 a42 a43,......,a4N b41 b42 b43,......,b4N

HRT a51 a52 a53,......,a5N b51 b52 b53,......,b5N

ORA a61 a62 a63,......,a6N b61 b62 b63,......,b6N

. . . .

. . . .

. . . .

γ aM1 aM2 aM3,......,aMN bM1 bM2 bM3,......,bMN

4. Changes in the estimated values of parameters for the next iteration is required. Therefore;

$$
\begin{aligned}
\eta_p &= \eta_p^o + \alpha_1^o \\
SRT &= SRT + \alpha_2^o \\
\Theta_d &= \Theta_d^o + \alpha_3^o \\
OLR &= OLR^o + \alpha_4^o \\
HRT &= HRT^o + \alpha_5^o \\
ORA &= ORA^o + \alpha_6^o \\
&\quad \cdot \quad \cdot\ \cdot \\
&\quad \cdot \quad \cdot\ \cdot \\
&\quad \cdot \quad \cdot\ \cdot \\
\gamma &= \gamma^o + \alpha_M^o
\end{aligned}
$$

$$(3.97)$$

in which superscript 1 represents new estimations and are the perturbations to be determined. A linear form is assumed for $k1$th cost functions;

$$
CCOST_{k1}^1 = CCOST_{k1}^o + a\,1k\,1.\alpha_1^o + \dots\dots + aMk\,1.\alpha_M^o \tag{3.98}
$$

$$
OM_k^1 = OM_{k1}^o + b\,1k\,1.\alpha^o + \dots\dots + bMk\,1.\alpha_M^o \tag{3.99}
$$

in which a_{ik_1} and b_{ik_1} are appropriate influence coefficient values calculated in step 3. $\alpha_1^o, \alpha_2^o, \alpha_3^o, \dots \alpha_M^o$ are determined by substituting equations (3.97) and (3.98) in the objective function. The linear programming formulation becomes;

$$\min \left\{ \sum_{k1=1}^{N} (CCOST_{k1}/\Gamma) \sum_{k1=1}^{N} OM_{k1} + VOPC \right\} \qquad (3.100)$$

subject to:

$$\pm (CCOST_{k1}^{o} + a\,1k\,1.\alpha_1^{o} + \ldots\ldots + aNk\,1.\alpha_M^{o}) \leq CCOST_{k1} \qquad (3.101)$$

$$\pm (OM_{k1}^{o} + b\,1k\,1.\alpha_1^{o} + \ldots\ldots + bNk\,1.\alpha_M^{o}) \leq OM_{k1}$$

$$CCOST_{k1}, OM_{k1}, \alpha_1^{o}, \ldots\ldots \alpha_M^{o} \geq 0 \qquad (3.102)$$

$$
\begin{array}{ccccc}
\eta_p L1 & < & \eta_p & < & \eta_p U1 \\
SRTL1 & < & SRT & < & SRTU1 \\
\Theta_d L1 & < & \Theta_d & < & \Theta_d L1 \\
OLRL1 & < & OLR & < & OLRU1 \\
HRTL1 & < & HRT & < & HRTU1 \\
ORAL1 & < & ORA & < & ORAU1 \\
\cdot & & \cdot & & \cdot \\
\cdot & & \cdot & & \cdot \\
\cdot & & \cdot & & \cdot \\
\gamma L1 & < & \gamma & < & \gamma U1 \\
\end{array}
$$

$$(3.103)$$

The variables are $CCOST_{k1}$, α_1^{o}, α_2^{o}, ...,α_M^{o}, OM_{k1} and slack variables. The quantities $CCOST_{k1}$, $a\,1k\,1, a\,2k\,2, \ldots\ldots, aMk\,1$, and OM_{k1} are known computationally. Solution obtained from linear programming include α_1^{o}, α_2^{o}, ...,α_M^{o}. Therefore, SRT, Θ_d, OLR, HRT, ORA,....,γ can be calculated using equation (3.97). This completes one cycle and this procedure (step 1-4) is repeated until the convergence criteria is satisfied.

IV. COST EQUATIONS FOR UNIT PROCESSES

The objective of this dissertation is to show that an initial design procedure which considers capital and operating costs, including costs calculated from dynamic treatment plant models, reduces overall, life time plant costs. In order to satisfy this objective, it was necessary to calculate typical treatment plant costs. A search of all available treatment plant cost data was made with the objective of creating a set of empirical equations describing costs as a function of key process variables, such as size.

Costs were divided into three categories: capital costs; fixed operating and maintenance costs, and variable operating costs. Fixed operating and maintenance costs are costs unaffected by the plant's operating strategy. Variable costs are substantially affected by treatment plant operations, such as aeration energy costs as affected by SRT.

Cost equations for capital, operating, and maintenance costs, excluding process energy, in terms of design variables for different unit processes, were developed using the data provided by Patterson and Banker (1971), Smith (1973), and Wasner et al. (1977). These costs do not include cost for special site work, land, legal, general contractor's overhead and profit, fiscal and administration. The fixed operation and maintenance costs include costs for energy (building electrical energy related), maintenance materials, and labor. The building energy requirements for each process are in terms of kW-hr/yr and are calculated using an average building related energy demand. Maintenance material costs include the cost of periodic replacement of component parts such as valves, motors, instrumentation and other process items of a similar nature to maintain good process operating conditions. These material costs do not

consider cost of chemicals for process operation. Labor requirements include both operation and maintenance labor and are represented in terms of hrs/yr.

Most engineers and planners are accustomed to updating costs using an index which is developed by tracking the costs of specific items and proportioning the costs according to a predetermined ratio. Most frequently utilized index in the construction industry is the *ENR* Construction Cost Index (CCI), and costs using this index can be updated as,

$$Updated\ Cost = \frac{(Construction\ Costs\ x\ Current\ CCI)}{(CCI\ of\ the\ Year\ of\ Available\ Data)} \quad (4.1)$$

The simplicity and ease of use of the ENR has made it popular with engineers and planners, but is limited when used for for water and wastewater treatment plant construction, because it does not include mechanical equipment, pipes or valves that are associated with such construction. The approach which is utilized to overcome the shortcomings of the ENR indices are to apply specific indices (e.g. EPA index for material and supply costs) and actual costs of labor ($/hr) and energy ($/kW-hr). Cost functions for the optimal design and operation of a treatment system are as follows:

Primary treatment (Screening, Grit removal, and Flow measurements)

$$CCOST = EXP\,[3.25972 + 0.61915\,x\,]*1000. \quad (4.2)$$

$$OHRS = EXP\,[6.39872 + 0.23096\,x + 0.16496\,x^2 - 0.0146\,x^3] \quad (4.3)$$

$$XMHRS = EXP\,[5.8461 + 0.20651\,x + 0.06884\,x^2 + 0.02382\,x^3 - 0.00441\,x^4] \quad (4.4)$$

$$TMSU = EXP\,[7.23566 + 0.39994\,x - 0.22498\,x^2 + 0.1101\,x^3 - 0.01103\,x^4] \quad (4.5)$$

$$EERG = EXP\,[6.30864 + 0.23453\,x - 0.35844\,x^2 + 0.00871\,x^3]$$

$$(4.6)$$

$$EERMS = EXP\,[7.1497 + 0.28856\,x - 0.07886\,x^2 + 0.014662\,x^3]$$

$$(4.7)$$

$$EER = EERG + EERMS$$

$$(4.8)$$

where

x	=	$ln(Q)$
Q	=	flow to the treatment plant, MGD,
$CCOST$	=	capital cost, \$,
$OHRS$	=	operation man-hour requirements, man-hr/yr,
$XMHRS$	=	maintenance man-hour requirements, man-hr/yr,
$TMSU$	=	total material and supply cost, \$,
$EERG$	=	electrical energy required for grit removal, kW-hr/yr
$EERMS$	=	electrical energy required for flow measurements and screening, kW-hr/yr,
EER	=	total electrical energy required, kW-hr/yr.

Primary Clarifier:

$$CCOST = EXP\,[3.71635 + 0.38986\,x + 0.08456\,x^2 - 0.00472\,x^3]*\,1000.$$

$$(4.9)$$

$$OHRS = EXP\,[5.84656 + 0.25841\,x + 0.1137\,x^2 - 0.01094\,x^3]$$

$$(4.10)$$

$$XMHRS = EXP\,[5.27342 + 0.22833\,x + 0.12265\,x^3 - 0.01167x^3]$$

$$(4.11)$$

$$TMSU = EXP\,[5.66988 + 0.7508\,x]$$

$$(4.12)$$

$$EER = EXP\,[11.0736 - 1.2574\,x + 0.16836\,x^2 - 0.004667\,x^3]$$

$$(4.13)$$

where

$$x = ln\,(AREAP)$$

AREAP = surface area, $1000 \, ft^2$.

Aeration:

$$CCOST = EXP\,[2.4144 + 0.17568 \, x + 0.08474 \, x^2 - 0.00267 \, x^3]* \, 1000.$$

(4.14)

$$CCOST1 = EXP\,[4.1488 + 0.71363 \, x_1 - 0.0526 \, x_1^2 + 0.014749 \, x_1^3]* \, 1000.$$

(4.15)

$$OHRS = EXP\,[6.9006 + 0.32373 \, x_1 + 0.05909 \, x_1^2 - 0.00493 \, x_1^3]$$

(4.16)

$$XMHRS = EXP\,[6.16994 + 0.29485 \, x_1 + 0.17599 \, x_1^2 - 0.04095 \, x_1^3 + 0.0033 \, x_1^4]$$

(4.17)

$$THSU = EXP\,[0.62138 + 0.48205 \, x_3]* \, 1000.$$

(4.18)

$$EER = EXP\,[-12.1285 + 10.9869 \, x_2 - 2.0285 \, x_2^2 + 0.17177 \, x_2^3$$

$$-0.00517 \, x_2^4]$$

(4.19)

where

x	=	$ln(V)$
V	=	liquid volume, $1000 \, ft^3$,
x_1	=	$ln \, (BCAP)$
$BCAP$	=	initial firm blower capacity, 1000 cfm,
$OCRT$	=	oxygen requirement, lbs of O_2/day,
x_2	=	$ln(OCRT)$
x_3	=	$ln \, (QA)$
QA	=	flow to the aeration tank, MGD,
$CCOST$	=	capital cost of the aeration tank (basin structure), \$,
$CCOST1$	=	capital cost of diffused air system, \$,

Secondary Clarifier:

$$CCOST = EXP[3.71635 + 0.38986\,x + 0.08456\,x^2 - 0.00472\,x^3]*1000.$$
(4.20)

$$OHRS = EXP[5.8466 + 0.25481\,x + 0.113703\,x^2 - 0.01094\,x^3]$$
(4.21)

$$XMHRS = EXP[5.27342 + 0.22833\,x + 0.12265\,x^2 - 0.011672\,x^3]$$
(4.22)

$$TMSU = EXP[5.66988 + 0.7508\,x]$$
(4.23)

$$EER = EXP[5.97902 + 0.37752\,x + 0.011138\,x^2 - 0.00084\,x^3]$$
(4.24)

where

x $= ln\,(AREAS)$

AREAS = surface area of the secondary clarifier, $1000\,ft^2$.

Anaerobic Digestion:

For digester volume $< 20,000\,ft^3$

$$CCOST = EXP[4.59422 + 0.12724\,x - 0.0040\,x^2]*1000.$$
(4.25)

$$OHRS = EXP[6.1638 + 0.166305\,x - 0.01247\,x^2]$$
(4.26)

$$XMHRS = EXP[5.72698 + 0.11367\,x]$$
(4.27)

$$TMSU = EXP[6.53162 + 0.19842\,x + 0.02166\,x^2]$$
(4.28)

For digester volume $\geq 20,000\,ft^3$

$$CCOST = EXP[7.67963 - 1.94969\,x + 0.40261\,x^2 - 0.01821\,x^3]*1000.$$
(4.29)

$$OHRS = EXP[9.12925 - 1.81674\,x + 0.37328\,x^2 - 0.01729\,x^3]$$
(4.30)

$$XMHRS = EXP\,[8.56675 - 1.76814\,x + 0.36317\,x^2 - 0.01662\,x^3]$$

(4.31)

$$TMSU = EXP\,[8.7028 - 1.18271\,x + 0.028269\,x^2 - 0.01367\,x^3]$$

(4.32)

$$EER = EXP\,[12.4365 - 2.0895\,x + 0.28\,x^2 - 0.008353\,x^3]$$

(4.33)

where

$x = ln(DV)$

DV = digester volume, 1000 ft^3.

Gravity Thickener:

$$COSTS = EXP\,[3.7259 + 0.39769\,x + 0.07574\,x^2 - 0.001977\,x^3$$

$$-0.000296\,x^4]* 1000.$$

(4.34)

For EXP(x) < 1

$$OHRS = 350.$$

(4.35)

$$XMHRS = 190.$$

(4.36)

$$TMSU = 250.$$

(4.37)

For EXP(x) ≥ 1

$$OHRS = EXP\,[5.84657 + 0.25481\,x + 0.11370\,x^2 - 0.01094\,x^3]$$

(4.38)

$$XMHRS = EXP\,[5.27342 + 0.22833\,x + 0.122646\,x^2 - 0.011672\,x^3]$$

(4.39)

$$TMSU = EXP\,[5.66988 + 0.7508\,x]$$

(4.40)

$$EER = EXP\,[-12.5085 + 6.72116\,x - 0.74406\,x^2 + 0.030546\,x^3]$$

(4.41)

where,

x = ln (AREAG)

$AREAG$ = surface area of the gravity thickener, 1000 ft^3.

Recirculation and Intermediate Pumping:

For initial firm pumping capacity ≥ 1 MGD

$$CCOST = EXP[3.48155 + 0.37749\,x + 0.09335\,x^2 - 0.00622\,x^3]* 1000.$$
(4.42)

$$OHRS = EXP[6.0973 + 0.25307\,x - 0.19366\,x^2 + 0.0782\,x^3 - 0.00668\,x^4]$$
(4.43)

$$XMHRS = EXP[5.91154 - 0.01316\,x + 0.07664\,x^2]$$
(4.44)

$$TMSU = EXP[5.05174 + 0.30161\,x + 0.19718\,x^2 - 0.01796\,x^3]$$
(4.45)

$$EERMS = EXP[7.14972 + 0.28856\,x - 0.07886\,x^2 + 0.01466\,x^3]$$
(4.46)

$$EER = EERP + EERMS$$
(4.47)

where,

x = ln(QR)

QR = recycle flow rate, MGD,

$EERP$ = electrical energy consumed by recirculation and intermediate pumps, kW-hr/yr.,

$EERMS$ = steady electrical energy (excluding pumps) required, kW-hr/yr.

Primary Sludge Pumping:

$$CCOST = EXP[-1.4455 + 2.3386\,x - 0.38263\,x^2 + 0.025888\,x^3]* 1000.$$
(4.48)

$$OHRS = EXP[4.365 + 0.70385\,x - 0.04225\,x^2 - 0.00193\,x^3]$$
(4.49)

$$XMHRS = EXP[1.83957 + 1.68369\,x - 0.23184\,x^2 + 0.014133\,x^3]$$
(4.50)

$$TMSU = EXP[31.1709 - 15.2236x + 3.07994x^2 - 0.19549x^3]$$

(4.51)

$$EER = EERP + EXP[7.14972 + 0.28856x_1 - 0.07886x_1^2 + 0.01466x_1^3]$$

(4.52)

where

x	=	ln (QI)
QI	=	firm pumping capacity, GPM,
x_1	=	ln (QI1)
QI1	=	pumping capacity, MGD.

Capital costs and fixed operation and maintenance costs are calculated using the average flow to the treatment plant and initial design parameters (primary clarifier overflow rate, solids retention time, hydraulic retention time, digester solids retention time, and secondary clarifier overflow rate), and variable operating costs, i.e. energy costs for oxygen transfer, sludge disposal costs and revenue from methane gas, are calculated using the present energy cost and sludge disposal cost. Costs using aforementioned cost equations and oxygen requirements, sludge production, and methane gas from anaerobic digestion and energy costs of $0.05/kW-hr and sludge disposal costs of $20/ton are shown in Table 4.1.

Most of the cost estimates depend upon initial designed parameters and unit sizes shown in Table 4.2. These are obtained from the steady state design of activated sludge process. In all cases, the dollar estimates are updated to 1984.

Capital costs per year are calculated for an interest rate i = 8% and planned project life of 20 years. Figure 4.1 shows the breakdown of costs (cap-

$$TMSU = EXP\,[31.1709 - 15.2236\,x + 3.07994\,x^2 - 0.19549\,x^3]$$

(4.51)

$$EER = EERP + EXP\,[7.14972 + 0.28856\,x_1 - 0.07886\,x_1^2 + 0.01466\,x_1^3]$$

(4.52)

where

x	=	ln (QI)
QI	=	firm pumping capacity, GPM,
x_1	=	ln (QI1)
QI1	=	pumping capacity, MGD.

Capital costs and fixed operation and maintenance costs are calculated using the average flow to the treatment plant and initial design parameters (primary clarifier overflow rate, solids retention time, hydraulic retention time, digester solids retention time, and secondary clarifier overflow rate), and variable operating costs, i.e. energy costs for oxygen transfer, sludge disposal costs and revenue from methane gas, are calculated using the present energy cost and sludge disposal cost. Costs using aforementioned cost equations and oxygen requirements, sludge production, and methane gas from anaerobic digestion and energy costs of $0.05/kW-hr and sludge disposal costs of $20/ton are shown in Table 4.1.

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Capital costs per year are calculated for an interest rate i = 8% and planned project life of 20 years. Figure 4.1 shows the breakdown of costs (cap-

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Table 4.1 Cost Estimates for Unit Processes [+]

Capital Costs ($):

Primary Treatment screening, grit removal, and flow measurements	=	0.27781×10^6
Primary Clarifier	=	0.35782×10^6
Aeration Basin	=	0.40532×10^6
Diffusers	=	0.74482×10^5
Secondary Clarifier	=	0.37533×10^6
Digester	=	0.52702×10^6
Thickener	=	0.34554×10^6
Recirculation and Mixing Pumps	=	0.15485×10^6
Sludge Pumps	=	0.48001×10^5

Operation and Maintenance Costs ($/yr)

Primary Treatment	=	0.45006×10^5
Primary Clarifier	=	0.24250×10^5
Aeration (Excluding oxygen transfer costs)	=	0.25824×10^5
Diffusers	=	0.25094×10^5
Secondary Clarifier	=	0.20496×10^5
Digester	=	0.28012×10^5
Thickener	=	0.23268×10^5
Recirculation and Mixing Pumps	=	0.20464×10^5
Sludge Pumps	=	0.40744×10^5

Variable Operating Costs ($/yr)

Energy (Oxygen Transfer)	=	0.25049×10^5
Sludge Disposal	=	0.12823×10^5
Revenue from Methane Gas	=	0.79175×10^3

+ Cost estimates are updated to 1984 dollars.

Table 4.2: Designed Parameters and Unit Sizes of Activated Sludge Treatment Plants

Input Parameter:

Flow	=	5 MGD = 788.55 m^3/hr
Influent suspended solids concentration	=	150 mg/L
Influent biochemical oxygen demand	=	250 mg/L
Influent ammonia concentration	=	25 mg/L

Initial designed parameteres and unit sizes:

Primary clarifier:

Overflow flow rate	=	1080 $gallons/ft^2/day$
Surface area	=	430.06 m^2
Depth	=	10 ft (average)

Aeration Basin:

Solids retention time	=	6.0 days
Hydraulic retention time	=	3.0 hours
Volume	=	$0.23656 x 10^4 \, m^3$

Secondary Clarifier:

Overflow rate	=	1000 $gallons/ft^2/day$
Surface area	=	464.47 m^2
Depth	=	10 ft (average)

Gravity Thickener:

Surface area	=	400 m^2

Anaerobic Digester:

Volume	=	330 m^3
Retention time	=	10.26 days

CAPITAL COSTS
($/YEAR)

(0.263204×10^6)

OPERATION AND
MAINTENANCE COSTS
($/YEAR)

(0.253158×10^6)

VOPC

$(\$ 0.3708 \times 10^6)$
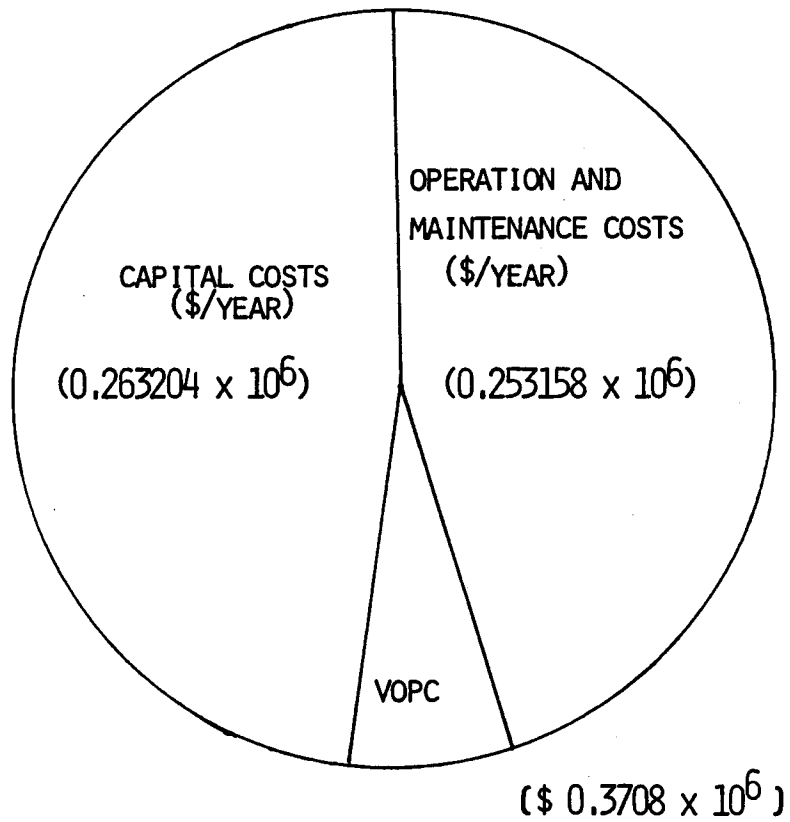
NOTE: VOPC = VARIABLE OPERATING COSTS

Fig. 4.1 Cost Breakdown (Capital fixed operation and maintenance and
variable operation)

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ital, fixed operation maintenance, and variable operation). Total cost per yr for the treatment of a 5 MGD wastewater is $0.553442 x 10^6$. Therefore, the cost for treating 1000 gallons of wastewater is $0.30. As indicated previously this cost does not include influent pumping, chlorination, chemicals, costs for legal, fiscal, administration, laboratory facilities, and cost of land.

The costs generated in this dissertation may be different than the cost of a typical treatment plant, since the costs shown here are a subset of the total costs. Furthermore, site specific costs have not been included. The costs provided are sufficiently accurate for comparisons and optimization; they should be applied to specific conditions only with extreme caution.

V. RESULTS AND DISCUSSION

A. Simulated Primary Sedimentation Basin Performance

The model of primary sedimentation basin represented by non-steady state diffusion equation along with a parameter at boundaries to describe the rate of scouring and resuspension is presented earlier. Dynamically, the primary sedimentation basin is the first processing unit to act on the influent flow and concentration. There are no feed-back loops involved in the primary sedimentation, hence, the responses of this process to influent parameter changes can be investigated independently of the dynamic responses of the remaining processing units.

The non-steady state diffusion equation is solved using ADI (Alternating Direction Implicit) method with a grid of 51 x 51 in x and z directions. The equation is simulated together with the effect of scouring parameter under various operating conditions (realistic influent flow rate and total suspended solids concentration) based on the assumption of homogeneous turbulence $(E_x = E_z = E)$ and uniform horizontal velocity (u = constant).

The efficiency of primary sedimentation basin is highly dependent on the settling velocity of suspended particles. The effect of settling velocity (W_p) of suspended particles on the efficiency of primary sedimentation basin is determined. The effect of horizontal velocity on removal efficiency is also determined and simulated results are shown in Figure 5.1 and 5.2, respectively.

Figure 5.3 shows the relationship between efficiency and depth for variable flow rate, constant width and constant volume of the sedimentation basin. It is apparent from the curves that the depth of the basin cannot be designed too
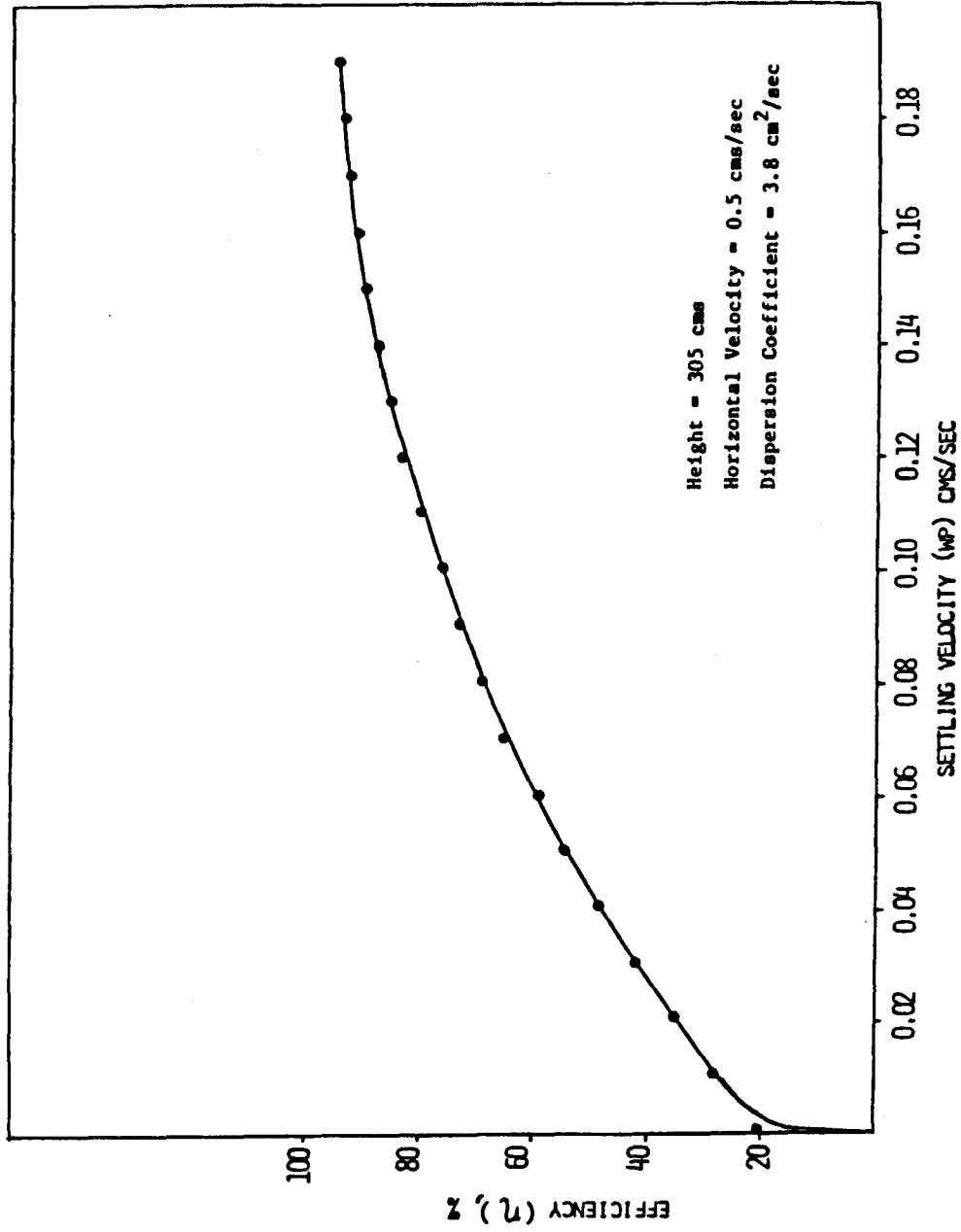
Fig. 5.1 Relationship Between Efficiency (%) and Settling Velocity, W_p, cms/sec

Height = 305 cms

Horizontal Velocity = 0.5 cms/sec

Dispersion Coefficient = 3.8 cm^2/sec

SETTLING VELOCITY (WP) CMS/SEC
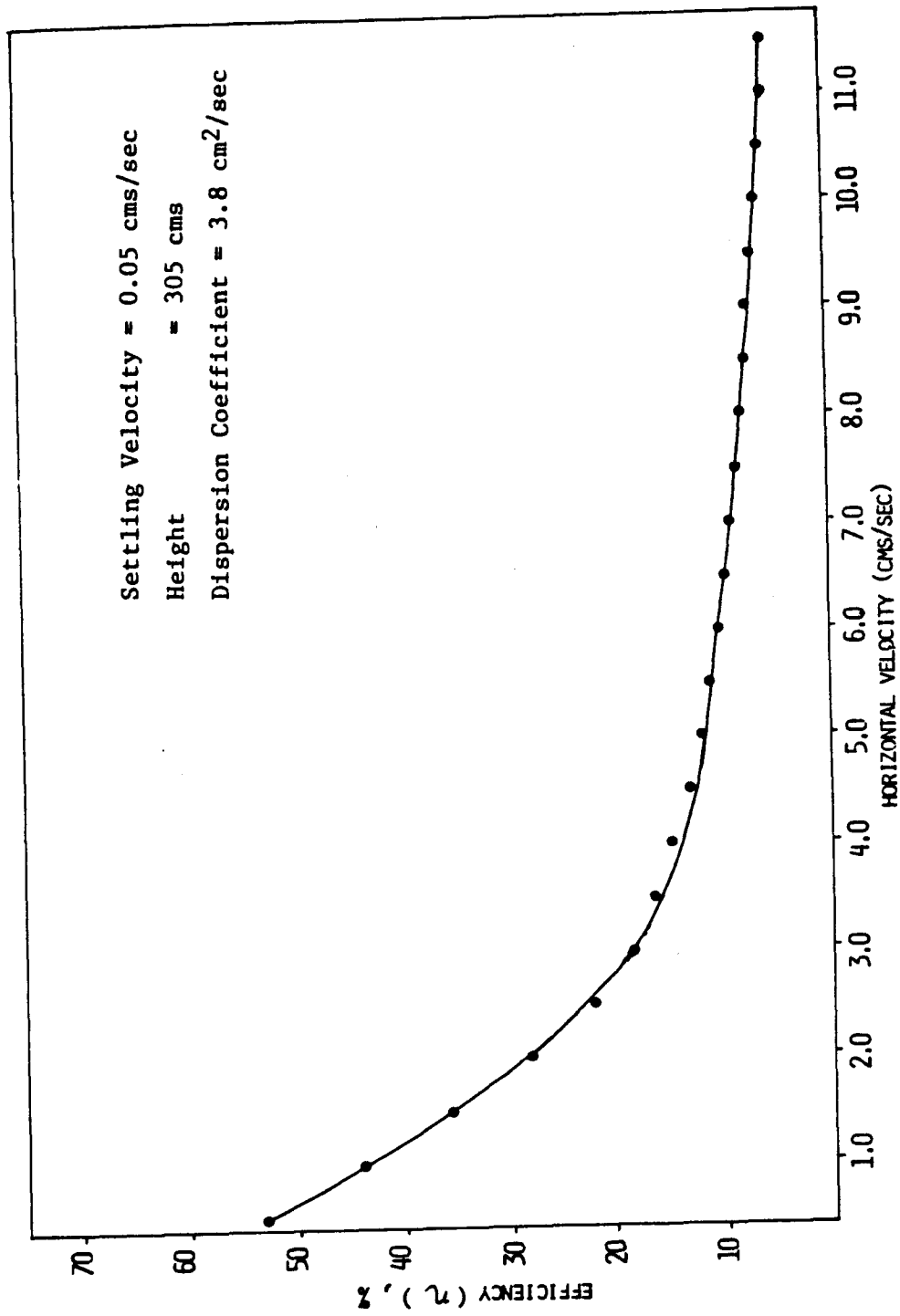
EFFICIENCY (η), %

Fig. 5.2 Relationship Between Efficiency (%) and Settling
Velocity, U, cms/sec

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EFFICIENCY(%) VS. DEPTH(CMS) FOR VARIABLE FLOW(CU.M/HR.)

VOLUME = 1803 M^3

WIDTH = 14.26 M.

$Q_1 < Q_2 < Q_3 < Q_4 < Q_5 < Q_6 < Q_7 < Q_8$
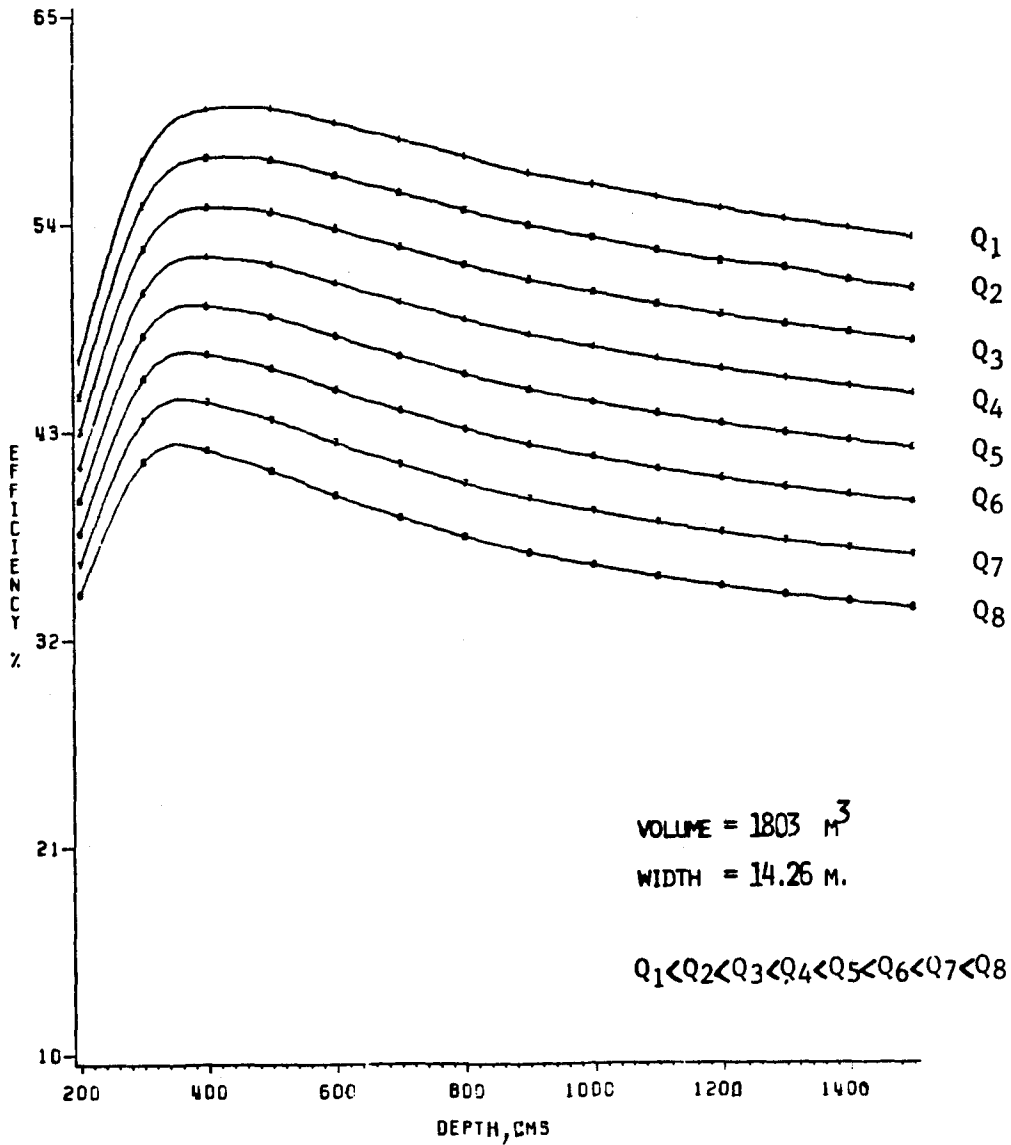
Fig. 5.3 Relationship Between Removal Efficiency (%) and Depth,
cms (V,W : Constant)

small. This result is expected because the mean horizontal velocity in the basin increases as the depth decreases causing an increase in mixing and turbulence and impact of water on particles of deposit. Therefore, depth is one of the most important design parameter for the design of primary sedimentation basin. Figure 5.4 shows the relationship between efficiency and depth for fixed flow rate and volume and variable width. In both Figures 5.3 and 5.4 there exists an optimum depth with maximum efficiency. Figure 5.5 shows that the effluent concentration is minimum (i.e. efficiency is maximum) at depth = 400 cms for dispersion coefficient, $Ex = 3.59 \exp(58.5*F)$. The effects of variable flow rate and concentration, as well as basin depth have been determined through simulations.

The direct use of non-steady state diffusion equation in the main optimization program is difficult to use because it solution requires extensive computer time. For this reason a regression model is developed to determine the effluent concentration from primary sedimentation basin. The second order model is

$$XEFF = B_0 + B_1*FLOW + B_2*HEIGHT$$
$$+ B_3*LENGTH + B_4*OVEL + B_5*OVEL^2$$

(5.1)

where,

B = statistical parameter estimates.

Statistical parameters are shown in the Table 5.1. The stepwise regression is used here for the development of the above model and the multiple R-square obtained is 0.9907.
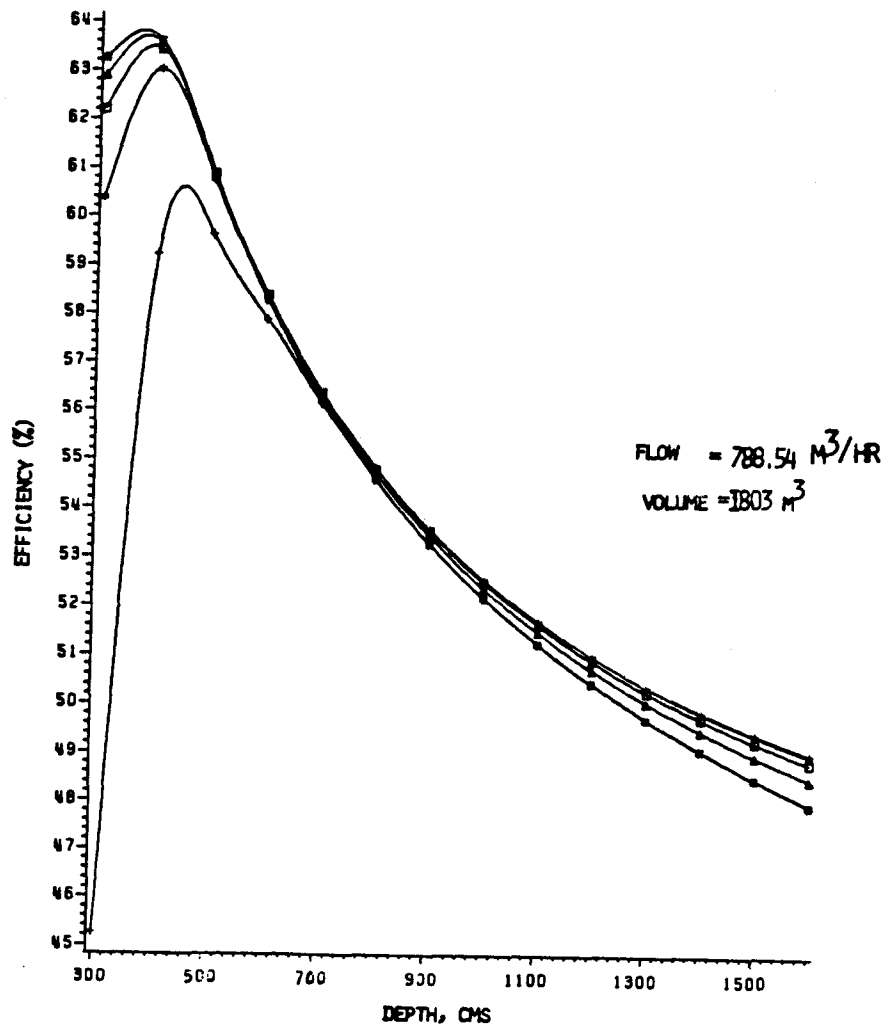
Fig. 5.4 Relationship Between Removal Efficiency (%) and Depth, cms (V,Q : Constant)

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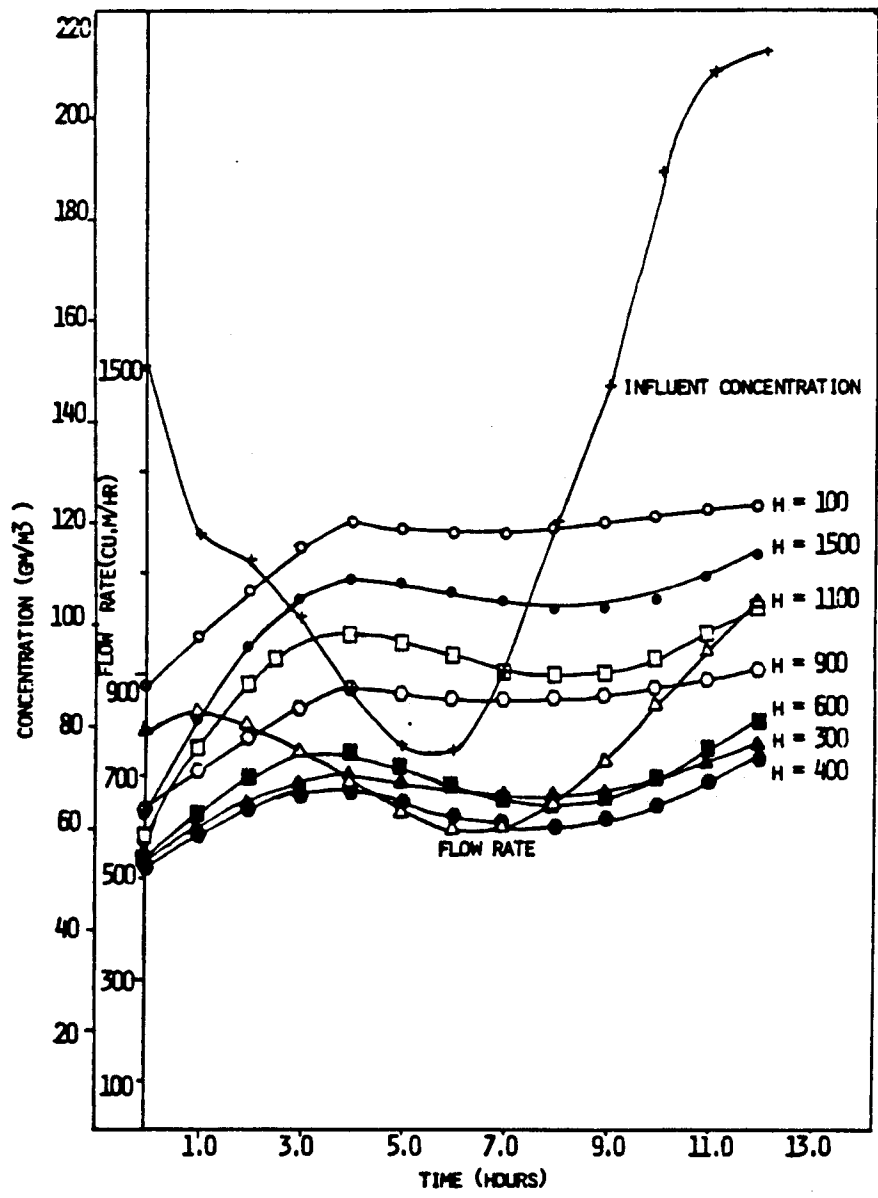
Fig. 5.5 Relationship Between Effluent Concentration and Depth
with Time for Variable Flow Rate and Influent
Concentration

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Table 5.1: Effluent Suspended Solids Model Parameters

Parameter	Parameter Estimate
B_0	10.9884
B_1	0.00247
B_2	0.00861
B_3	0.00849
B_4	0.00096
B_5	-0.1287

B. Simulation of Activated Sludge Process:

The mathematical model to simulate the activated sludge plant is described earlier. This is described by a complex set of nonlinear, simultaneous differential equations. The activated sludge is modeled as (a) a continuous flow stirred tank reactor (CFSTR), and (b) a plug flow reactor (PFR), approximated by three CFSTR's in series.

The biological model parameters and coefficients for the simulation of heterotrophic bacteria is presented in Table 5.2. Numerical values of these parameters are the best estimates from the literature whenever these were available or it could be calculated. In certain cases there was no estimate of parameters available in the literature and in these instances, parameters and coefficients were estimated in such a way that the model should conform to well known observations.

Table 5.3 presents the numerical values for the nitrification model. Parameters used here are same as those proposed by Poduska (1972).

The simultaneous nonlinear differential equations are solved using numerical techniques. Four integration methods have been used including variable step methods for obtaining steady state results. Time requirements of different integration methods are different depending upon the values of coefficients and parameters. Finally, the variable step, Milne method is used for its minimum time requirement.

The steady state solutions are obtained using the numerical values presented in Tables 5.2 and 5.3. Average influent BOD_5 and suspended solids concentration are 250 mg/l and 150 mg/l respectively. Influent particulate

Table 5.2: Parameters and Coefficients for Heterotrophic Bacteria

Terms	Value	Description
f_s^*	0.5	maximum fraction of stored mass,
KT	0.005	Transport rate coefficient, 1/gm. XA.hr.,
RS	0.001	Direct growth rate coefficient, 1/gm.XA.hr.,
RH	0.01	Hydrolysis rate coefficient, $hr.^{-1}$,
RXA	0.015	Storage growth rate coefficient,
Y_1	0.60	Mass of XA produced per unit mass of XA or SD utilized,
Y_2	0.20	Mass of XI produced per unit mass of XA destroyed,
Y_3	1.00	Conversion factor, gm of XS or SD/gm of XA.

Table 5.3: Parameters and Coefficients for Nitrifying Bacteria

Terms	Value	Description
μ_{NS}^{*}	0.02	Maximum specific growth rate of *Nitrosomonas*, (T^{-1})
K_{DNS}	0.005	*Nitrosomonas* decay coefficient, T^{-1}
Y_{NS}	0.05	Yield coefficient, mass of *Nitrosomonas* formed per unit mass of ammonium nitrogen oxidized.
μ_{NB}^{*}	0.04	Maximum specific growth rate of *Nitrobactor*, T^{-1}
K_{DNB}	0.005	*Nitrobacter* decay coefficient, T^{-1}
Y_{NB}	0.02	Yield coefficient, mass of *Nitrobacter* formed per unit mass of nitrite nitrogen oxidized.
KN	0.07	Ammonia nitrogen released in decay of XA, $gm\ NH_4^{+} - N/gm\ XA$

substrate concentration, inert mass, and non-volatile solid mass are calculated using the coefficient in Figure 3.3. The ammonium influent concentration is 30 mg/l.

Different values of RXA, RH, KT, RSD, and f_s^* are used for simulations and RXA = 0.15, RH = 0.01, RSD = 0.001, and KT = 0.005 are considered as the properly adjusted parameters because it conforms well with the documented observations. These steady state results are dependent on the size of solid liquid separator and for the purpose of these simulations the size of the solid liquid separator is considered adequate for thickening and clarification. Steady state results of activated sludge process after final adjustments of parameters are shown in Table 5.4. Figures 5.6 and 5.7 show steady state mass (particulate, active, stored, inert, and total) concentrations, soluble substrate concentration, nitrite, nitrate, and ammonia concentrations at different sludge retention time (SRT), days.

The model predicts essentially the same effluent concentration for sludge ages above 6 days which is in agreement with the field observations. Therefore, for defining an optimum sludge age for operation, the decision should be based upon the criteria, such as the aeration capacity, sludge production rate, and sludge thickening and production characteristics, rather than soluble substrate concentration.

Figure 5.8 shows the steady state results for nitrification using the parameters and coefficients shown in Table 5.2. It is observed from the Table 5.4 that the washout sludge age for the nitrifiers is higher than washout sludge age for heterotrophs.
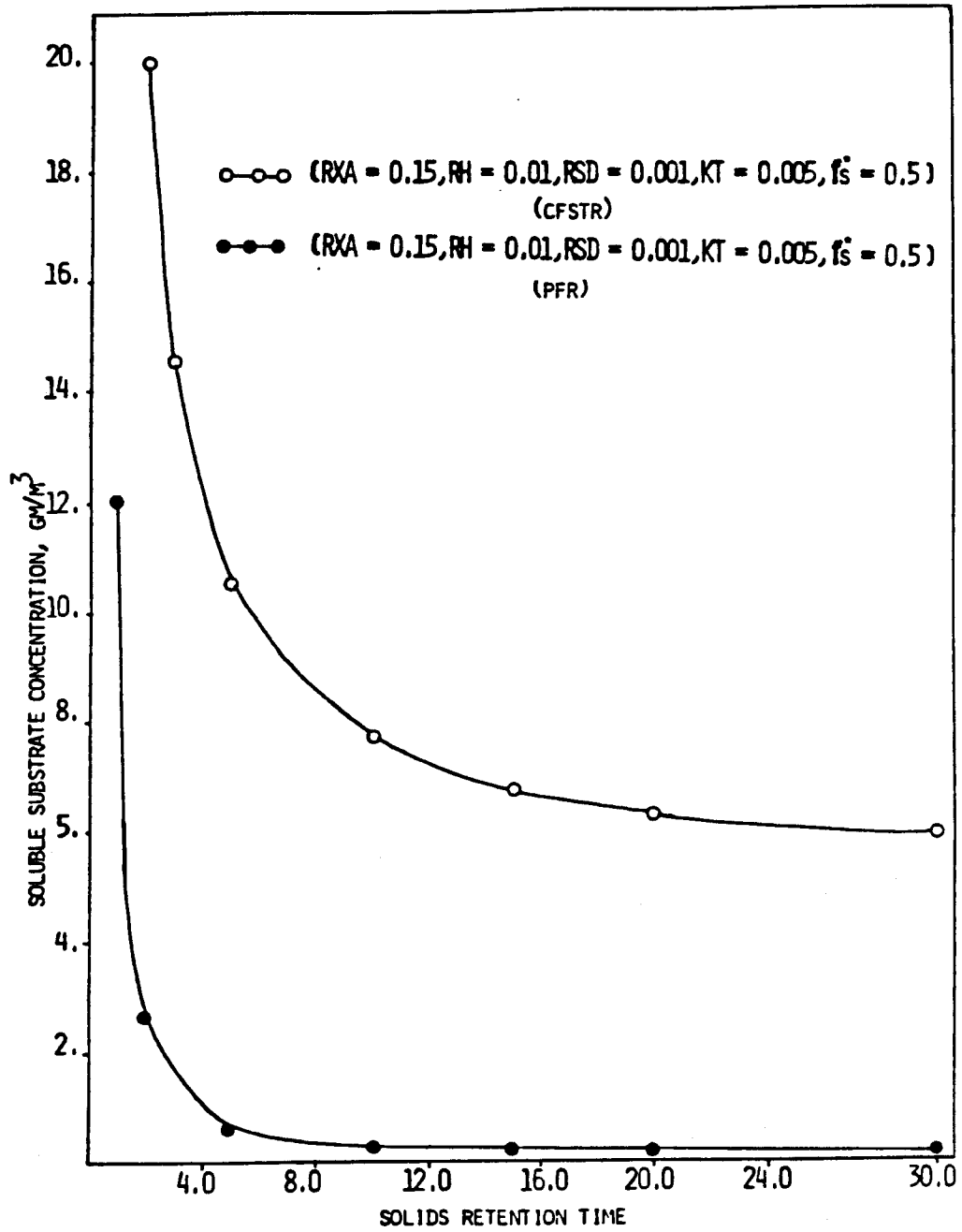
Fig. 5.6 Steady State Effluent Soluble Substrate Concentration, gm/m^3
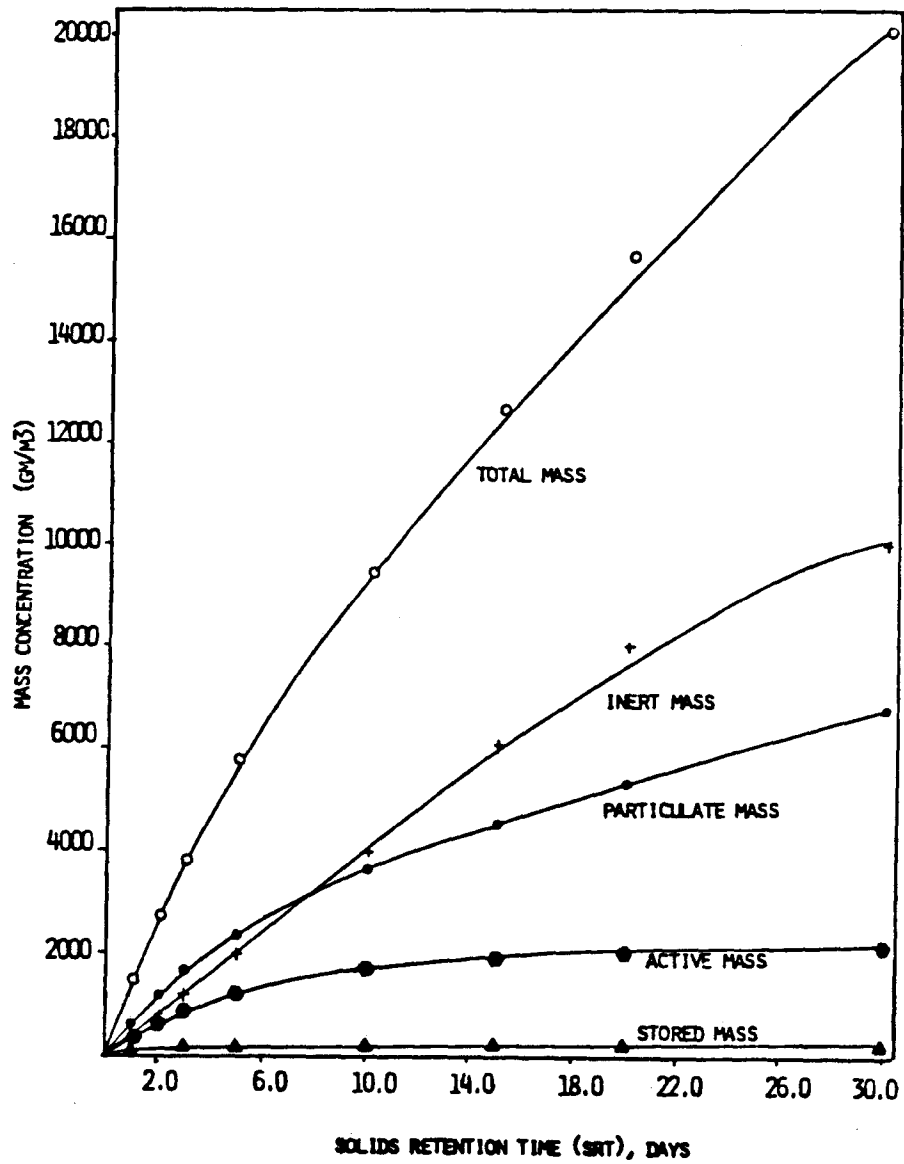
Fig. 5.7 Steady State Mass Concentrations (RXA = 0.15, RH = 0.01, RSD = 0.001, KT = 0.005, $f_s^* = $ .5)
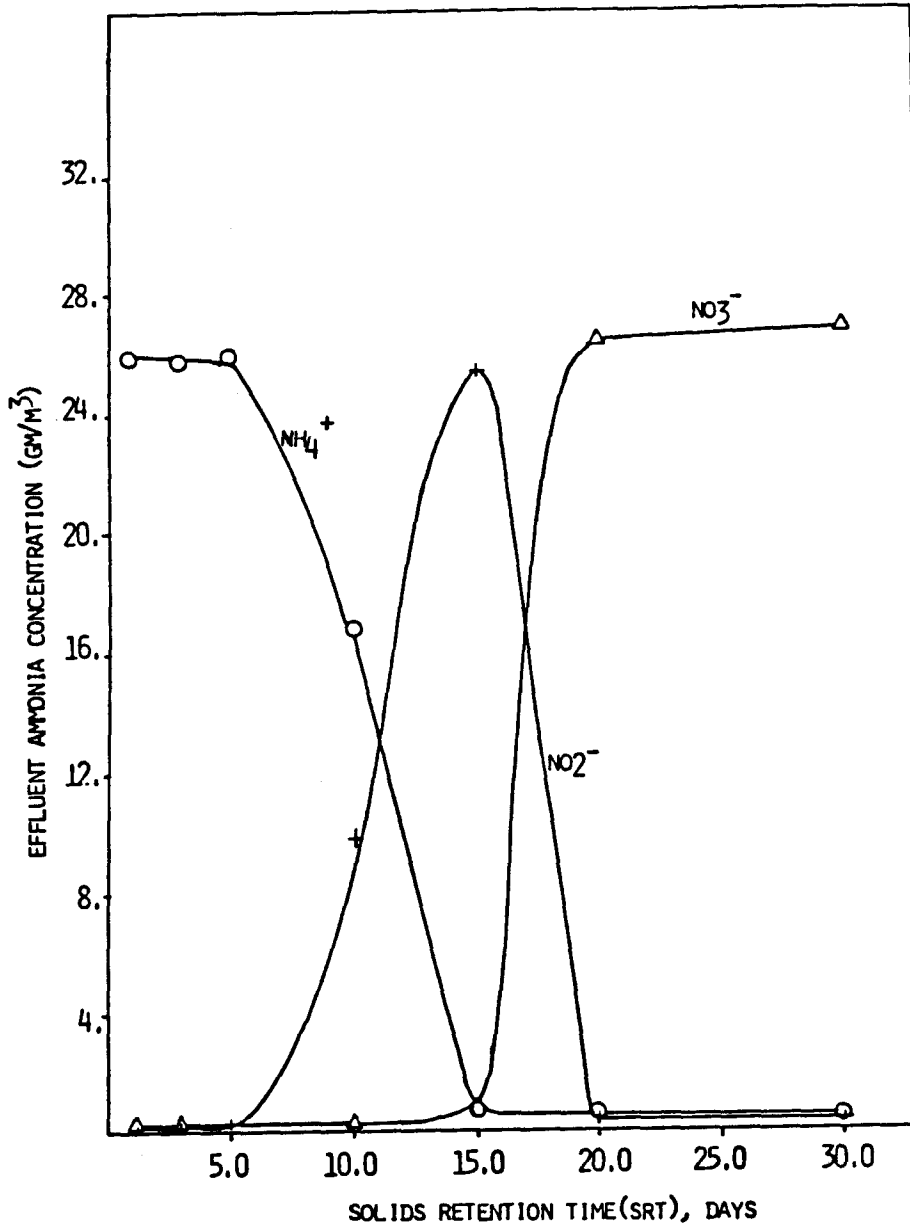
Fig. 5.8 Steady State Effluent Ammonia Concentrations for
Variable Solids Retention Time (SRT), Days

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Table 5.4 Steady State Results of Complete Mixing Activated Sludge

Process Simulation.

Species	Solids Retention Time (SRT), Days						
	1	3	5	10	15	20	30
XA	321.7	892.9	1222.5	1650.7	1861.8	1987.8	2130.4
XP	674.7	1642.0	2354.2	3636.7	4644.1	5530.7	6828.7
XI	343.1	1143.8	1989.1	4006.4	6018.9	8012.0	11064.0
XS	109.8	155.9	172.9	192.8	202.3	208.0	214.4
XN	283.4	845.3	1388.4	2617.4	3812.6	4957.0	6704.6
XNS	3.9×10^{-2}	8.2×10^{-3}	6.9×10^{-2}	6.7	40.7	46.7	52.3
XNB	3.5×10^{-3}	3.7×10^{-3}	4.5×10^{-8}	6.8×10^{-10}	0.13	17.4	20.7
XT	1449.3	3838.6	5738.8	9486.6	12727.0	15738.0	20238.0
S_1	30.8	11.0	7.95	5.82	5.14	4.8	4.48
SN_1	47.6	47.6	47.6	47.6	47.6	47.6	47.6
NH_{41}	25.9	25.76	26.0	16.88	0.676	0.554	0.474
N_{21}	6.5×10^{-2}	1.3×10^{-2}	0.104	9.80	25.41	0.233	0.192
N_{31}	2.4×10^{-3}	3.3×10^{-9}	3.5×10^{-10}	4.4×10^{-7}	0.89	26.34	26.71

Notes:

RXA=K*RSD, RXA=0.15, KT=0.005, RSD=0.001

C. Dynamic Characteristics of Anaerobic Digestion:

Parameters for this model were obtained from the literature whenever they were available. In some cases they were calculated from the reported stoichiometry or reaction rates. Many of the parameters are not available in the literature and in these instances they were estimated in such a way that the model would conform to well known observations. The biological parameters and coefficients for the simulation of anaerobic digestion is presented in Appendix A.

Effects of sludge retention time and loading rates are shown in Figures 5.9 - 5.12. In each case the model is operated for a sufficient period of time to obtain steady state results. The response of effluent soluble substrate and effluent biodegradable solids to organic and hydraulic loading is shown in Figure 5.9. Overloading situations cause soluble substrate to increase. If the overloading is too high, the process may be unstable, causing an increase in volatile acids concentration, leading to increased un-ionized acids concentration and reduced pH. Inhibition results in increased un-ionized volatile acids and possibility of process failure. It can be observed that if QCH_4, μ_M, and μ are decreasing and effluent soluble substrate is increasing, then there is a higher probability for the failure to occur. If QCH_4, μ_M, and μ are decreasing and percent of CO_2 and percent of H_2 are increasing then failure is ensue. Percent of CO_2 and percent of H_2 can be measured and both can be used as indicators for process conditions. Gas production per unit of VSS destroyed, percent of VSS destroyed, and pH decrease and total volatile acids (propionic, n-butyric, and acetic), un-ionized acids, and percent of H_2 increase at lower sludge retention time (SRT) as shown in Figure 5.12.
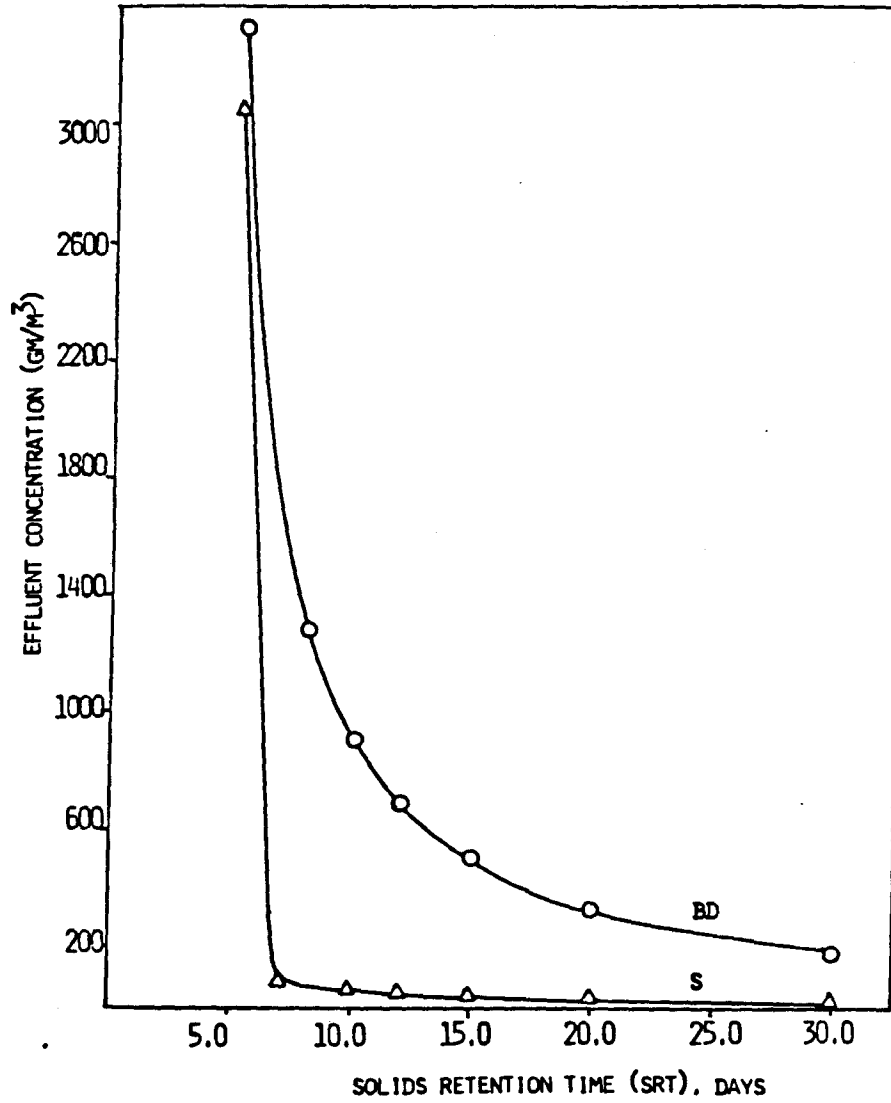
Fig. 5.9 Steady State Effluent Concentrations (Biodegradable
        Solid (BD) and Soluble Substrate (S)) for Variable
        SRT, Days

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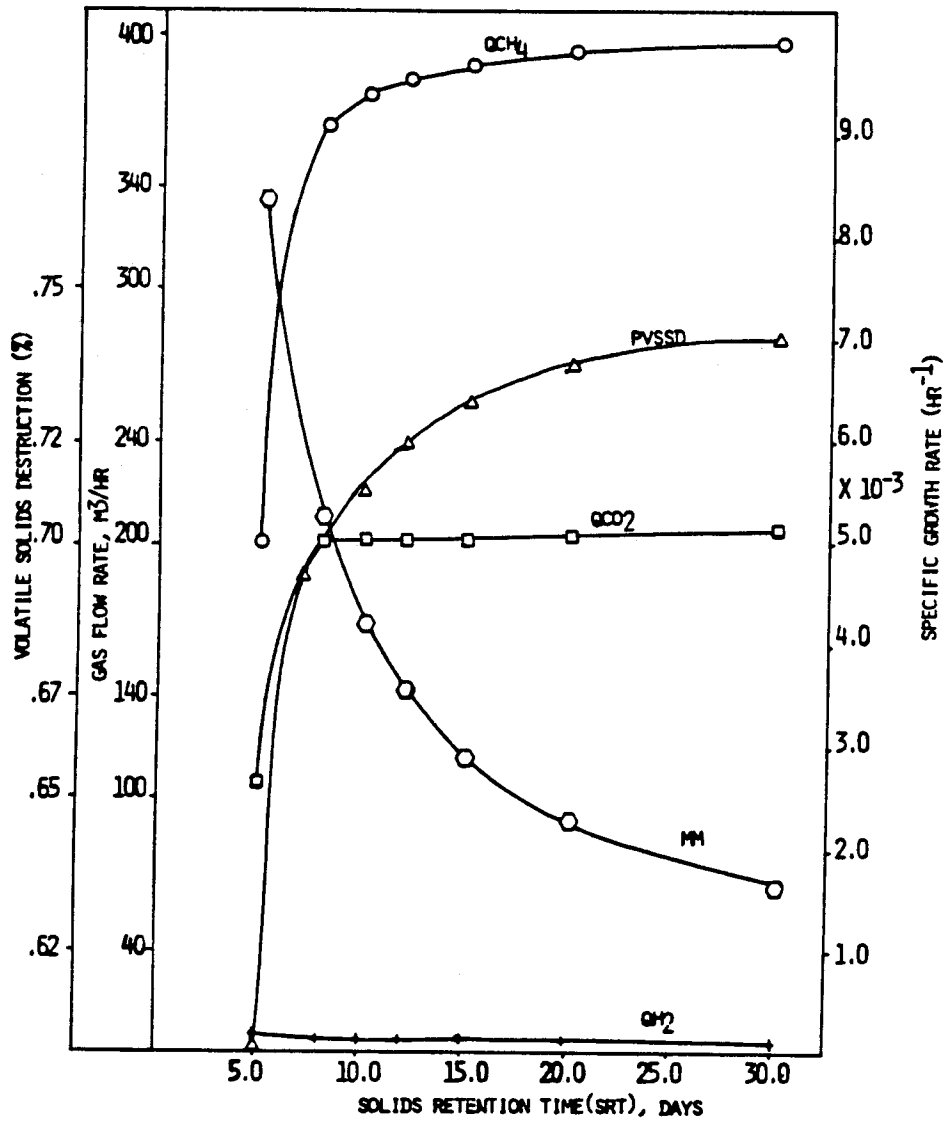
Fig. 5.10 Steady State Volatile Solids Destruction, Gas Flow
Rate (QCH_4, QCO_2, and QH_2), and
Specific Growth Rate of Methanogens for Variable SRT,
Days

124
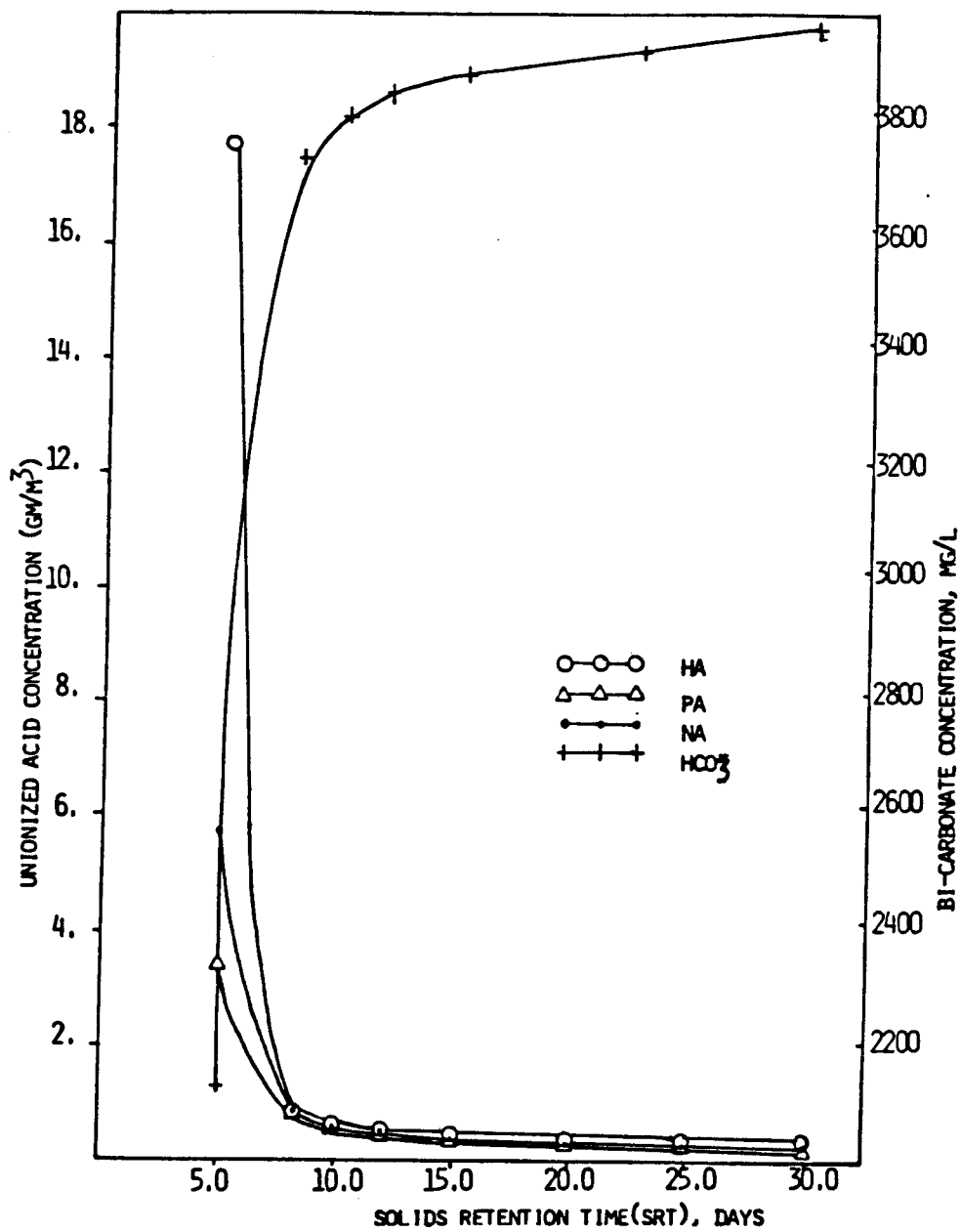
Fig. 5.11 Steady State Un-ionized Acids Concentration (Acetic (HA),
Propionic (PA), and N-Butyric Acids Concentration),
and Bi-carbonate Concentration (HCO_3) for Variable
SRT, Days

125
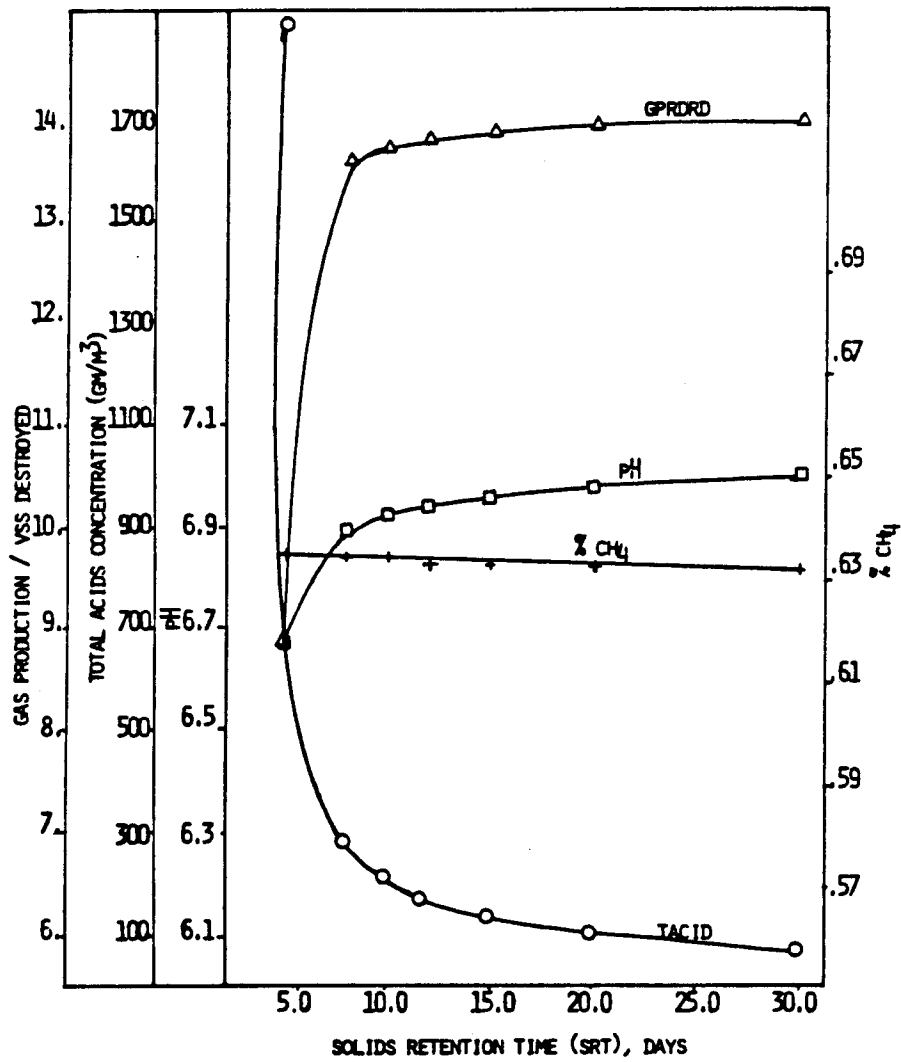
Fig. 5.12 Steady State Gas Production/VSS Destroyed, Total Acids
Concentration, pH, and % CH_4 for Variable SRT,
Days

It is important to recognize that the results of simulations might be adequate to show the qualitative validity of the model, but quantitative conclusions are tentative until more accurate values of the parameters are established.

D. Optimization

The objective function used in the previously described optimization procedure was based entirely upon cost. Amortised capital and operating costs, and both fixed and variable operating costs were combined into a single function.

Three distinct exercises were performed using the optimization procedure. The first was to verify that global minimums could be obtained. The second was to investigate the effects of the three major economic parameters: labor, energy and solids disposal costs. The final exercise was to perform an optimization on subsets of the objective function. This procedure was divided into two parts: capital cost and fixed operating costs only, and variable operating and maintenance cost only. These two cases were then compared to results obtained in the sensitivity study. The two cases of capital and fixed operating costs, and variable costs only, are roughly equivalent to current design procedures, or operating procedures, respectively.

It is far too complicated, and perhaps impossible, to prove that the objective function used in this dissertation has a global minimum. Therefore a different approach was used to insure that a global minimum was obtained. Several different sets of initial parameters were used, and results for the different sets were compared. For all practical purposes, the results were the same. The final values of primary clarifier overflow rate (POFR), hydraulic

retention time (Θ_h), and secondary clarifier overflow rate (OFR) remained virtually the same for all values of the starting parameters. The other two parameters, digester volume (DV) and solids retention time (SRT) changed slightly with different initial conditions, but changes observed were less than 10%. If the optimization technique increased SRT, DV was decreased. The two parameters were slightly correlated, and an increase in SRT was compensated by a decrease in digester volume. The final cost for different starting conditions did not vary by more than 1%. It has been assumed that global optimums have been obtained for all results presented here.

Optimization of a 5 MGD wastewater treatment plant considering the economic parameters shown in Table 5.5 indicates that the size of the primary and secondary clarifiers and aeration basin should be made as small as possible. It all cases the upper constraints for these three parameters were active (1200 and 1000 gallons/ft^2–day, three hours Θ_h). As can be observed from Figure 5.13 the solids retention time (SRT) and digester solids retention time (Θ_d) are 2.4 and 12.1 days, respectively. The cost of wastewater treatment considering the economic parameters in Table 5.6 is $0.2992 per 1000 gallons.

Sensitivity analysis of the economic parameters showed similar results. The cost of electricity was varied and the impact of the increased cost on the design parameters is shown in Figure 5.13. As in the previous case, the two overflow rates and hydraulic retention time approached their limits. Increasing SRT increases oxygen demand and reduces sludge production. Therefore, for lower energy cost the solids retention time should increase with a corresponding decrease in digester solids retention time. As expected Figure 5.13 shows this trend.

Table 5.5: Economic Parameters Used for Optimal Design and Operation

Construction cost index	=	246 (December 1984)
Material and supply cost index	=	1610.18 (December 1984)
Discount rate	=	0.10185
Planning period	=	20 years
Interest rate	=	8%
Hourly labor rate	=	$20.84/hr
Cost of sludge disposal	=	$20.0/ton
Cost of electricity	=	$0.05/Kw-hr
Efficiency of converting heat value of fuels to equivalent electrical energy	=	0.50
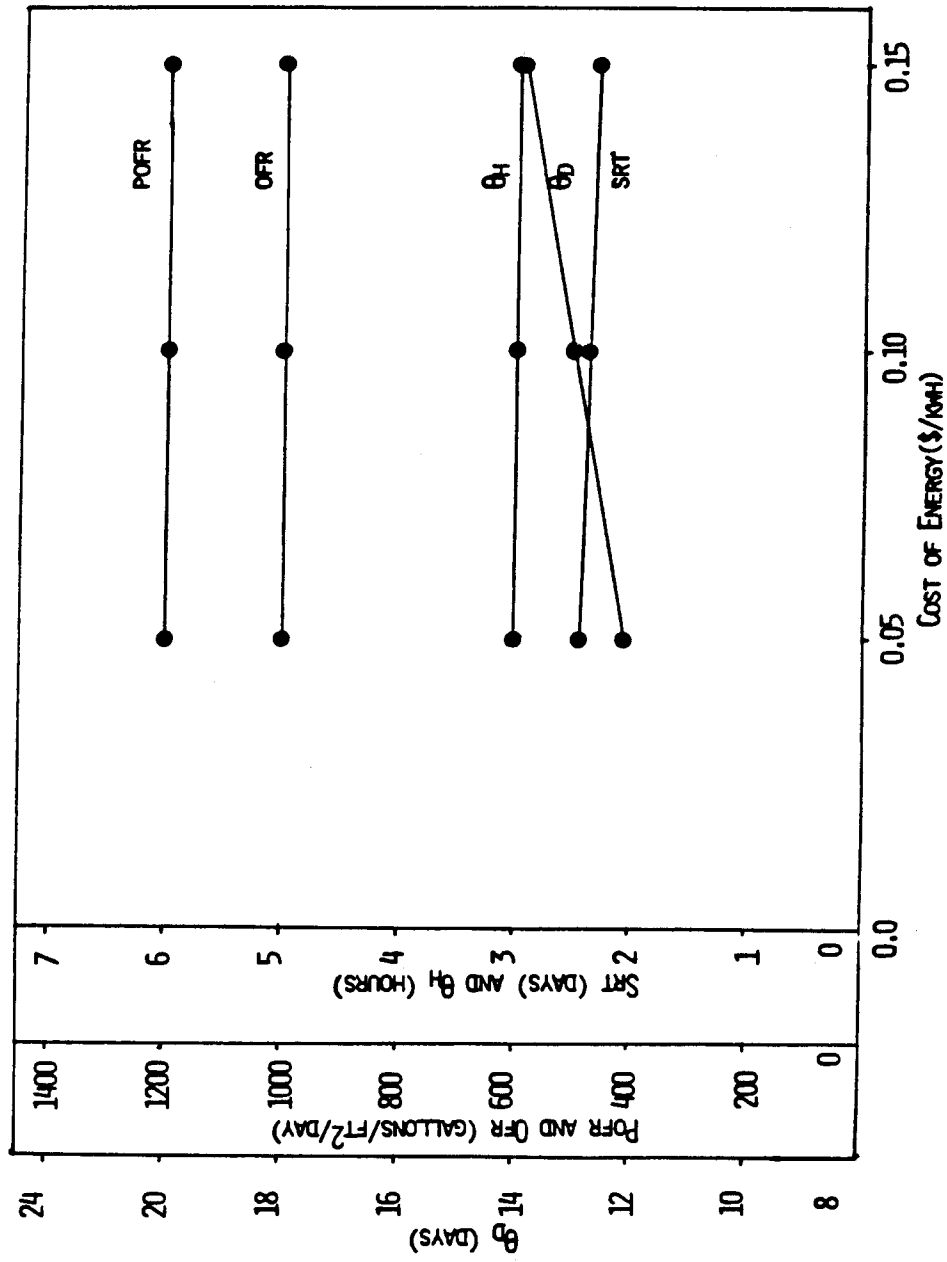
Fig. 5.13 Optimal Design and Operating Parameters with Varying
Oxygen Transfer Costs

The effect of increased sludge disposal costs is shown in Figure 5.14. For increased cost, the optimization algorithm selected higher SRT's to reduce the sludge production. Moreover, the digester volume increased resulting in increased volatile solids destruction and further reduction in sludge production.

The influence of labor rate on design and operating parameters is shown in Figure 5.15. At lower labor rate the digester volume increased, creating greater revenue from methane gas and less sludge production. This indicates that the labor requirements for operation and maintenance of an anaerobic digester is more than for an aeration basin.

In all cases shown in Figures 5.13, 5.14, and 5.15, the maximum solids retention time for all ranges of all costs is less than 2.5 days. In practice SRT's are usually more than three days and less than ten days. To investigate higher SRT the lower constraint was increased. This also caused nitrification to occur.

This case and the influence of higher cost of energy cost are shown in Figure 5.16. The cost of treatment with energy cost at $0.05/kW and the increased lower constraint was $0.3672 per 1000 gallons. This compared to to $0.2992 per 1000 gallons in the previous case.

The most important objective of this research was to compare costs and design and operating parameters for objective functions a) capital costs only, b) capital costs and operation and maintenance costs, and c) operation and maintenance costs only. Results of these aforementioned objectives are shown in Table 5.6. This table indicates that the cost of treatment considering the objective function with capital and operation and maintenance costs is $0.2992 per 1000 gallons compared to $0.3087 and $0.3005 per 1000 gallons for objective
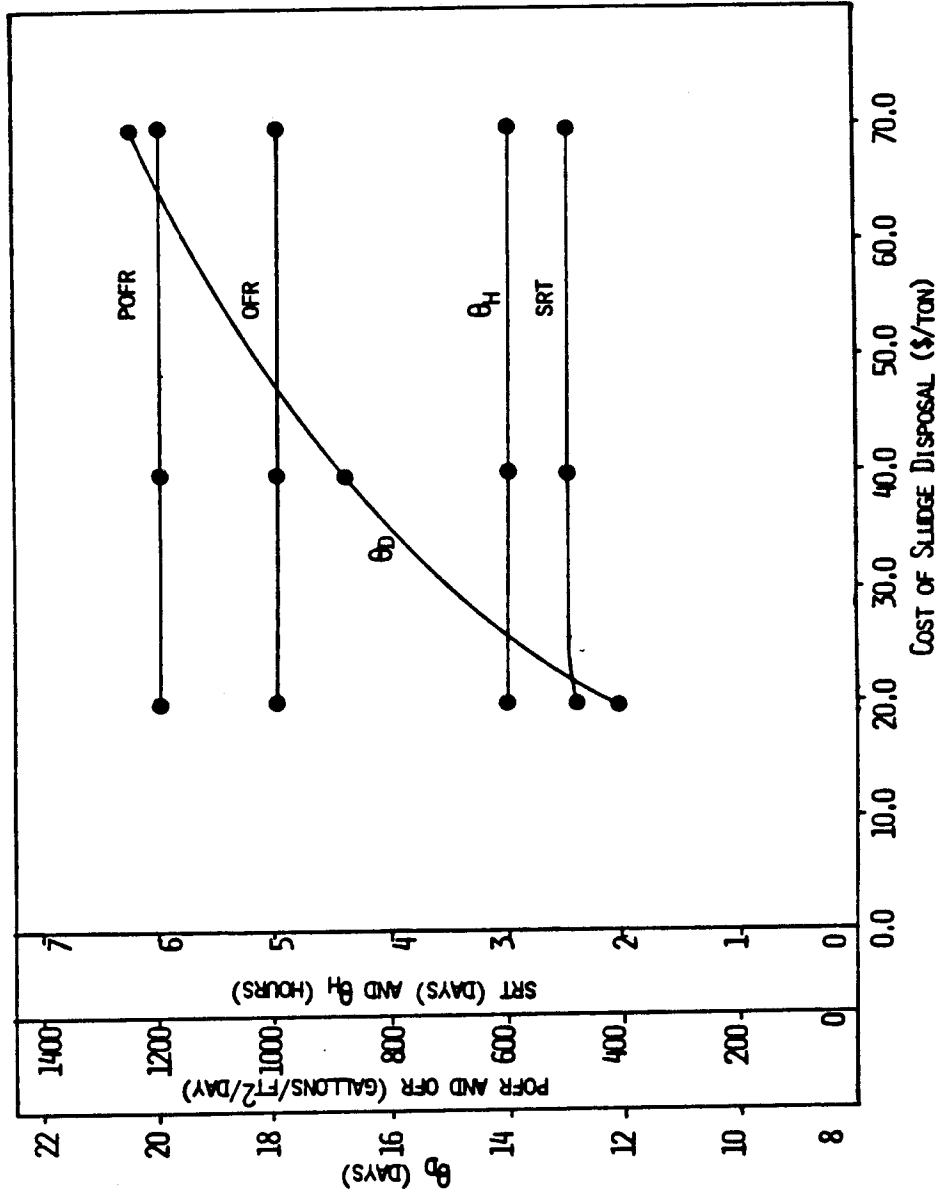
Fig. 5.14 Optimal Design and Operating Parameters with Varying
Sludge Disposal Costs
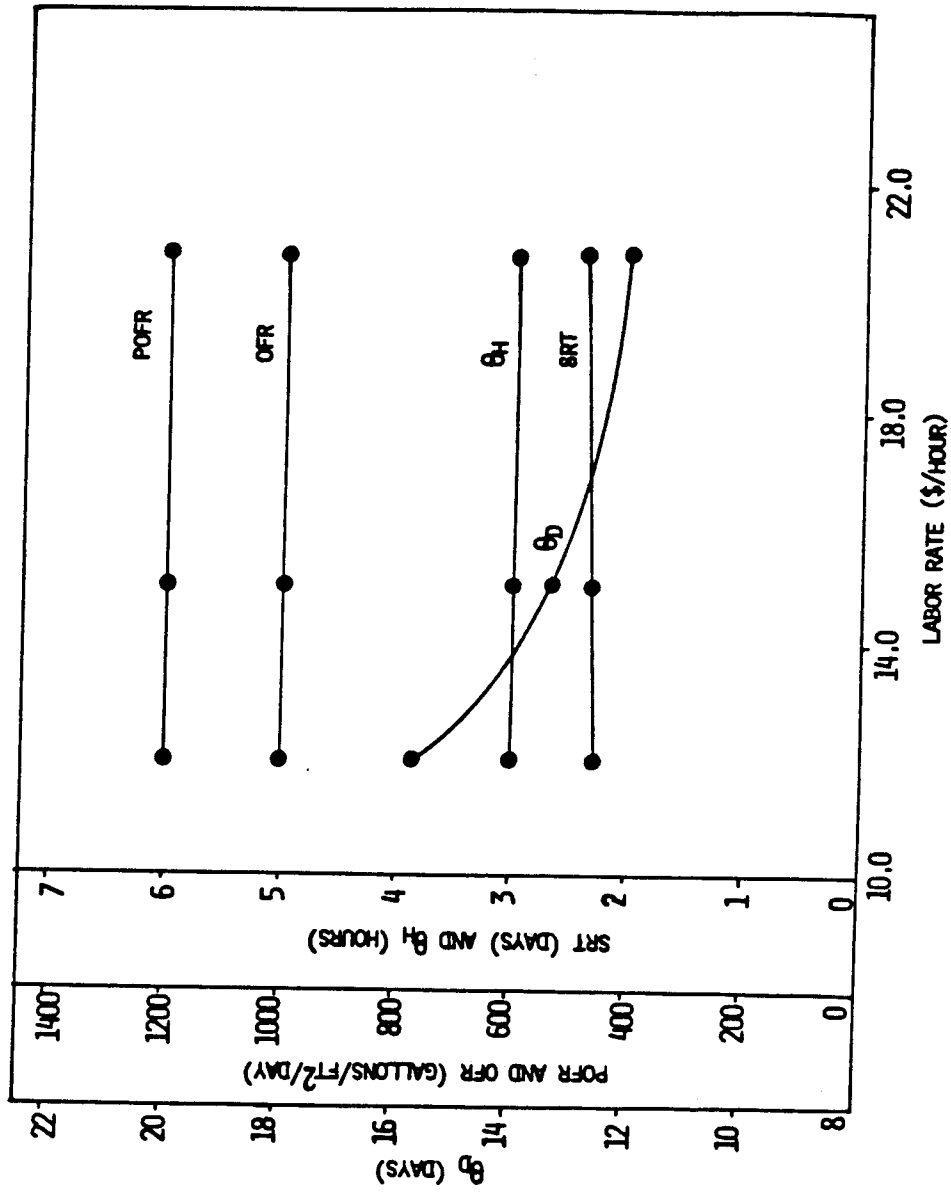
Fig. 5.15 Optimal Design and Operating Parameters with Varying
Labor Rate
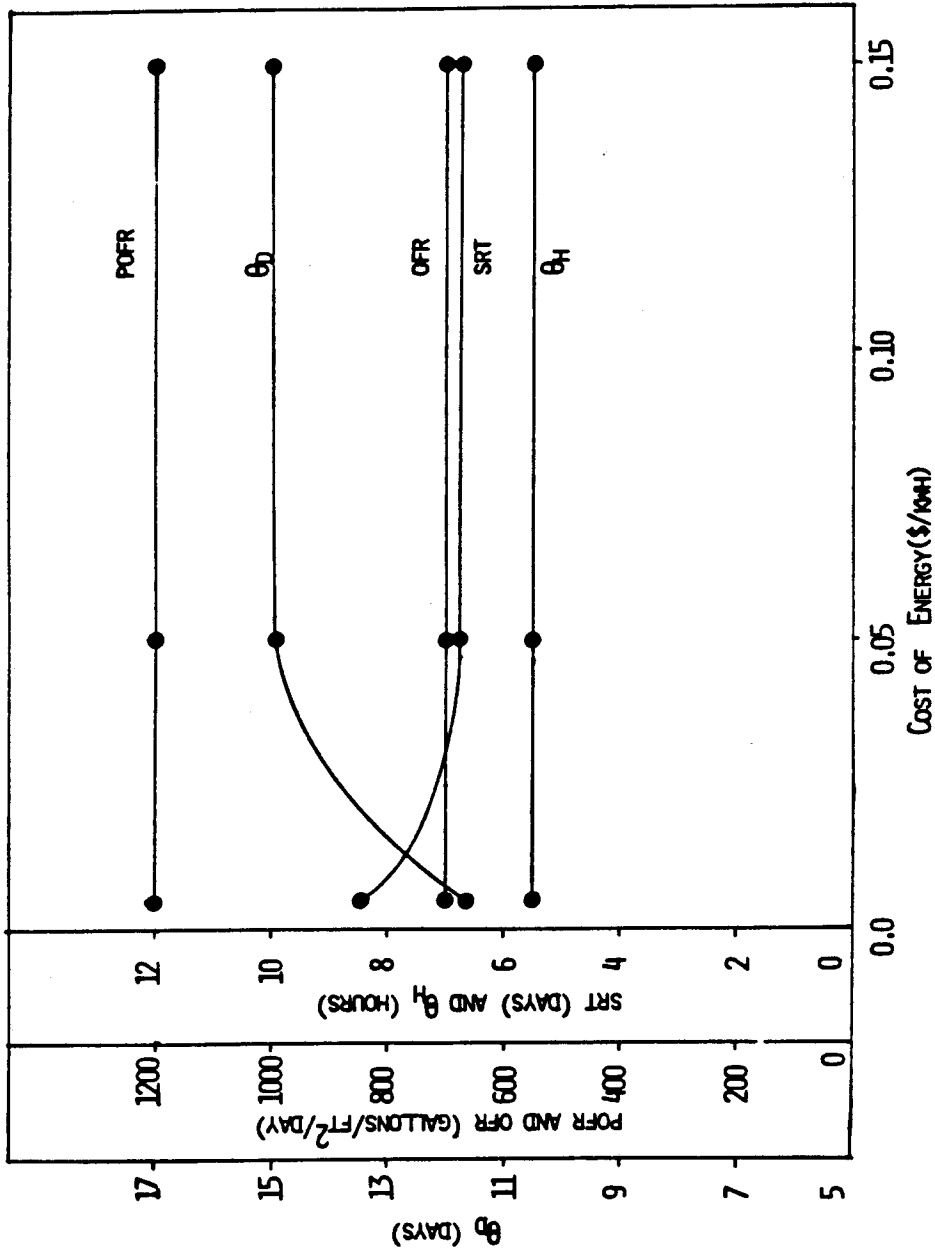
Fig. 5.16 Influence of Oxygen Transfer Costs on Optimal Design and
Operating Parameters for Higher SRT Systems

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Table 5.6: Comparison of Optimization Cases.

Cost	Case 1	Case 2	Case 3
Total Capital Costs ($/yr)	0.274663×10^6	0.25995×10^6	0.263625×10^6
Total Operating Costs ($/yr)	0.288805×10^6	0.28609×10^6	0.284761×10^6
Total Costs ($/yr)	0.563468×10^6	0.54604×10^6	0.548386×10^6
Cost $/1000 gallons	0.3087	0.2992	0.3005

Notes:

Case 1: Objective function considering only capital costs.

Case 2: Objective function considering both capital costs and operation and maintenance costs.

Case 3: Objective function considering only operation and maintenance costs.

functions with capital costs only and operations and maintenance costs only, respectively. The table shows that using the dynamic plant models coupled with cost functions that include both fixed and variable costs produces the least cost design. Optimization using either the steady state models for operating costs, or optimizing after plant construction produces a higher cost design.

VI: SUMMARY AND CONCLUSIONS

The two major objectives of this dissertation were realized. A dynamic model for the entire wastewater treatment system was developed. Process dynamics were incorporated into cost estimates for the design and operation of the treatment system. Secondly, an optimization technique was employed to obtain the minimum, total discounted cost. Both fixed and variable costs were considered in a single objective function.

The first step for development of the wastewater treatment plant model was to obtain a realistic input functions. Time series data (influent flow rate, BOD_5, and TSS) were obtained and analyzed using Fourier transforms, and from the Fourier coefficients an input function model was developed. Inputs were also perturbed with random noise to obtain a realistic input condition.

The first unit process, the primary clarifier was modeled using a non-steady state advection-diffusion equation, considering turbulence, deposit resuspension and transient inputs (flow rate, BOD_5, and TSS).

The dynamic model of the activated sludge process is capable of describing the rapid removal of substrates observed in contact stabilization, as well as the lag in specific growth rate at high loading rates was used. This model separates the removal of soluble and particulate substrates, and considers floc-phase substrate storage. The model of the solid-liquid separator is based on the solids-flux theory, as presented by Dick (1970). A flux limit between layers in the separator was used to insure that the limiting flux was not exceeded. The relationship developed by Cashion (1981) was used to determine the effluent suspended solids concentration.

The sludge treatment models included gravity thickening and anaerobic digestion. The dynamic model of anaerobic digestion uses the new concepts of acetoclastic methanogenesis. The model also considers Monod (1942) kinetics with inhibition by un-ionized acids, and includes the carbonate material balance for theoretical pH calculations.

Finally, the entire wastewater treatment system was optimized using the influence coefficient method with total plant cost as an objective function. Capital, fixed, and variable operation and maintenance costs were included. Variable operating costs are costs which are significantly affected by operating strategy, such as changes in mean cell retention time. Revenue from methane production was also included.

A sensitivity analysis of economic parameters, i.e. cost of energy, cost of sludge disposal, and labor rate, indicated that minimum sizes of the clarifiers and aeration tank should be used. No correlation among these parameters was detected. Solids retention times of the activated sludge process (SRT) and digester (Θ_d), however, have an inverse correlation; when SRT increases the volume of the digester decreases.

The optimization algorithm developed is capable of handling objective functions with a) only capital costs, b) both capital and operation and maintenance costs, and c) only operation and maintenance costs. The cost of treatment is minimized if both fixed and variable costs are considered.

A. Conclusions

The following results and conclusions are noteworthy.

1. A non-steady state advection-diffusion equation considering turbulence, deposit resuspension, and realistic inputs was used to model the primary clarifier. The solution of this equation indicates that the depth is an important parameter, and that there exists a depth for which the efficiency is maximum.

2. A structured model of the activated sludge process was developed which distinguishes between particulate and soluble substrates and includes material balances on active, inert, stored, and non-volatile biomass. A model of nitrification which includes material balances on *Nitrosomonas*, *Nitrobacter*, ammonia, nitrite, and nitrate was also used.. These models were coupled with a solid-liquid separator model.

3. A dynamic model of anaerobic digestion was developed upon the new concepts that methanogens do not metabolize organic acids, except acetate and formate, and that hydrogen production and utilization has a central position in the fermentation of acetate and formate. This model includes material balances of biodegradable and non-biodegradable solids, soluble organics, acids (propionic, n-butyric, and acetic) and hydrogen, as well as biodegradable solids hydrolyzers, propionic acid, n-butyric acid, soluble substrate oxidizers, hydrogen consumers and methane formers. The model also includes inhibition by un-ionized acids and calculates the theoretical pH considering carbonate equilibria.

4. The optimization methodology predicts optimal design and operating

parameters for which the total discounted cost is minimum. This methodology is also capable of predicting optimal design and operating parameters for proposed treatment plants, as well as for existing plants.

5. The optimal design and operation of a 5 MGD wastewater treatment requires that both clarifiers be designed with high overflow rates, with low hydraulic and solids retention times of the aeration basin, and higher digester solids retention time for anaerobic digestion.

6. A sensitivity analysis of economic parameters such as cost of energy, sludge disposal and labor shows no impact on clarifiers (primary and secondary) overflow rates and hydraulic retention time, and an inverse relationship between the other two parameters, SRT and Θ_d.

B. Recommendations

In developing this methodology it became apparent that there is a need for research in the following areas:

1. An improved design of a primary clarifier to consider the non-uniform horizontal velocity in the basin.

2. Development of a better equation to calculate the effluent suspended solids concentration from the secondary clarifier.

3. Experimental data from treatment plants should be collected to better estimate the structured activated sludge process model parameters.

4. Improve the dynamic anaerobic digestion model parameters with the additional treatment data.

5. The solid-liquid separator should be modeled incorporating a second partial differential equation which describes the settling velocity as a function of concentration and compaction.

6. Expand the dimension of the problem to include multiple sludge treatment and disposal alternatives.

7. Incorporate implicit constraints on optimization parameters.

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Appendix A   Digester Parameters

Appendix A

Parameters and Coefficients for Anaerobic Digestion.

Parameters	Value	Description
μ_{BD}^*	0.0125	Maximum growth rate of biodegradable hydrolyzers hydrolyzers, 1/hr
μ^*	0.0166	Maximum specific growth rate for soluble substrate oxidizers,1/hr
μ_p^*	0.018	Maximum specific growth rate for propionic acid oxidzers, 1/hr
μ_B^*	0.02	Maximum specific growth rate for n-butyric acid oxidizers, 1/hr
μ_M^*	0.0166	Maximum specific growth rate for methane formers, 1/hr
μ_H^*	0.045	Maximum specific growth rate for hydrogen consumers, 1/hr
K_{DBD}	0.0001	Decay coefficient for biodegradable solids hydrolyzers, 1/hr
K_{DS}	0.0001	Decay coefficient for soluble substrate oxidzers, 1/hr
K_{DP}	0.0001	Decay coefficient for propionic acid oxidzers, 1/hr
K_{DB}	0.0001	Decay coefficient for n-butyric acid oxidizers, 1/hr
K_{DH_2}	0.0001	Decay coefficient for hydrogen consumers, 1/hr
K_{DM}	0.0001	Decay coefficient for methane formers, 1/hr
QII	41.617	Flow rate, m^3/hr

VD	QII*SRT	Volume of the digester, m^3
VG	10% of VD	Volume of the gas of the digester, m^3
K_{SBD}	3000.0	Saturation coefficient for biodegradable solids hydrolyzers, gm/m^3
K_S	150.0	Saturation coefficient for soluble substrate oxidizers, gm/m^3
K_{SP}	2.0	Saturation coefficient for propionic acid oxidizers, gm/m^3
K_{SB}	2.0	Saturation coefficient for n-butyric acid oxidizers, gm/m^3
K_{TA}	5.0	Saturation coefficient for methane formers,. gm/m^3
K_{H_2}	1.0	Saturation coefficient for hydrogen consumers, gm/m^3
K_{1P}	40.0	Inhibition for propionic acid, gm/m^3
K_{1B}	40.0	Inhibitiion for n-butyric acid, gm/m^3
K_{1A}	40.0	Inhibition for acetic acid, gm/m^3
K_{SI}	2580.0	Inhibition coefficient for soluble substrate, gm/m^3
K_{H_2I}	2.0	Inhibition coefficient for hydrogen, gm/m^3
Y_{CH_4X}	47.0	Methane yield coefficient
Y_{XH_2}	1.05	Yield coefficient of hydrogen consumers
Y_{MH}	2.0	Yield coefficient of methane
Y_{XSO}	0.05	Soluble organic yield coefficient, gm of organism / gm of soluble substrate
Y_{XS}	0.03	Yield coefficient for acid formers
Y_{PACS}	0.36	Yield coefficient of propionic acid, gm of PAC / gm of soluble substrate
Y_{NBACS}	0.386	Yield coefficient n-butyric acid, gm of NBAC / gm of soluble substrate

Y_{XPAC}	0.02	Yield coefficient, gm of organism/ gm of soluble substrate
Y_{XNBAC}	0.02	Yield coefficient, gm of organism/ gm of soluble substrate
Y_{XA}	0.0466	Yield coefficient of methane, gm of organism/ gm of acetic acid
Y_{AP}	0.8106	Yield coefficient of HAC from PAC, gm of HAC/ gm of PAC
Y_{ANB}	1.363	Yield coefficient of HAC from NBAC, gm of HAC/ gm of NBAC
Y_{HP}	0.081	Yield coefficient of hydrogen from PAC, gm of hydrogen/ gm of PAC
Y_{HNB}	0.0454	Yield coefficient of hydrogen from NBAC, gm of hydrogen/ gm of NBAC
Y_{H_2S}	0.010	Yield coefficient of hydrogen, gm of hydrogen/ gm of soluble substrate
Y_{NH_4}	0.1212	Yield coefficient of ammonia, gm of ammonia/ gm of organism
$Y_{CO_{21}}$	0.05	Yield coefficient of CO_2 from biodegradable solids hydrolyzers
$Y_{CO_{22}}$	0.050	Yield coefficient of CO_2 from soluble substrate oxidizers
Y_{CO_2X}	47.0	Yield coefficient of CO_2 from methane formers, mole of CO_2/ mole of organism
$K_L A$	0.4167	Gas transfer coefficient of CO_2, 1/hr
$K_L A_1$	0.4167	Gas transfer coefficient of H_2, 1/hr
K_{HAC}	$1.738 \, x \, 10^{-5}$	Ionization constant of acetic acid at $25^o C$
K_{PAC}	$1.349 \, x \, 10^{-5}$	Ionization constant of propionic acid at $25^o C$
K_{NBAC}	$1.479 \, x \, 10^{-5}$	Ionization constant of n-butyric acid at $25^o C$
K_{CO_2}	$3.230 \, x \, 10^{-5}$	Henry's law constant of CO_2, moles /

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		mm Hg.l at $25^o C$
K_{HH_2}	$0.9 \, x \, 10^{-6}$	Henry's law constant of hydrogen, moles/ mm Hg.l at $38 \, ^o C$
K_1	$3.98 \, x \, 10^{-7}$	Ionization constant of CO_2 at $25^o C$
TP	730.0	Total pressure, mm Hg
D	22.4	Standard volume of gas, liter / mole at $25^o C$
CF	10	conversion factor, gm of soluble substrate / gm of biodegradable solids.

Appendix B   Computer Programs

```fortran
C       SOLUTION OF THE ADVECTION-DIFFUSION EQUATION CONSIDERING
C              TURBULENCE AND DEPOSIT RESUSPENSION
C
C
C       INITIAL CONDITION: 100 MG/L
C       BOUNDARY CONDITIONS:
C                           C=100 MG/L FOR X=0
C                           DC/DX=0 FOR X=IMAX
C                           EZ*DC/DZ+SCOUR*WP*C=0 FOR Z=0
C                           EZ*DC/DZ+WP*C=0 FOR Z=H
C
C
C       THIS PROGRAM SOLVES TWO DIMENSIONAL PARABOLIC PARTIAL DIFFERENTIAL
C       EQUATION USING ADI(ALTERNATING DIRECTION IMPLICIT) METHOD.
C
C       THE PROGRAM IS DEVELOPED BY PRASANTA K. BHUNIA
C
C       THE PARAMETERS ARE:
C       IMAX: NUMBER OF ROWS OF NODES IN THE GRID,
C       JMAX: NUMBER OF COLUMNS OF NODE IN THE GRID,
C       KMAX: NUMBER OF TIME STEPS,
C       DX: IS DELTA X, GRID SIZE IN THE X DIRECTION,
C       DZ: IS DELTA Z, GRID SIZE IN THE Z DIRECTION,
C       DT: IS DELTA T, THE SIZE OF THE TIME STEP,
C       C1(I,J) IS THE VALUE OF THE SOLUTION. A( ),B( ),C( ) ARE
C       COEFFICIENTS RESPECTIVELY, ON THE LOWER,MAIN AND UPPER DIAGONALS.
C       D( ) IS THE RIGHT SIDE OF AX=D.
        COMMON LAST,I,J,KPLUS1,C1(51,51),A(60),B(60),C(60),D(60)
        DIMENSION C01(51,51),D01(51,51),ECONC6(200),H1(200),Q1(200)
        DIMENSION SCONC2(4),ECONC2(51),HVEL1(200),XMAX1(200),EX1(200)
        DIMENSION WIDTH1(200),SSIN1(200),OVEL1(200),ECONC7(200)
        INTEGER EVEN
        READ(15,100) ALPHA,BETA1,HVEL,HEIGHT,WP,CO,XMAX,BC1
100     FORMAT(6F8.4,F8.3,F8.4)
        READ(15,105) DENSTY,PSLDGE,WIDTH
105     FORMAT(2F7.2,F8.2)
        WRITE(6,121) ALPHA,BETA1,HVEL,HEIGHT,WP,CO,XMAX,BC1
121     FORMAT(7(F10.5,3X))
        WRITE(6,122) DENSTY,PSLDGE,WIDTH
122     FORMAT(3(F10.5,3X))
        TSSAV=150.
        QAV=788.54
        GACC=981.0
        IMAX=51
        JMAX=51
        DO 200 I=1,IMAX
        READ(15,111) (C01(I,J),J=1,JMAX)
111     FORMAT(6E13.5)
200     CONTINUE
        VOL=1802.689E+06
        DO 202 I=1,IMAX
        DO 202 J=1,JMAX
        D01(I,J)=C01(I,J)
```

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```
202   CONTINUE
      HEIGHT=325.
123   Q=QAV
      SSIN=TSSAV
      Q1(1)=Q
      ETIME=1.
      II=1
      SSIN1(1)=SSIN
      H1(1)=HEIGHT
      FRUDN1=SQRT(GACC*HEIGHT)
      XMAX=VOL/(WIDTH*HEIGHT)
      XMAX1(1)=XMAX
      DO 203 I=1,IMAX
      DO 203 J=1,JMAX
      CO1(I,J)=DO1(I,J)
203   CONTINUE
      WRITE(6,1019) WIDTH,HEIGHT,XMAX
1019  FORMAT(/10X,'WIDTH=',E13.5,4X,'HEIGHT=',E13.5,4X,'LENGTH=',E13.5)
      HVEL=Q*100./(.36*WIDTH*HEIGHT)
      OVEL=Q*24.E 04/(WIDTH*XMAX)
      OVEL1(1)=OVEL
      HVEL1(1)=HVEL
      EX=3.59*EXP(FRUDN3)
      EX1(1)=EX
      SCOUR1=-(BETA1/EX)
      SCOUR=ALPHA*EXP(SCOUR1)
      SCOUR=1.0
      PECLET=(HVEL*XMAX)/EX
      WRITE(6,1321)
1321  FORMAT(/20X,' VARIABLE WIDTH,  VARIABLE HEIGHT')
      WRITE(6,1100) ALPHA,BETA1,HVEL,HEIGHT,WP,CO,EX,SCOUR,XMAX,PECLET
1100  FORMAT(///25X,'ALPHA=',F5.2,30X,'BETA=',F5.2//25X,
     1'HORIZONTAL VELOCITY IN CMS/SEC=',F8.4,4X,'BASIN DEPTH=',F8.2//
     225X,'SETTLING VELOCITY OF THE SS CMS/SEC=',
     3E13.5//25X,'CONCENTRATION OF SUSPENDED SEDIMENT AT THE INLET IN
     4MG/L=',F8.1//25X,'DISPERSION COEFFICIENT IN CM**2/SEC=',F8.1//
     525X,'SCOURING PARAMETER=',F10.5//25X,'BASIN LENGTH IN CMS=',F8.2
     6//25X,'PECLET NUMBER=',F10.2//)
C     ESTABLISH THE GRID SIZE
      KMAX=36
C.. SET THE TIME= TO ZERO INITIALLY
      TIME=0.
      PRINTI=0.0
      DX=XMAX/(IMAX-1)
      DX1=DX*DX
      DX2=1./DX1
      DZ=HEIGHT/(JMAX-1)
      DZ11=1./DZ
      DT=100.0
      DZ1=DZ*DZ
      DZ2=1./DZ1
      DT1=1./DT
777   HVEL=Q*100./(.36*WIDTH*HEIGHT)
```

```
202    CONTINUE
       HEIGHT=325.
 123   Q=QAV
       SSIN=TSSAV
       Q1(1)=Q
       ETIME=1.
       II=1
       SSIN1(1)=SSIN
       H1(1)=HEIGHT
       FRUDN1=SQRT(GACC*HEIGHT)
       XMAX=VOL/(WIDTH*HEIGHT)
       XMAX1(1)=XMAX
       DO 203 I=1,IMAX
       DO 203 J=1,JMAX
       C01(I,J)=D01(I,J)
 203   CONTINUE
       WRITE(6,1019) WIDTH,HEIGHT,XMAX
1019   FORMAT(/10X,'WIDTH=',E13.5,4X,'HEIGHT=',E13.5,4X,'LENGTH=',E13.5)
       HVEL=Q*100./(.36*WIDTH*HEIGHT)
       OVEL=Q*24.E 04/(WIDTH*XMAX)
       OVEL1(1)=OVEL
       HVEL1(1)=HVEL
       EX=3.59*EXP(FRUDN3)
       EX1(1)=EX
       SCOUR1=-(BETA1/EX)
       SCOUR=ALPHA*EXP(SCOUR1)
       SCOUR=1.0
       PECLET=(HVEL*XMAX)/EX
       WRITE(6,1321)
1321   FORMAT(/20X,' VARIABLE WIDTH,  VARIABLE HEIGHT')
       WRITE(6,1100) ALPHA,BETA1,HVEL,HEIGHT,WP,CO,EX,SCOUR,XMAX,PECLET
1100   FORMAT(///25X,'ALPHA=',F5.2,30X,'BETA=',F5.2//25X,
      1'HORIZONTAL VELOCITY IN CMS/SEC=',F8.4,4X,'BASIN DEPTH=',F8.2//
      225X,'SETTLING VELOCITY OF THE SS CMS/SEC=',
      3E13.5//25X,'CONCENTRATION OF SUSPENDED SEDIMENT AT THE INLET IN
      4MG/L=',F8.1//25X,'DISPERSION COEFFICIENT IN CM**2/SEC=',F8.1//
      525X,'SCOURING PARAMETER=',F10.5//25X,'BASIN LENGTH IN CMS=',F8.2
      6//25X,'PECLET NUMBER=',F10.2//)
C      ESTABLISH THE GRID SIZE
       KMAX=36
C.. SET THE TIME= TO ZERO INITIALLY
       TIME=0.
       PRINTI=0.0
       DX=XMAX/(IMAX-1)
       DX1=DX*DX
       DX2=1./DX1
       DZ=HEIGHT/(JMAX-1)
       DZ11=1./DZ
       DT=100.0
       DZ1=DZ*DZ
       DZ2=1./DZ1
       DT1=1./DT
 777   HVEL=Q*100./(.36*WIDTH*HEIGHT)
```

```
            OVEL=Q*24.E 04/(WIDTH*XMAX)
            FRUDN2=HVEL/FRUDN1
            FRUDN3=58.5*FRUDN2
            EX=3.59*EXP(FRUDN3)
            EZ=EX
            EZ1=1./EZ
            FRAC1=2.*DT1
            FRAC21=EZ*DZ2
            FRAC2=2.*FRAC21
            FRAC3=FRAC1+FRAC2
            FRAC31=FRAC1-FRAC2
            FRAC4=WP/(2.*DZ)
            FRAC5=(-FRAC4-FRAC21)
            FRAC6=-FRAC21+FRAC4
            FRAC7=HVEL/(2.*DX)
            FRAC8=EX*DX2
            FRAC81=2.*FRAC8
            FRAC9=FRAC7+FRAC8
            FRAC10=FRAC1-FRAC81
            FRAC12=FRAC1+FRAC81
            FRAC14=WP*SCOUR*DZ11
            FRAC15=WP*WP*SCOUR*EZ1
            FRAC16=FRAC3-2.*FRAC14+FRAC15
            FRAC17=FRAC31+2.*FRAC14-FRAC15
            FRAC18=FRAC31-2.*WP*DZ11-WP*WP*EZ1
            FRAC78=-FRAC7+FRAC8
            FRACY1=FRAC3+WP*WP*EZ1+2.*WP*DZ11
            FRACY2=2.*DZ*SCOUR*EZ1
            FRAC88=FRACY2*WP
            FRAC19=-FRAC8+FRAC1-FRAC7
            FRAC20=FRAC8+FRAC1+FRAC7
            FRACY3=2.*WP*DZ*EZ1
            CFACT1=0.000001
      C     INITIAL BOUNDARY CONDITION
            BC=C0
            JLAST1=JMAX-1
            JLAST=JMAX-2
            LAST=IMAX-1
            IMAX1=IMAX-2
            JMAX1=JMAX-19
            IMAX2=IMAX-4
      C     K=1, DEFINES AN ODD TRAVERSAL
      C     K=2, DEFINES AN EVEN TRAVERSAL OF THE GRID
            DO 220 KPLUS1=2,KMAX
            SCONC3=0.0
            ECONC3=0.0
            K=KPLUS1-1
            EVEN=K/2
            EVEN=EVEN*2
            IF(K.EQ.EVEN) GO TO 300
      C     THE FOLLOWING SEGMENT IS EXECUTED FOR THE ODD VALUES OF K.
      C     THE INLET BOUNDARY CONDITION.
            STEP=1.0
```

```
C       X.....EXPLICIT AND Y....IMPLICIT
        I=2
        J=2
        I2=I+1
        A(2)=0.0
        B(2)=FRAC16
        C(2)=-FRAC2
        D(2)=BC1*FRAC9+C01(I,J)*FRAC10+C01(I2,J)*FRAC78
        DO 231 J=3,JLAST
        A(J)=FRAC6
        B(J)=FRAC3
        C(J)=FRAC5
        D(J)=BC1*FRAC9+C01(I,J)*FRAC10+C01(I2,J)*FRAC78
231     CONTINUE
        A(JLAST1)=-FRAC2
        B(JLAST1)=FRACY1
        C(JLAST1)=0.0
        D(JLAST1)=BC1*FRAC9+C01(I,JLAST1)*FRAC10+C01(I2,JLAST1)*FRAC78
        CALL TDA(STEP)
        DO 240 I=3,LAST
        J=2
        I1=I-1
        I2=I+1
        A(2)=0.0
        B(2)=FRAC16
        C(2)=-FRAC2
        D(2)=C01(I1,J)*FRAC9+C01(I,J)*FRAC10+C01(I2,J)*FRAC78
C       THE INTERIOR OF THE GRID
        DO 250 J=3,JLAST
        A(J)=FRAC6
        B(J)=FRAC3
        C(J)=FRAC5
        D(J)=C01(I1,J)*FRAC9+C01(I,J)*FRAC10+C01(I2,J)*FRAC78
250     CONTINUE
C       THE EXTERIOR BOUNDARY CONDITION
        A(JLAST1)=-FRAC2
        B(JLAST1)=FRACY1
        C(JLAST1)=0.0
        D(JLAST1)=C01(I1,JLAST1)*FRAC9+C01(I,JLAST1)*FRAC10+
       1C01(I2,JLAST1)*FRAC78
        CALL TDA(STEP)
240     CONTINUE
        I=IMAX
        I1=I-1
        A(2)=0.0
        B(2)=FRAC16
        C(2)=-FRAC2
        D(2)=C01(I1,J)*FRAC9+C01(I,J)*FRAC19
        DO 251 J=3,JLAST
        A(J)=FRAC6
        B(J)=FRAC3
        C(J)=FRAC5
        D(J)=C01(I1,J)*FRAC9+C01(I,J)*FRAC19
```

```
251     CONTINUE
        A(JLAST1)=-FRAC2
        B(JLAST1)=FRACY1
        C(JLAST1)=0.0
        D(JLAST1)=C01(I1,JLAST1)*FRAC9+C01(I,JLAST1)*FRAC19
        CALL TDA(STEP)
        DO 242 I=2,IMAX
        C1(I,1)=C1(I,3)+C1(I,2)*FRAC88
242     C1(I,JMAX)=C1(I,JLAST)-FRACY3*C1(I,JLAST1)
        DO 285 I=2,IMAX
        DO 285 J=1,JMAX
        C01(I,J)=C1(I,J)
        C01(1,J)=BC1
285     CONTINUE
        DO 611 J=1,JMAX
        I=LAST
        C01(IMAX,J)=C1(I,J)
611     CONTINUE
        GO TO 218
C       THE FOLLOWING SEGMENT IS EXECUTED FOR THE EVEN VALUES OF K.
300     STEP=2.0
C       X.......IMPLICIT AND Y...... EXPLICIT
        J=2
        I=2
        J2=J+1
        A(2)=0.0
        B(2)=FRAC12
        C(2)=-FRAC78
        D(2)=C01(I,J)*FRAC17+C01(I,J2)*FRAC2+BC1*FRAC9
        DO 254 I=3,LAST
        A(I)=-FRAC9
        B(I)=FRAC12
        C(I)=-FRAC78
        D(I)=C01(I,J)*FRAC17+C01(I,J2)*FRAC2
254     CONTINUE
        A(IMAX)=-FRAC9
        B(IMAX)=FRAC20
        C(IMAX)=0.0
        D(IMAX)=C01(IMAX,J)*FRAC17+C01(IMAX,J2)*FRAC2
        CALL TDA(STEP)
        DO 260 J=3,JLAST
        J1=J-1
        J2=J+1
C       INLET BOUNDARY CONDITION
        A(2)=0.0
        B(2)=FRAC12
        C(2)=-FRAC78
        I=2
        D(2)=C01(I,J1)*(-FRAC6)+C01(I,J)*FRAC31+C01(I,J2)*(-FRAC5)
     1+BC1*FRAC9
C       THE INTERIOR GRID
        DO 270 I=3,LAST
        A(I)=-FRAC9
```

```fortran
      B(I)=FRAC12
      C(I)=-FRAC78
      D(I)=C01(I,J1)*(-FRAC6)+C01(I,J)*
     1FRAC31+C01(I,J2)*(-FRAC5)
270   CONTINUE
C     THE EXTERIOR BOUNDARY CONDITION
      A(IMAX)=-FRAC9
      B(IMAX)=FRAC20
      C(IMAX)=0.0
      D(IMAX)=C01(IMAX,J1)*(-FRAC6)+C01(IMAX,J)*FRAC31+C01(IMAX,J2)*
     1(-FRAC5)
      CALL TDA(STEP)
260   CONTINUE
      J=JLAST1
      J1=J-1
      I=2
      A(2)=0.0
      B(2)=FRAC12
      C(2)=-FRAC78
      D(2)=BC1*FRAC9+C01(I,J1)*FRAC2+C01(I,J)*FRAC18
      DO 255 I=3,LAST
      A(I)=-FRAC9
      B(I)=FRAC12
      C(I)=-FRAC78
      D(I)=C01(I,J1)*FRAC2+C01(I,J)*FRAC18
255   CONTINUE
      A(IMAX)=-FRAC9
      B(IMAX)=FRAC20
      C(IMAX)=0.0
      D(IMAX)=C01(IMAX,J1)*FRAC2+C01(IMAX,J)*FRAC18
      CALL TDA(STEP)
      DO 262 I=2,IMAX
      C1(I,1)=C1(I,3)+FRAC88*C1(I,2)
262   C1(I,JMAX)=C1(I,JLAST)-FRACY3*C1(I,JLAST1)
      DO 263 I=2,IMAX
      C01(I,1)=C1(I,1)
263   C01(I,JMAX)=C1(I,JMAX)
      DO 295 I=2,IMAX
      DO 295 J=1,JMAX
      C01(I,J)=C1(I,J)
      C01(1,J)=BC1
295   CONTINUE
      DO 612 J=1,JMAX
      I=LAST
      C01(IMAX,J)=C1(I,J)
612   CONTINUE
C
C     CALCULATION OF THE EFFLUENT CONCENTRATION FROM THE PRIMARY
C     SEDIMENTATION TANK
C
      DO 305 J=20,JMAX
      ECONC1=0.0
      DO 310 I=3,IMAX
```

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```
            ECONC1=ECONC1+C01(I,J)
310     CONTINUE
            ECONC2(J)=ECONC1/IMAX1
            ECONC3=ECONC3+ECONC2(J)
305     CONTINUE
            ECONC4=ECONC3/JMAX1
            ECONC5=((SSIN-ECONC4)/SSIN)*100.
C
C       CALCULATION OF SLUDGE CONCENTRATION, DRY SLUDGE MASS(IN GRAM)
C       AND VOLUME OF SLUDGE(IN CUBIC METER) IN THE BOTTOM OF THE
C       PRIMARY SEDIMENTATION TANK
C
            DO 320 J=1,3
            SCONC1=0.0
            DO 330 I=3,IMAX
            SCONC1=SCONC1+C01(I,J)
330     CONTINUE
            SCONC2(J)=SCONC1/IMAX2
            SCONC3=SCONC3+SCONC2(J)
320     CONTINUE
            SCONC4=SCONC3/3.
            DMASS=SCONC4*XMAX*3.*DZ*WIDTH*CFACT1
            SVOL=(DMASS/(DENSTY*PSLDGE))*CFACT1
218     TIME=TIME+DT
            IF(TIME.LE.3599.) GO TO 220
            IF(TIME.EQ.3600.) TIME1=1.0
            H1(II)=HEIGHT
            SSIN1(II)=SSIN
            Q1(II)=Q
            XMAX1(II)=XMAX
            HVEL1(II)=HVEL
            ECONC6(II)=ECONC5
            ECONC7(II)=ECONC4
            WIDTH1(II)=WIDTH
            EX1(II)=EX
            OVEL1(II)=OVEL
            II=II+1
            II2=II-1
            ETIME=ETIME+TIME1
            Q=QAV*FLOW(ETIME)
            SSIN=TSSAV*TSS(ETIME)
            PRINTI=PRINTI+TIME
C           CALL PRINTA(C01,IMAX,JMAX,PRINTI,DX)
C           WRITE(6,1190) ECONC4
C1190   FORMAT(////2X,'EFFLUENT CONCENTRATION OF THE PSD',
C       1' TANK IN MG/L=',F10.5)
C           WRITE(6,1200) SCONC4
C1200   FORMAT(/2X,'SLUDGE CONCENTRATION IN THE PSD',
C       1' TANK IN MG/L=',F10.5)
C           WRITE(6,1210) DMASS
C1210   FORMAT(/2X,'DRY MASS OF SLUDGE IN THE PSD',
C       1' TANK IN GRAM=',E13.5)
C           WRITE(6,1220) SVOL
```

```
C1220  FORMAT(/2X,'SLUDGE VOLUME IN THE PSD TANK IN',
C     1' CUBIC METER=',E13.5)
       TIME=0.0
220    CONTINUE
       IF(ETIME.LT.20.) GO TO 777
       DO 681 I=1,IMAX
       WRITE(26,6662) (CO1(I,J),J=1,JMAX)
6662   FORMAT(10E13.5)
681    CONTINUE
       DO 666 I=1,II2
       WRITE(6,2221) Q1(I),SSIN1(I),H1(I),XMAX1(I),HVEL1(I),EX1(I),
      1OVEL1(I),ECONC7(I),ECONC6(I)
2221   FORMAT(/2X,9(1X,F10.3))
666    CONTINUE
       DO 671 I=1,II2
       WRITE(26,2222) Q1(I),SSIN1(I),H1(I),XMAX1(I),HVEL1(I),EX1(I),
      1OVEL1(I),ECONC7(I),ECONC6(I)
2222   FORMAT(2X,9(2X,F10.3))
671    CONTINUE
       DHT=100.
       HEIGHT=HEIGHT+DHT
       IF(HEIGHT.LT.400.) GO TO 123
       STOP
       END
C
C
C
       SUBROUTINE TDA(STEP)
C      TRIDIAGONAL ALGORITHM. THIS SUBROUTINE IMPLEMENTS THE TRIDIAGONAL
C      ALGORITHM.
       COMMON LAST,I,J,KPLUS1,C1(51,51),A(60),B(60),C(60),D(60)
       DIMENSION BETA(100),GAMMA(100)
       BETA(2)=B(2)
       GAMMA(2)=D(2)/B(2)
       LAST1=LAST+1
       LAST2=LAST-1
       IF(STEP.GT.1.5) GO TO 12
       DO 10 I1=3,LAST
       ILESS1=I1-1
       BETA(I1)=B(I1)-(A(I1)*C(ILESS1)/BETA(ILESS1))
       GAMMA(I1)=(D(I1)-A(I1)*GAMMA(ILESS1))/BETA(I1)
10     CONTINUE
       GO TO 14
12     DO 11 I2=3,LAST1
       ILESS2=I2-1
       BETA(I2)=B(I2)-(A(I2)*C(ILESS2)/BETA(ILESS2))
       GAMMA(I2)=(D(I2)-A(I2)*GAMMA(ILESS2))/BETA(I2)
11     CONTINUE
14     IF(STEP.GT.1.5) C1(LAST1,J)=GAMMA(LAST1)
       IF(STEP.LE.1.5) C1(I,LAST)=GAMMA(LAST)
       IF(STEP.LE.1.5) GO TO 2
       DO 30 K4=1,LAST2
       I3=LAST1-K4
```

```fortran
      IPLUS2=I3+1
      C1(I3,J)=GAMMA(I3)-(C(I3)*C1(IPLUS2,J)/BETA(I3))
30    CONTINUE
      GO TO 40
2     DO 20 K3=2,LAST2
      I4=LAST1-K3
      IPLUS1=I4+1
      C1(I,I4)=GAMMA(I4)-(C(I4)*C1(I,IPLUS1)/BETA(I4))
20    CONTINUE
40    RETURN
      END
C
C
C
C
      SUBROUTINE PRINTA(ARRAY,IMAX,JMAX,PRINTI,DELTX)
      DIMENSION ARRAY(IMAX,JMAX)
      DATA ICOUNT/1/
      NJ=6
      WRITE(NJ,1010) PRINTI,ICOUNT
1010  FORMAT(////10X,'    TIME=',F12.1,10X,' PRINT NO=',I3)
      WRITE(NJ,1020)
1020  FORMAT(/50X,'   DEPTH')
      ICOUNT=ICOUNT+1
C     CALCULATE THE SPACING FOR PRINTING
      L=JMAX/10
      WRITE(NJ,1030)(J,J=1,JMAX,L)
1030  FORMAT(/11(4X,I3,4X))
      DO 10 I=1,IMAX
      WRITE(NJ,1040) (ARRAY(I,J), J=1,JMAX,L)
1040  FORMAT('0',11F11.5)
10    CONTINUE
      RETURN
      END
C
C
C
      FUNCTION TSS(TIME)
      DIMENSION A(5),B(5),C(5)
      DATA A/0.0,-6.96097E-02,-.176173,.14660,-9.67005E-02/,
     1B/0.0,2.60089E-02,-.274343,4.09673E-02,2.49002E-02/,
     2C/1.,2.,7.,14.,21./,F/3.73999E-02/
      TSS=1.0
      DO 10 I=1,5
      THETA=F*C(I)*TIME
10    TSS=TSS+A(I)*COS(THETA)+B(I)*SIN(THETA)
      RETURN
      END
C
      FUNCTION FLOW(TIME)
      DIMENSION A(5),B(5),C(5)
      DATA A/0.0,5.41989E-02,-.036769,-.052324,.0618556/,B/0.0,
     1-1.3742E-03,2.57417E-02,-.201479,.155797/,C/1.,2.,5.,7.,14./,
```

```
      2F/.0373999/
       FLOW=1.0
       DO 10 I=1,5
       THETA=F*TIME*C(I)
10     FLOW=FLOW+A(I)*COS(THETA)+B(I)*SIN(THETA)
       RETURN
       END
```

```
C
C
C
C                    DYNAMIC MODEL OF ANAEROBIC DIGESTION
C
C                       DEVELOPED BY PRASANTA K.BHUNIA
C
C
C
MACRO XBDJ,XPTJ,XBTJ,XSJ,XH2J,XMJ,BDJ,SJ,PTJ,NTJ,HTJ,H2J,DHTJ,...
THJ,DPTJ,DNTJ,BDOJ,NBDOJ,XNVOJ,XNCDJ,BTOJ,SPJ,PPJ,NTPJ,HTPJ,DH2J,...
BNJ=DT1(XPI,XBI,XSI,XH2I,XMI,SI,BSI,PTI,NTI,HTI,H2I,MA,MP,MB,MM,DTHJ,...
MH,MU,MBD,VD,XAR,XPR,XSR,X1R,X2R,XNR,XIR,PCC,QII,C11,PCI,XNCDI,BNDI,SRT)
*       ANAEROBIC DIGESTER
*       FLOW IS IN M**3/HR, VOLUME IS IN M**3
*
*       MASS BALANCES ON THE MICROBIAL CONCENTRATIONS OF PROPIONIC ACID,
*       N-BUTYRIC ACID,ACETIC ACID, H2 AND METHANE FORMERS
        MLSSR1=XAR+XPR+XSR+X1R+X2R
        MLSSR2=MLSSR1+XIR+PCC+XNR
        BDOJ=C11*((MLSSR1+CONBD*PCC)/MLSSR2)
        NBDOJ=C11*((XIR+CONNB*PCC)/MLSSR2)
        XNVOJ=C11*((XNR+CONNV*PCC)/MLSSR2)
        VD=SRT*QII*24.
*
*       INVERSE OF RETENTION TIME (1/HOURS)
        THJ=QII/VD
*
*       BIODEGRADABLE SOLIDS HYDROLYZERS
        DXBDJ=THJ*(0.0-XBDJ)+(MBD-KDBD)*XBDJ
        XBDJ=INTGRL(XBDI,DXBDJ)
*
*       PROPIONIC ACID OXIDIZERS
        DXPTJ=THJ*(0.0-XPTJ)+(MP-KDP)*XPTJ
        XPTJ=INTGRL(XPI,DXPTJ)
*
*       N-BUTYRIC ACID OXIDIZERS
        DXBTJ=THJ*(0.0-XBTJ)+(MB-KDB)*XBTJ
        XBTJ=INTGRL(XBI,DXBTJ)
*
*       SOLUBLE SUBSTRATE OXIDIZERS
        DXSJ=THJ*(0.0-XSJ)+(MU-KDS)*XSJ
        XSJ=INTGRL(XSI,DXSJ)
*
*       HYDROGEN CONSUMERS
        DXH2J=THJ*(0.0-XH2J)+(MH-KDH2)*XH2J
        XH2J=INTGRL(XH2I,DXH2J)
*
*       METHANE FORMERS
        DXMJ=THJ*(0.0-XMJ)+(MM-KDM)*XMJ
        XMJ=INTGRL(XMI,DXMJ)
*
*       BIODEGRADABLE SOLIDS MASS BALANCE
```

```
        RXN1=MBD*XBDJ/YXSO
        DBDJ=THJ*(BDOJ-BDJ)-RXN1
        BTOJ=BDOJ*QII
        BDJ=INTGRL(BSI,DBDJ)
*
*       NON-BIODEGRADABLE SOLIDS MASS BALANCE
        DBN=THJ*(NBDOJ-BNJ)
        BNJ=INTGRL(BNDI,DBN)
*
*       NON-VOLATILE SOLIDS MASS BALANCE
        DXNCD=THJ*(XNVOJ-XNCDJ)
        XNCDJ=INTGRL(XNCDI,DXNCD)
*
*       SOLUBLE ORGANICS MASS BALANCE
        RXN2=MU*XSJ/YXS
        TMYXSC=(1.-YXSO-YCO21)
        RXN11=TMYXSC*RXN1
        DSJ=THJ*(0.0-SJ)-RXN2+RXN11
        SPJ=RXN11*VD
        SJ=INTGRL(SI,DSJ)
*
*       PROPIONIC ACID MASS BALANCE
        RXN4=MP*XPTJ/YXPAC
        RXN21=RXN2*(1.-YXS-YCO22)
        PPJ=(RXN21*YPACS)*VD
        DPTJ=THJ*(PTIN-PTJ)-RXN4+RXN21*YPACS
        PTJ=INTGRL(PTI,DPTJ)
*
*       N-BUTYRIC ACID MASS BALANCE
        RXN5=MB*XBTJ/YXNBAC
        NTPJ=(RXN21*YNBACS)*VD
        DNTJ=THJ*(NTIN-NTJ)-RXN5+RXN21*YNBACS
        NTJ=INTGRL(NTI,DNTJ)
*
*       ACETIC ACID MASS BALANCE
        RXN6=MM*XMJ/YXA
        RXN41=RXN4*(1.-YXPAC)
        RXN51=RXN5*(1.-YXNBAC)
        HTPJ=(RXN41*YAP+RXN51*YANB+RXN21*YHCS)*VD
        DHTJ=THJ*(HTIN-HTJ)-RXN6+RXN41*YAP+RXN51*YANB+RXN21*YHCS
        HTJ=INTGRL(HTI,DHTJ)
*
*       MASS BALANCE FOR H2
        RXN7=MH*XH2J/YXH2
        DH2J=THJ*(H2N-H2J)-RXN7+RXN41*YHP+RXN51*YHNB+RXN21*YH2S+DTHJ
        H2J=INTGRL(H2I,DH2J)
ENDMACRO
MACRO CMJ,CTJ,QCJ,Q4J,PCJ,CAJ,CPJ,CBJ,CCJ,CAMJ,HCO3J,HAJ,PAJ,...
NBAJ,HOJ,C2J,QJ,BDCJ,Q4MJ,Q4HJ,PHJ,QH2J,TH2J,DTHJ=DT2(PCI,CTI,...
N4N,C2N,HCO3IN,VD,QII,CMI,CAI,CAMI,XMJ,XH2J,XSJ,MM,MU,MH,MBD,ZI,...
CPI,CCI,HTJ,PTJ,NTJ,DHTJ,DPTJ,XBDJ,BDCI,DNTJ,TP,H2J,PHI,THI,CBI)
*
*       CARBONATE AND AMMONIA SYSTEM AND PH RATE OF CO2 FORMATION
```

```
*        BY METHANE FORMATION,GRAMS/M**3.HR
*

         VG=PVG*VD
         DCMJ=MM*XMJ*YCO2X*44./XMW
         CMJ=INTGRL(CMI,DCMJ)
*
*        CO2 PRODUCTION FROM BIOLOGICAL SOLIDS AND SOLUBLE SUBSTRATES
         DBDCJ=(MBD*XBDJ/YXSO)*YCO21+(MU*XSJ/YXS)*YCO22
         BDCJ=INTGRL(BDCI,DBDCJ)
*
         CO2S=KHCO2*PCJ*44.E+03
*        RATE OF GAS TRANSFER TO GASEOUS PHASE,GRAMS/M**3.HR
         DCTJ=KLA*(CO2S-C2J)
         CTJ=INTGRL(CTI,DCTJ)
         H2S=KHH2*PHJ*MH2*1.E+03
         DTHJ=KLA1*(H2S-H2J)
         TH2J=INTGRL(THI,DTHJ)
*        TOTAL FLOW OF CO2 AND CH4 IN M**3/HR
         QCJ=-D*DCTJ*VD*.02272E-03
         Q4MJ=(MM*XMJ*YCH4X/XMW)*D*VD*1.E-03
         Q4HJ=((MH*XH2J/YXH2)*YMH/CH4M)*D*VD*1.E-03
         Q4J=Q4MJ+Q4HJ
         QH2J=-DTHJ*VD*D*1.E-03/MH2
         QJ=Q4J+QCJ+QH2J
         DPCJ=-TP*D*(VD/VG)*DCTJ*.02272E-03-(PCJ/VG)*QJ
         PCJ=INTGRL(PCI,DPCJ)
         DPHJ=-TP*D*(VD/VG)*DTHJ*1.E-03/MH2-(PHJ/VG)*QJ
         PHJ=INTGRL(PHI,DPHJ)
*
*        RATE OF CO2 PRODUCTION FROM HCO3- BY ACETIC ACID FORMATION
         DCAJ=DHTJ
         CAJ=INTGRL(CAI,DCAJ)
*
*        RATE OF CO2 PRODUCTION FROM HCO3- BY PROPIONIC ACID FORMATION
         DCPJ=DPTJ
         CPJ=INTGRL(CPI,DCPJ)
*
*        RATE OF CO2 PRODUCTION FROM HCO3- N-BUTYRIC ACID FORMATION
         DCBJ=DNTJ
         CBJ=INTGRL(CBI,DCBJ)
*        RATE OF CO2 PRODUCTION FROM HCO3- BY CATION FORMATION
         DZJ=((QII/VD)*(ZI-CCJ))
         DCCJ=DZJ
         CCJ=INTGRL(CCI,DCCJ)
*
*        RATE OF CO2 FORMATION BY AMMONIA
         DNH4J=(QII/VD)*(N4N-CAMJ)+MU*XSJ*YNH4
         DCAMJ=DNH4J
         CAMJ=INTGRL(CAMI,DCAMJ)
*
         DHCO3J=DZJ+DNH4J-DPTJ-DNTJ-DHTJ
         HCO3J=INTGRL(HCO3I,DHCO3J)
         ALH1=KCO2*C2J/HCO3J
```

```
            K1=ALH1/K
            HAJ=HTJ*K1
            PAJ=PTJ*K1
            NBAJ=NTJ*K1
            HOJ=HCO3J+HAJ+PAJ+NBAJ
            DHC31J=(QII/VD)*(HCO3IN-HOJ)
            DC21J=(QII/VD)*(C2N-C2J)
            DC2J=DC21J+DCMJ+DCTJ+DCAJ+DCPJ+DCBJ-DCCJ+DNH4J+DHC31J+DBDCJ
            C2J=INTGRL(C2I,DC2J)
      ENDMACRO
      INITIAL
            PARAM XAR=8637.,XPR=5443.,XSR=1161.,X1R=25.8,X2R=.1,XNR=10880.
            PARAM XIR=17515.,PCC=5500.,C11=43662.
            PARAM QII=41.617,MU=.01667,YXSO=0.08,YXS=.05
            PARAM MBD=0.0125,KDBD=0.0001,XBDI=1615.3,KSBD=3000.
            PARAM YHCS=0.235,YPACS=0.36,YNBACS=0.386,YH2S=0.01
            PARAM MP=.018,MB=.02,MA=.01625,MH=.045,MM=.016667
            PARAM YXA=.0466,YXPAC=.02,YXNBAC=.02,YHP=.08099,YHNB=.0454
            PARAM YAP=0.8106,YANB=1.363,YXH2=1.05,KDP=.00001,KDB=.00001
            PARAM KDS=.00001,KDH2=.00001,KDM=.00001,K1P=45.,K1B=45.
            PARAM K1A=39.,KSP=2.,KSB=2.,KSA=2.,KH2=1.,YCO2X=47.,YMH=2.
            PARAM XMW=113.,KHCO2=3.23E-05,KLA=.41667,D=25.7,CH4M=16.
            PARAM SRT=5.,TP=730.,YCO21=0.05,BDCI=0.0,YCO22=0.05
            PARAM YNH4=0.1212,K=1.4725E-05
            PARAM LFDM=3204.2,KCO2=1.E-06,YCH4X=47.,H2N=0.
            PARAM XNCDI=3292.,XPI=146.,XBI=146.,XSI=145.,XH2I=469.,XMI=269.
            PARAM BSI=337.,SI=17.,PTI=23.0,NTI=21.,HTI=24.
            PARAM H2I=0.2,CTI=-7041.,PCI=290.,CMI=4128.,HCO3IN=0.,HCO3I=4016.
            PARAM CAI=10.0,CPI=14.,CBI=11.3,CCI=50.
            PARAM NH4I=5.0,C2N=0.,BNDI=9100.,ZI=50.0,CAMI=129.,C2I=456.
            PARAM N4N=30.0,KN=0.0,KS=150.,KTA=5.
            PARAM QCH4I=0.0,QCO2I=0.0,TOTLQI=0.0
            PARAM CONBD=0.7,CONNB=0.3,CONNV=0.35
            PARAM PTIN=0.0,NTIN=0.0,HTIN=0.0,KLA1=0.416667
            PARAM CONVF1=16018.7,CONVF2=35.3147,CLB1=453.6,KSI=2580.
            PARAM BTI=0.,SRPI=0.,PTRI=0.,NTRI=0.,HTRI=0.,Q4MI=0.0
            PARAM Q4HI=0.0,PVG=0.1,EPS1=0.00003,EPS2=0.00003,BDII1=300.
            PARAM XBDII1=1500.,MH2=2.,PHI=.2,THI=.05,KHH2=.9E-06,KH2I=2.
      FN=0.0
      *
      DYNAMIC
      PROCEDURE DIFF1,BDII2,DIFF2,XBDII2=CHECK(EPS1,EPS2)
            IF(KEEP-1) 306,310,310
      310   BDII2=BD1
            XBDII2=XBD1
            DIFF1=ABS(BDII2-BDII1)
            DIFF2=ABS(XBDII2-XBDII1)
            IF((DIFF1.LT.EPS1).AND.(DIFF2.LT.EPS2)) FN=1.0
            BDII1=BDII2
            XBDII1=XBDII2
      306   CONTINUE
      ENDPROCEDURE
      *
```

```
      XBD1,XPT1,XBT1,XS1,XH21,XM1,BD1,S1,PT1,NT1,HT1,H21,DHT1,...
      TH1,DPT1,DNT1,BDO1,NBDO1,XNVO1,XNCD1,BTO1,SP1,PP1,NTP1,HTP1,DH21,...
      BN1=DT1(XPI,XBI,XSI,XH2I,XMI,SI,BSI,PTI,NTI,HTI,H2I,M1,M2,M3,M4,DTH1,...
      M5,M6,M7,VD,XAR,XPR,XSR,X1R,X2R,XNR,XIR,PCC,QII,C11,PCI,XNCDI,BNDI,SRT)
      CM1,CT1,QC1,Q41,PC1,CA1,CP1,CB1,CC1,CAM1,HCO31,HA1,PA1,...
      NBA1,HO1,C21,Q1,BDC1,Q4M1,Q4H1,PH1,QH21,TH21,DTH1=DT2(PCI,CTI,...
      N4N,C2N,HCO3IN,VD,QII,CMI,CAI,CAMI,XM1,XH21,XS1,M4,M6,M5,M7,ZI,...
      CPI,CCI,HT1,PT1,NT1,DHT1,DPT1,XBD1,BDCI,DNT1,TP,H21,PHI,THI,CBI)
            TACID=PT1+NT1+HT1
            VBNBI=NBDO1-XNVO1
            VSSIN=BDO1+VBNBI
            VBNBO=BN1-XNCD1
            VSSO=BD1+VBNBO
*
*         % OF VSS DESTROYED
          PVSSD=(VSSIN-VSSO)/VSSIN
*
*         RATE OF VSS DESTROYED IN LB VSS/HR
          RVSSD=QII*(VSSIN-VSSO)/CLB1
*
*         OLR : ORGANIC LOADING RATE IN GRAMS/M**3 DAY
*         OLR1: ORGANIC LOADING RATE IN LB/FT**3 DAY
          OLR=VSSIN*QII*24./VD
          OLR1=OLR/CONVF1
*
*         GPRDAP: GAS PRODUCTION / VSS APPLIED IN FT**3/LB VSS APPLIED
*         GPRDRD: GAS PRODUCTION/ VSS DESTROYED IN FT**3/LB VSS DESTROYED
          GPRDAP=(Q1*CLB1/(QII*VSSIN))*CONVF2
          GPRDRD=(Q1/RVSSD)*CONVF2
          BDT1=INTGRL(BTI,BTO1)
          SRP1=INTGRL(SRPI,SP1)
          PTR1=INTGRL(PTRI,PP1)
          NTR1=INTGRL(NTRI,NTP1)
          HTR1=INTGRL(HTRI,HTP1)
          Q4MT=INTGRL(Q4MI,Q4M1)
          Q4HT=INTGRL(Q4HI,Q4H1)
          QCH4=INTGRL(QCH4I,Q41)
          QCO2=INTGRL(QCO2I,QC1)
          TOTLQ=INTGRL(TOTLQI,Q1)
          PQCH4=TP-PC1-PH1
          PRCO2=PC1/TP
          PRCH4=PQCH4/TP
*
*         INCORPORATION OF INHIBITION FUNCTION BY THE UNIONIZED ACIDS
*         IN THE SPECIFIC GROWTH RATE OF PROPIONIC,N-BUTYRIC,ACETIC ACID,
*         HYDROGEN, AND METHANE FORMERS RESPECTIVELY.
          DMU=PA1/K1P+NBA1/K1B+HA1/K1A
          TA1=PA1+NBA1+HA1
          DMU1=1.+KS/S1+TACID/KSI
          DMP=1.+KSP/PA1+DMU+H21/KH2I
          M2=MP/DMP
          M6=MU/DMU1
          DMB=1.+KSB/NBA1+DMU+H21/KH2I
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XBD1,XPT1,XBT1,XS1,XH21,XM1,BD1,S1,PT1,NT1,HT1,H21,DHT1,...
TH1,DPT1,DNT1,BDO1,NBDO1,XNVO1,XNCD1,BTO1,SP1,PP1,NTP1,HTP1,DH21,...
BN1=DT1(XPI,XBI,XSI,XH2I,XMI,SI,BSI,PTI,NTI,HTI,H2I,M1,M2,M3,M4,DTH1,...
M5,M6,M7,VD,XAR,XPR,XSR,X1R,X2R,XNR,XIR,PCC,QII,C11,PCI,XNCDI,BNDI,SRT)
CM1,CT1,QC1,Q41,PC1,CA1,CP1,CB1,CC1,CAM1,HCO31,HA1,PA1,...
NBA1,HO1,C21,Q1,BDC1,Q4M1,Q4H1,PH1,QH21,TH21,DTH1=DT2(PCI,CTI,...
N4N,C2N,HCO3IN,VD,QII,CMI,CAI,CAMI,XM1,XH21,XS1,M4,M6,M5,M7,ZI,...
CPI,CCI,HT1,PT1,NT1,DHT1,DPT1,XBD1,BDCI,DNT1,TP,H21,PHI,THI,CBI)
        TACID=PT1+NT1+HT1
        VBNBI=NBDO1-XNVO1
        VSSIN=BDO1+VBNBI
        VBNBO=BN1-XNCD1
        VSSO=BD1+VBNBO
*
*       % OF VSS DESTROYED
.       PVSSD=(VSSIN-VSSO)/VSSIN
*
*       RATE OF VSS DESTROYED IN LB VSS/HR
        RVSSD=QII*(VSSIN-VSSO)/CLB1
*
*       OLR : ORGANIC LOADING RATE IN GRAMS/M**3 DAY
*       OLR1: ORGANIC LOADING RATE IN LB/FT**3 DAY
        OLR=VSSIN*QII*24./VD
        OLR1=OLR/CONVF1
*
*       GPRDAP: GAS PRODUCTION / VSS APPLIED IN FT**3/LB VSS APPLIED
*       GPRDRD: GAS PRODUCTION/ VSS DESTROYED IN FT**3/LB VSS DESTROYED
        GPRDAP=(Q1*CLB1/(QII*VSSIN))*CONVF2
        GPRDRD=(Q1/RVSSD)*CONVF2
        BDT1=INTGRL(BTI,BTO1)
        SRP1=INTGRL(SRPI,SP1)
        PTR1=INTGRL(PTRI,PP1)
        NTR1=INTGRL(NTRI,NTP1)
        HTR1=INTGRL(HTRI,HTP1)
        Q4MT=INTGRL(Q4MI,Q4M1)
        Q4HT=INTGRL(Q4HI,Q4H1)
        QCH4=INTGRL(QCH4I,Q41)
        QCO2=INTGRL(QCO2I,QC1)
        TOTLQ=INTGRL(TOTLQI,Q1)
        PQCH4=TP-PC1-PH1
        PRCO2=PC1/TP
        PRCH4=PQCH4/TP
*
*       INCORPORATION OF INHIBITION FUNCTION BY THE UNIONIZED ACIDS
*       IN THE SPECIFIC GROWTH RATE OF PROPIONIC,N-BUTYRIC,ACETIC ACID,
*       HYDROGEN, AND METHANE FORMERS RESPECTIVELY.
        DMU=PA1/K1P+NBA1/K1B+HA1/K1A
        TA1=PA1+NBA1+HA1
        DMU1=1.+KS/S1+TACID/KSI
        DMP=1.+KSP/PA1+DMU+H21/KH2I
        M2=MP/DMP
        M6=MU/DMU1
        DMB=1.+KSB/NBA1+DMU+H21/KH2I
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          M3=MB/DMB
          DMA=1.+KSA/HA1+DMU
          M1=MA/DMA
          DMH2=1.+KH2/H21+DMU
          M5=MH/DMH2
          DMM=1.+KTA/TA1+DMU
          M4=MM/DMM
          M7=MBD/(1.+(KSBD/BD1))
*
*      HYDROGEN ION CONCENTRATION CALCULATED BY THE CARBONATE EQUILIBRIA
          LKCO2=ALOG10(KCO2)
          LCO2=ALOG10(C21)
          LHCO3=ALOG10(HCO31)
          LH=LKCO2+LCO2-LHCO3
          PH=-LH
NOSORT
          CALL DEBUG(1,250.)
*
TERMINAL
          THETAD=VD/QII
*
*      CONSTRAINT ON THE MAXIMUM PERMISSIBLE LOADING RATE
          LFD=BD1
          VD1=QII*THETAD
          VD2=LFD*QII/LFDM
          VD3=AMAX1(VD1,VD2)
METHOD MILNE
TIMER FINTIM=1.,DELT=.01,PRDEL=1.0,OUTDEL=1.0,DELMIN=0.25E-10
FINISH FN=1.0
PRINT XBD1,XPT1,XBT1,XS1,XH21,XM1,BD1,S1,PT1,NT1,HT1,H21,...
CM1,CT1,QC1,Q41,PC1,CA1,CP1,CB1,CC1,CAM1,HCO31,HO1,HA1,PA1,NBA1,...
C21,BN1,XNCD1,QCH4,QCO2,PQCH4,PRCO2,PRCH4,PH,PVSSD,OLR,OLR1,...
BDT1,SRP1,PTR1,NTR1,HTR1,Q4MT,Q4HT,TOTLQ,GPRDAP,GPRDRD
OUTPUT QH21,TH21,PH1
OUTPUT TACID,PT1,NT1,HT1,PRCH4
OUTPUT PRCO2,PH,HCO31,X1
OUTPUT QCH4,QCO2,M4,M7
OUTPUT HA1,PA1,NBA1,PH
OUTPUT M1,M2,M3,M5,M6
END
PARAM SRT=20.,BDII1=300.
TIMER FINTIM=1.,DELT=.01,PRDEL=1.0,OUTDEL=1.0,DELMIN=0.25E-10
END
PARAM SRT=15.,BDII1=300.
TIMER FINTIM=1.,DELT=.01,PRDEL=1.0,OUTDEL=1.0,DELMIN=0.25E-10
END
PARAM SRT=12.,BDII1=300.
TIMER FINTIM=1.,DELT=.01,PRDEL=1.0,OUTDEL=1.0,DELMIN=0.25E-10
END
PARAM SRT=10.,BDII1=300.
TIMER FINTIM=1.,DELT=.01,PRDEL=1.0,OUTDEL=1.0,DELMIN=0.25E-10
END
PARAM SRT=8.,BDII1=300.
```

```
TIMER FINTIM=1.,DELT=.01,PRDEL=1.0,OUTDEL=1.0,DELMIN=0.25E-10
END
PARAM SRT=5.,BDII1=300.
TIMER FINTIM=1.,DELT=.01,PRDEL=1.0,OUTDEL=1.0,DELMIN=0.25E-10
END
STOP
ENDJOB
```

```
/      DIMENSION ER(11,3),CINF(3,5,11),PAROLD(5),PARL(5),PARU(5),
/     1CCOST(11),OM(11),ERP(3),WEIGH(3)
*
*     ACTIVATED SLUDGE PROCESS COUPLED WITH OPTIMIZATION PROCEDURE
*     IS USED TO FIND OPTIMAL DESIGN AND OPERATING PARAMETERS
*     OF A TREATMENT SYSTEM.
*     THE PROGRAM IS CREATED BY PRASANTA K. BHUNIA
*
*     ACTIVATED SLUDGE SIMULATION CONSIDERING ZERO VOLUME REACTOR
*                    (PLUG FLOW REACTORS)
*
MACRO QTJ,SJ,XSJ,XAJ,XIJ,XPJ,XTJ,VJ,X1J,X2J,DJ,XNJ,OHJ,ONJ,...
N4J,N3J,N2J=AP(Q1J,QR2J,SOJ,XPOJ,XAOJ,XIOJ,SRJ,XSRJ,XSOJ,XPRJ,...
XARJ,XIRJ,N4OJ,N2OJ,N3OJ,RN4J,RN2J,RN3J,XR1J,XR2J,SIJ,XSIJ,XPIJ,CKAJ,...
XAIJ,XIIJ,N4IJ,N2IJ,N3IJ,X1OJ,X1IJ,X2IJ,X2OJ,XNOJ,XNIJ,XNRJ,DOJ,DIJ,DRJ)
*
*     CARBONACEOUS SYSTEM
*
*     V = VOLUME OF THE AERATION TANK, M**3.
*     QAV = AVERAGE FLOW, M**3/HR.
*
      QTJ=QR2J+Q1J
      XTJ=(XSJ+XAJ+XIJ+XPJ)
      FSJ=XSJ/(XTJ-XPJ-XIJ)
      FPJ=XPJ/(XTJ-XIJ)
*
*     BIODEGRADABLE SOLUBLE SUBSTRATE MASS BALANCE
*
      RSR1=KT*XAJ*SJ*(FSH-FSJ)
      RSR2=RS*XAJ*SJ
      DSJ=((Q1J*SOJ+QR2J*SRJ-QTJ*SJ)/VJ)-RSR1-RSR2
      SJ=INTGRL(SIJ,DSJ)
*
*     STORED PARTICULATE SUBSTRATE
*
      RXPHY=RH*XAJ*(FPJ/(KSP+FPJ))*Y3
      DXPJ=((Q1J*XPOJ+QR2J*XPRJ-QTJ*XPJ)/VJ)-RXPHY
      XPJ=INTGRL(XPIJ,DXPJ)
*
*     STORED MASS
*
      RXSP=RSR1+RXPHY
      RXA1=RXA*XAJ*FSJ/Y1
      DXSJ=((Q1J*XSOJ+QR2J*XSRJ-QTJ*XSJ)/VJ)+RXSP-RXA1
      XSJ=INTGRL(XSIJ,DXSJ)
*
*     ACTIVE MASS
*
      KDXA=KD*XAJ
      RXAF1=Y1*(RXA1+RSR2)
      RXAF=RXAF1-KDXA
      DXAJ=((Q1J*XAOJ+QR2J*XARJ-QTJ*XAJ)/VJ)+RXAF
      XAJ=INTGRL(XAIJ,DXAJ)
```

```
*
*       INERT MASS
*

        RXIF=Y2*KDXA
        DXIJ=((Q1J*XIOJ+QR2J*XIRJ-QTJ*XIJ)/VJ)+RXIF
        XIJ=INTGRL(XIIJ,DXIJ)
*
*       NON-VOLATILE SOLIDS
*

        DXNJ=((Q1J*XNOJ+QR2J*XNRJ-QTJ*XNJ)/VJ)
        XNJ=INTGRL(XNIJ,DXNJ)
*
*       NITROGENEOUS SYSTEM
*       AMMONIA NITROGEN BY NITROSOMONAS
*

        MUNS=MUHNS*(N4J/(KSNS+N4J))
        MUNS1=MUNS*X1J/YNS
        RHNH4=(-Y1*(RXA1+RSR2)+Y2P*KDXA)*KN
        DN4J=((Q1J*N4OJ+QR2J*RN4J-QTJ*N4J)/VJ)-MUNS1+RHNH4
        N4J=INTGRL(N4IJ,DN4J)
*
*       NITRITE NITROGEN BY NITROBACTER
*

        MUNB=MUHNB*(N2J/(KSNB+N2J))
        MUNB1=MUNB*X2J/YNB
        DN2J=((Q1J*N2OJ+QR2J*RN2J-QTJ*N2J)/VJ)+MUNS1-MUNB1
        N2J=INTGRL(N2IJ,DN2J)
*
*       NITRATE NITROGEN
*

        DN3J=((Q1J*N3OJ+QR2J*RN3J-QTJ*N3J)/VJ)+MUNB1
        N3J=INTGRL(N3IJ,DN3J)
*
*       ORGANISM (NITROSOMONAS AND NITROBACTER)
*       NITROSONOMAS
        DX1J=((Q1J*X1OJ+QR2J*XR1J-QTJ*X1J)/VJ)+X1J*(MUNS-KDNS)
        X1J=INTGRL(X1IJ,DX1J)
*
*       NITROBACTER
*

        DX2J=((Q1J*X2OJ+QR2J*XR2J-QTJ*X2J)/VJ)+X2J*(MUNB-KDNB)
        X2J=INTGRL(X2IJ,DX2J)
*
*       OXYGEN UTILIZATION BY HETEROTROPIC ORGANISM
*

        OURC1=Y1P*(RXA1+RSR2)
        OURC2=Y2P*KDXA
        OHJ=OURC1+OURC2
*
*       OXYGEN CONSUMPTION RATE DUE TO NITRIFIERS
        ONJ=MUNS1*YNSO2+MUNB1*YNBO2
*
*       OXYGEN INPUT RATE
```

```
        KLATJ=KLAO+CKAJ
        OURIJ=KLATJ*(DOS-DJ)
*
*       DO BALANCE
        DDJ=((Q1J*DOJ+QR2J*DRJ-QTJ*DJ)/VJ)-OHJ-ONJ+OURIJ
        DJ=INTGRL(DIJ,DDJ)
ENDMACRO
*       THIS MACRO CONTAINS MASS BALANCES FOR NON-BIODEGRADABLE
*       SOLUBLE SUBSTRATE
MACRO SNJ=ASP1(Q1J,QR2J,QTJ,SNOJ,SNIJ,VJ,SNRJ)
*
*       NON-BIODEGRADABLE SOLUBLE SUBSTRATE
*
        DSNJ=((Q1J*SNOJ+QR2J*SNRJ-QTJ*SNJ)/VJ)
        SNJ=INTGRL(SNIJ,DSNJ)
ENDMACRO
*
*       THIS MACRO CALUCULATES RUNNING MEANS AND RUNNING VARIANCES
MACRO XBARJ,VBARJ=STAT(XJ,INDEPJ,TRIGJ)
        CALC10=MODINT(0.0,TRIGJ,1.0,XJ)
        CALC11=MODINT(0.0,TRIGJ,1.0,(XJ**2))
PROCEDURE XBARJ,VBARJ=LOGIC(CALC10,CALC11)
        IF(INDEPJ) 340,350,340
340     XBARJ=CALC10/INDEPJ
        VBARJ=(CALC11-((CALC10)**2)/INDEPJ)/INDEPJ
350     CONTINUE
ENDPROCEDURE
ENDMACRO
*       THIS MACRO MIXES FLOWS AND CONCENTRATIONS FOR THE STEP FEED
*       OPERATION
MACRO QTL,SL,SNL,XPL,XSL,XAL,XNL,XIL,N4L,N2L,N3L,X1L,X2L,DL=STEP(...
QTK,QK,SK,SNK,XPK,XSK,XAK,XIK,XNK,N4K,N2K,N3K,X1K,X2K,SOK,SNOK,...
XPOK,XSOK,XAOK,XNOK,XIOK,N4OK,N2OK,N3OK,X1OK,X2OK,DK,DOK)
*
NOSORT
        QTL=QTK+QK
        QX1=QTK/QTL
        QX2=1.-QX1
*
*       BYPASS CALCULATION IF THERE IS NO MIXING
        IF(QX2) 10,10,20
10      SL=SK
        SNL=SNK
        XPL=XPK
        XSL=XSK
        XAL=XAK
        XNL=XNK
        XIL=XIK
        N4L=N4K
        N2L=N2K
        N3L=N3K
        X1L=X1K
        X2L=X2K
```

```
         DL=DK
         GO TO 30
20       SL=QX1*SK+QX2*SOK
         SNL=QX1*SNK+QX2*SNOK
         XPL=QX1*XPK+QX2*XPOK
         XSL=QX1*XSK+QX2*XSOK
         XAL=QX1*XAK+QX2*XAOK
         XNL=QX1*XNK+QX2*XNOK
         XIL=QX1*XIK+QX2*XIOK
         N4L=QX1*N4K+QX2*N4OK
         N2L=QX1*N2K+QX2*N2OK
         N3L=QX1*N3K+QX2*N3OK
         X1L=QX1*X1K+QX2*X1OK
         X2L=QX1*X2K+QX2*X2OK
         DL=QX1*DK+QX2*DOK
30       CONTINUE
SORT
ENDMACRO
*
INITIAL
         STORAGE VS(10),SFLUX(10),TFLUX(10),A1(10),Z(10)
         FIXED NELEM,M,NELEM1,I,I1,I2,IFLAGD,IFIRST,ILEVEL,ITMAX,J,IPH
         FIXED NCE,NEF,ITER,NP,NP2
*
*        CARBONACEOUS PARAMETERS
         PARAM KT=0.0125,FSH=0.7,RS=0.002,K=150.,KD=0.015
         PARAM Y1=0.6,Y2=0.2,Y3=1.0,RH=0.015
         PARAM SI1=24.,SI2=8.2,SI3=3.6,SNI1=10.0,SNI2=10.0,SNI3=10.0
         PARAM XNI1=179.,XNI2=179.,XNI3=179.,XAI1=570.,XAI2=570.,XAII1=100.
         PARAM XAI3=570.,XII1=445.,XII2=445.,XII3=445.,XSI1=150.,XSI2=115.
         PARAM XSI3=45.,XPI1=285.,XPI2=280.,XPI3=275.
         PARAM XAO1=0.0,XSO1=0.0,MLSS=2500.0
         PARAM FRACV=0.79,FRACB=0.70,KOEX=1.5,KOES=0.63,FRACB1=0.8
         PARAM FRAC4=0.4,FRANV=.21,FRANB=.3,XMTI1=0.0
*
*        NITROGENEOUS PARAMETERS
         PARAM MUHNS=0.02,KSNS=1.0,MUHNB=0.04,KSNB=1.0,KDNS=0.005
         PARAM KDNB=0.005,YNS=0.05,YNB=0.02,KN=0.07
         PARAM N2I1=0.5,N2I2=0.5,N2I3=0.5,N4I1=13.9,N4I2=9.4,N4I3=5.9
         PARAM N3I1=7.1,N3I2=10.5,N3I3=13.75,N3O1=0.0,N2O1=0.0
         PARAM X1I1=6.3,X1I2=6.3,X1I3=6.3,X1O1=0.0
         PARAM X2I1=2.4,X2I2=2.4,X2I3=2.4,X2O1=0.0
         PARAM YNSO2=3.42,YNBO2=1.14
         PARAM NELEM=10,HCLAR=3.048,FA=1.8052,QII=4.,VD=900.
         PARAM ROW=0.3,SRT=10.,MXTS=0.0,QI=4.0
         PARAM SNH4AV=30.0,SCODA=250.0,TSSAV=150.
         PARAM T1=24.,T2=24.,T3=6.,TDEL=0.025,DTIME=.25,CKG=1.E+03
         PARAM TPRED=2.,ITYPE=3,ESP=0.001,KSP=0.05
         PARAM FGATE1=1.,FGATE2=0.,FGATE3=0.,RGATE1=1.,RGATE2=0.,RGATE3=0.
         PARAM QAV=788.55,XEFF=17.975,SAGE1=9.
         PARAM ABO=83.1,AB1=-7.19,AB2=-3.33,AB3=-1.50,AB11=-0.626
         PARAM AB22=-0.304,AB33=0.014,AB12=1.44,AB13=0.132,AB23=0.024
         PARAM IFLAGD=2,HEIGHT=4.0,PPUMPF=3.,REFFP=0.2
```

```
      PARAM CXTPU=5.0E04,IXNPU=8.E06,IXVPU=35.0E06
      PARAM SSI=150.,BOD5=250.,NH4=25.,THETAH=6.0
      PARAM XR=10000.
      PARAM OFR=800.,POFR=850.
      PARAM OMEFFT=0.05,PUMPT=4.,CXTTU=1.E+05
      PARAM IMTNVS=1.E+03,IMTBD=1.E+03,IMTNB=1.E+03,ITMSIT=1.E+08
      PARAM AGT=400.
      PARAM CONBD=0.7,CONNB=0.30,CONNV=0.21
*
*     DISSOLVED OXYGEN PARAMETERS
*
      PARAM CKA1=20.0,CKA2=20.0,CKA3=20.0,KLAO=0.1
      PARAM DR1=0.0,DO1=0.0,DOS=8.0
      PARAM DI1=4.0,DI2=4.0,DI3=4.0
*
*     COST AND OPTIMIZATION PARAMETERS
*
      PARAM CKWH=0.05,COL=10000.0,CSD=20.0,DHR=20.84,HEAD=3.0
      PARAM IFIRST=1,ILEVEL=-1,DBTIME=0.0
*
      PARAM SUMOLD=1.E+14,EPS=1.E+35,EPSI=0.10
      PARAM ITMAX=4,DP=0.1,ITER=0
      PARAM AINR=0.08,IPH=20,FVOPC1=0.0,EFFG=0.6
*
      PARAM FLAGC=1.,FLAGO=1.
*
*     INITIAL SEGEMENT OF THE REACTOR
      NEF=3
      NCE=11
      NP=5
      NP2=10
      S3C=SI3
      XA3C=XAI3
      XP3C=XPI3
      XS3C=XSI3
      XI3C=XII3
      XT3C=XA3C+XP3C+XS3C+XI3C
      XN3C=XNI3
      X13C=X1I3
      X23C=X2I3
      XAR=XAI3/ROW
      XPR=XPI3/ROW
      XSR=XSI3/ROW
      XIR=XII3/ROW
      XTR=XAR+XSR+XPR+XIR
      X1R=X1I3/ROW
      X2R=X2I3/ROW
NOSORT
*
*     PRIMARY AND SECONDARY CLARIFIER OVERFLOW RATES ARE IN M**3/M**2/
*     DAY WHEN USED IN THE OPTIMIZATION PROGRAM
      PARL(1)=400.
      PARL(2)=9.
```

```
                    PARL(3)=5.5
                    PARL(4)=300.
                    PARL(5)=400.
                    PARU(1)=1200.
                    PARU(2)=20.0
                    PARU(3)=15.
                    PARU(4)=2500.0
                    PARU(5)=700.
                    DO 101 I=1,NELEM
                    TFLUX(I)=0.0
                    SFLUX(I)=0.0
                    A1(I)=0.0
                    Z(I)=DX*I
        101         CI(I)=800.
                    CI(NELEM-1)=4000.
                    CI(NELEM)=8000.
                    CU=CI(NELEM)
        SORT
                    GAMMA=((1.-(1.+AINR)**(-IPH)))/AINR
                    QO=QAV
                    N4O1=SNH4AV
                    QPP=QO
                    SO11=SCODA*(1.-REFFP)
                    SO12=SO11/KOES
                    SO1=SO12*FRAC4
                    SNO1=FRANB*SO1
                    STIME=0.0
                    SSIN=TSSAV
                    XPOO=SSIN*FRACV*FRACB*KOEX
                    XIOO=SSIN*FRACV*FRANB*KOEX
                    XNOO=SSIN*FRANV*KOEX
        *           FN=0.0
                    Y1P=1.-Y1
                    Y2P=1.-Y2
                    YSB=YNSO2+YNBO2
                    RXA=K*RS
                    DX=HCLAR/NELEM
                    M=NELEM-1
                    V1=V/3.
                    V2=V1
                    V3=V1
PROCEDURE AREAP,V,THETAH,A3,FLUX,XAI1,XAI2,XAI3,XPI1,XPI2,XPI3,...
XII1,XII2,XII3,XSI1,XSI2,XSI3,XNI1,XNI2,XNI3,X1I1,X1I2,X1I3,X2I1,...
X2I2,X2I3,XTI1,XTI2,XTI3,THETAD=STD1(SSI,BOD5,NH4,XR,VD,...
QII,POFR,OFR,ROW,SRT,TSSAV,SCODA,MLSS)
                    IF(IFIRST.GT.1) GO TO 200
                    PAROLD(1)=POFR
                    PAROLD(2)=SRT
                    PAROLD(3)=THETAH
                    PAROLD(4)=VD
                    PAROLD(5)=OFR
                    CALL STEADY(SSI,BOD5,NH4,AREAP,V,SRT,THETAH,QAV,XR,...
                          A3,THETAD,VD,QII,MLSS,POFR,OFR,IFIRST)
```

```
              IFIRST=IFIRST+1
              GO TO 210
  200     POFR=PAROLD(1)
          SRT=PAROLD(2)
          THETAH=PAROLD(3)
          VD=PAROLD(4)
          OFR=PAROLD(5)
          CALL STEADY(SSI,BOD5,NH4,AREAP,V,SRT,THETAH,QAV,XR,...
                A3,THETAD,VD,QIIIA,MLSS,POFR,OFR,0)
  *       CALL SICOND(TSSAV,BOD5,SRT,XAI1,XAI2,XAI3,XSI1,XSI2,XSI3,...
  *       XPI1,XPI2,XPI3,XII1,XII2,XII3,XNI1,XNI2,XNI3,X1I1,X1I2,X1I3,...
  *       X2I1,X2I2,X2I3,XTI1,V,THETAH)
  210     CONTINUE
ENDPROCEDURE
*
*
DYNAMIC
*
*         DYNAMIC SEGMENT
          TRG6=0.5-IMPULS((T3+TDEL),T3)
          TRG24=0.5-IMPULS((T1+TDEL),T1)
          TRG168=0.5-IMPULS((T2+TDEL),T2)
          T6=MODINT(0.0,TRG6,1.0,1.0)
          T24=MODINT(0.0,TRG24,1.0,1.0)
          T168=MODINT(0.0,TRG168,1.0,1.0)
*
*         INPUT SECTION TO THE MODEL
PROCEDURE Q0,QPP,SSIN,SO1,N4O1,XIOO,XNOO,XPOO,SO11,SO12,DIFF1,XAAI2=...
INPUT(ITYPE,T6,T24,T168,FRACV,FRACB,KOEX,FRACB1,KOES,SNH4AV)
          IF(IFLAGD.EQ.1) FA=0.0
          IF(KEEP-1) 3060,3000,3060
  3000  IF(TIME-STIME) 3060,3010,3010
  3010  STIME=TIME+DTIME
          XAAI2=XA1
  *       DIFF1=ABS(XAAI2-XAII1)
  *       IF(DIFF1.LT.ESP) FN=1.0
          XAII1=XAAI2
          IF(ITYPE-2) 3020,3060,3060
*
*         TIME VARYING INPUT
  3020  SSIN=TSSAV*TSS(T24)
          SO11=SCODA*VBOD(T24)*(1.-REFFP)
          SO12=SO11/KOES
          SO1=SO12*FRAC4
          SNO1=FRANB*SO1
          N4O1=SNH4AV*VSNH4(T24)
          XPOO=SSIN*FRACV*FRACB*KOEX
          XIOO=SSIN*FRACV*FRANB*KOEX
          XNOO=SSIN*FRANV*KOEX
          Q0=QAV*FLOW(T24)
          QPP=QAV*FLOW(T24+TPRED)
  3060  CONTINUE
ENDPROCEDURE
```

```
*
*       PRIMARY CLARIFIER SEGMENT(TWO DIMENSIONAL ADVECTION-DIFFUSION
*       EQUATION IS SOLVED USING ALTERNATING DIRECTION IMPLICIT(ADI)
*       METHOD AND THE EMPIRICAL EQUATION IS DEVELOPED USING THE RESULT
*       OF THIS ADVECTION-DIFFUSION EQUATION
*
*       RE: REMOVAL EFFICIENCY OF THE PRIMARY CLARIFIER
*
        RE=(SSIN-XEFFP1)/SSIN
        SSOUT=(1.-RE)*SSIN
        XPO1=SSOUT*FRACV*FRACB*KOEX
        XIO1=SSOUT*FRACV*FRANB*KOEX
        XNO1=SSOUT*FRANV*KOEX
*
*       UNDERFLOW CONCENTRATION
*       HSPS= HEIGHT OF SLUDGE IN THE PRIMARY SEDIMENTATION TANK
        CXNPU=CXTPU*(XNPU/(XNPU+XVPU))
        CXVPU=CXTPU-CXNPU
        HSPS=(XNPU+XVPU)/(AREAP*CXTPU)
        DXNPU=QAV*SSIN*FRANV*RE-QI*CXNPU
        XNPU=INTGRL(IXNPU,DXNPU)
        DXVPU=QAV*SSIN*FRACV*RE-QI*CXVPU
        XVPU=INTGRL(IXVPU,DXVPU)
PROCEDURE XEFFP1,LENGTH=PSD(QAI,HEIGHT,AREAP,SSIN,POFR)
        CALL PSD1(XEFFP1,LENGTH,POFR,QAI,HEIGHT,AREAP,SSIN)
ENDPROCEDURE
*
*       SECONDARY CLARIFIER
*       FLOW IS IN M**3/HR , AREA IS IN M**2 ,
*       AND FLUX IS IN KG/HR.M**2
*       SRT : SOLIDS RETENTION TIME, DAYS
*       ORA : OVERFLOW RATE, METERS/DAY
*       HRT : HYDRAULIC RETENTION TIME, HR
        XT3C=XS3C+XP3C+XA3C+XI3C
        MLVSS=XT3C+X13C+X23C
        MLSS=MLVSS+XN3C
        HRT=THETAH
        ORA=(QR/A3)*24.
        NUM=V*MLVSS+MXTS
        CONST2=AB1+AB12*HRT+AB13*ORA
        CONST1=ABO+AB2*HRT+AB3*ORA+AB22*(HRT**2)+AB33*(ORA**2)+AB23...
        *HRT*ORA
        CONST3=CONST1
        QAI=QO+FA
        ASRT=SRT*QAI*24.
        PI=((NUM/ASRT)-XEFF)/(CU-XEFF)
        Q1=QAI-QI
        Q2=(1.+ROW)*Q1
        Q3=Q2
        QR1=(ROW+PI)*Q1
        QRO=PI*Q1
        QR2=QR1-QRO
        QR=Q3-QR1
```

```
*
*       VELOCITY IS IN CM/HOUR,
*       AREA IS IN M**2 AND CONCENTRATION IS IN GM/M**3
        BODEFF=(S3C+XEFF*((XA3C+XS3C+XP3C)/XT3C))*KOES
        C=INTGRL(CI,CDOT,10)
PROCEDURE CDOT,TFLUX,SFLUX,THETA,VS,A,A2,SAGE1,SAGE2=SEC2(MXTS,...
MLSS,MLVSS,XT3C,Q3,QR1,A3,QR,XEFF,DX,NELEM)
        A=A3
        U=QR1*100./A
        FLUXIN=(Q3*MLSS-(Q3-QR1)*XEFF)*0.001/A
        DO 1000 I=1,NELEM
        VS(I)=SVS(C(I))
1000    SFLUX(I)=(C(I)*VS(I))*0.00001
        TFLUX(1)=(U*C(1))*0.00001+AMIN1(SFLUX(1),SFLUX(2))
        CDOT(1)=(FLUXIN-TFLUX(1))*1000./DX
        DO 1010 I=2,M
        TFLUX(I)=(U*C(I))*0.00001+AMIN1(SFLUX(I),SFLUX(I+1))
1010    CDOT(I)=(TFLUX(I-1)-TFLUX(I))*1000./DX
        CDOT(NELEM)=(TFLUX(M)-(U*C(NELEM)*0.00001))*1000./DX
        TFLUX(NELEM)=(U*C(NELEM))*0.00001+SFLUX(NELEM)
        A2=A
        THETA=0.0
        MXTS=0.0
        DO 1050 I=1,NELEM
        MXTS=MXTS+DX*A2*C(I)
*       THETA IS IN HOURS
1050    THETA=THETA+DX*100./(VS(I)+U)
        IF (TSWR) 2010,2010,2005
*       TSWR IS IN  GMS/HR, SAGE1,SAGE2 ARE IN DAYS.
2005    SAGE1=MTA/(TSWR*24.)
        SAGE2=MT/(TSWR*24.)
2010    CONTINUE
ENDPROCEDURE
*
*       RECYCLE SLUDGE CONCENTRATION
        VEL=HCLAR*100./THETA
        XPRP=PIPE(250,XPI3,HCLAR,VEL,XP3C,1)
        XARP=PIPE(250,XAI3,HCLAR,VEL,XA3C,1)
        XSRP=PIPE(250,XSI3,HCLAR,VEL,XS3C,1)
        XIRP=PIPE(250,XII3,HCLAR,VEL,XI3C,1)
        XTRP=XPRP+XSRP+XARP+XIRP
        X1RP=PIPE(250,X1I3,HCLAR,VEL,X13C,1)
        X2RP=PIPE(250,X2I3,HCLAR,VEL,X23C,1)
        XNRP=PIPE(250,XNI3,HCLAR,VEL,XN3C,1)
        MLSSRP=XTRP+X1RP+X2RP+XNRP
        MLVSRP=MLSSRP-XNRP
PROCEDURE XAR,XPR,XSR,XIR,XTR,XNR,X1R,X2R,SR1,SNR1,MLSSR,RN41,RN31,...
RN21,MLVSSR,FAC1,XTRDI,MTNVS,MTBD,MTNB,TMSIT,HST,XNVO1,BDO1,...
NBDO1,PRIMC2=THICK(XARP,XSRP,XPRP,XIRP,XNRP,X1RP,X2RP,FA,QII,...
XTRP,MLSSRP,MLVSRP,C(NELEM),CXTPU,CONBD)
*
*       THIS PROCEDURE IS USED FOR THE SIMULATION OF GRAVITY SLUDGE
*       THICKENER INCLUDING THE MIXING OF THICKENER RETURN SUPERNATANT
```

```
          GO TO (510,520),IFLAGD
*         LOW RATE DIGESTION WITHOUT THICKENER
510       XTRDI=C(NELEM)
515       FAC1=C(NELEM)/MLSSRP
          XAR=FAC1*XARP
          XSR=FAC1*XSRP
          XPR=FAC1*XPRP
          XIR=FAC1*XIRP
          XTR=FAC1*XTRP
          XNR=FAC1*XNRP
          X1R=FAC1*X1RP
          X2R=FAC1*X2RP
          MLSSR=FAC1*MLSSRP
          MLVSSR=FAC1*MLVSRP
          GO TO 530
520       CONTINUE
*
*         HIGH RATE DIGESTION WITH THICKENER SUPERNATANT RECYCLE
          DMTNVS=QI*CONNV*CXTPU+C(NELEM)*FRANV*QRO-FA*OMEFFT*C(NELEM)*FRANV
          MTNVS=INTGRL(IMTNVS,DMTNVS)
          DMTBD=QI*CONBD*CXTPU+C(NELEM)*FRACB*QRO-FA*OMEFFT*C(NELEM)*FRACB
          MTBD=INTGRL(IMTBD,DMTBD)
          DMTNB=QI*CONNB*CXTPU+C(NELEM)*FRANB*QRO-FA*OMEFFT*C(NELEM)*FRANB
          MTNB=INTGRL(IMTNB,DMTNB)
          TMASS=MTNVS+MTBD+MTNB
          DTMSIT=QI*CXTPU+C(NELEM)*QRO-QII*CXTTU-FA*OMEFFT*C(NELEM)
          TMSIT=INTGRL(ITMSIT,DTMSIT)
          HST=TMSIT/(AGT*CXTTU)
          PRIMC2=IMPULS(0.0,6.0)
          QII=PUMPT*INSW((HST-1.),0.,1.)*PULSE(2.,PRIMC2)
          IF(QIIIA.EQ.0.0) GO TO 540
          XNVO1=DMTNVS/QIIIA
          BDO1=DMTBD/QIIIA
          NBDO1=DMTNB/QIIIA
          GO TO 550
540       XNVO1=0.0
          BDO1=0.0
          NBDO1=0.0
550       FA1=QRO+QI-QII
          FA=INSW(FA1,0.,FA1)
          SR1=S3C
          SNR1=SN3
          RN41=N43
          RN21=N23
          RN31=N33
          GO TO 515
530       CONTINUE
ENDPROCEDURE
          QIIIA,QIIIV=STAT(QII,T24,TRG24)
*
*         FLOW DIVIDE SEGMENT
*         THIS PROCEDURE DIVIDES THE INFLUENT AND RECYCLE FLOWS FOR STEP
*         FEED
```

```
      PROCEDURE QX,QY,QZ,QRX,QRY,QRZ=FLOW(FGATE1,FGATE2,...
FGATE3,RGATE1,RGATE2,RGATE3,Q2,QR2)
          FRACF=Q1/(FGATE1+FGATE2+FGATE3)
          FRACR=QR2/(RGATE1+RGATE2+RGATE3)
          QX=FGATE1*FRACF
          QY=FGATE2*FRACF
          QZ=FGATE3*FRACF
          QRX=RGATE1*FRACR
          QRY=RGATE2*FRACR
          QRZ=RGATE3*FRACR
ENDPROCEDURE
*
*
*       AERATOR SEGMENT
*       FIRST REACTOR
QT1,S1,XS1,XA1,XI1,XP1,XT1,V1,X11,X21,D1,XN1,OH1,ON1,...
N41,N31,N21=AP(QX,QRX,SO1,XPO1,XAO1,XIO1,SR1,XSR,XSO1,XPR,...
XAR,XIR,N4O1,N2O1,N3O1,RN41,RN21,RN31,X1R,X2R,SI1,XSI1,XPI1,CKA1,...
XAI1,XII1,N4I1,N2I1,N3I1,X1O1,X1I1,X2I1,X2O1,XNO1,XNI1,XNR,DO1,DI1,DR1)
SN1=ASP1(QX,QRX,QT1,SNO1,SNI1,V1,SNR1)
*
*       MIXING AFTER THE FIRST REACTOR
QTB,SB,SNB,XPB,XSB,XAB,XNB,XIB,N4B,N2B,N3B,X1B,X2B,DB=STEP(...
QT1,QY,S1,SN1,XP1,XS1,XA1,XI1,XN1,N41,N21,N31,X11,X21,SO1,SNO1,...
XPO1,XSO1,XAO1,XNO1,XIO1,N4O1,N2O1,N3O1,X1O1,X2O1,D1,DO1)
*
*       SECOND REACTOR
QT2,S2,XS2,XA2,XI2,XP2,XT2,V2,X12,X22,D2,XN2,OH2,ON2,...
N42,N32,N22=AP(QTB,QRY,SB,XPB,XAB,XIB,SR1,XSR,XSB,XPR,...
XAR,XIR,N4B,N2B,N3B,RN41,RN21,RN31,X1R,X2R,SI2,XSI2,XPI2,CKA2,...
XAI2,XII2,N4I2,N2I2,N3I2,X1B,X1I2,X2I2,X2B,XNB,XNI2,XNR,DB,DI2,DR1)
SN2=ASP1(QTB,QRY,QT2,SN1,SNI2,V2,SNR1)
*
*       MIXING AFTER THE SECOND REACTOR
QTC,SC,SNC,XPC,XSC,XAC,XNC,XIC,N4C,N2C,N3C,X1C,X2C,DC=STEP(...
QT2,QZ,S2,SN2,XP2,XS2,XA2,XI2,XN2,N42,N22,N32,X12,X22,SO1,SNO1,...
XPO1,XSO1,XAO1,XNO1,XIO1,N4O1,N2O1,N3O1,X1O1,X2O1,D2,DO1)
*
*       THIRD REACTOR
QT3,S3,XS3,XA3,XI3,XP3,XT3,V3,X13,X23,D3,XN3,OH3,ON3,...
N43,N33,N23=AP(QTC,QRZ,SC,XPC,XAC,XIC,SR1,XSR,XSC,XPR,...
XAR,XIR,N4C,N2C,N3C,RN41,RN21,RN31,X1R,X2R,SI3,XSI3,XPI3,CKA3,...
XAI3,XII3,N4I3,N2I3,N3I3,X1C,X1I3,X2I3,X2C,XNC,XNI3,XNR,DC,DI3,DR1)
SN3=ASP1(QTC,QRZ,QT3,SN2,SNI3,V3,SNR1)
*
*   ANAEROBIC DIGESTION SEGMENT
PROCEDURE Q4MT,TACID,BD1,BN1,SS1,XNCD1,PVSSD,OLR,OLR1,VD,XEFF...
=DIGST(THETAD,QIIIA,XAR,XPR,XSR,XIR,XNR,X1R,XNVO1,BDO1,NBDO1,...
X2R,CXTPU,XTRDI,AB11,CONST3,CONST1,SRT,MLSS,XR,A2)
CALL DIGST1(Q4MT,TACID,BD1,BN1,SS1,XNCD1,PVSSD,THETAD,OLR,OLR1,VD,...
QIIIA,XAR,XPR,XSR,X1R,X2R,CXTPU,XIR,XNR,XNVO1,BDO1,NBDO1,...
XTRDI,IFLAGD)
*
```

```
*       EFFLUENT TSS CONCENTRATION
        XEFF=CONST3+CONST2*SAGE1+AB11*(SAGE1**2)
        IF(XEFF.LT.0.0) XEFF=4.5+4.2*(MLSS*QR*0.001/A2)
ENDPROCEDURE
*NOSORT
*       CALL DEBUG(1,DBTIME)
*SORT
*
*       INVENTORY SECTION OF THE MODEL
*       OXYGEN CONSUMPTION CALCULATIONS
        IN1=(XIO1+XPO1+SO1+(N4O1+KN*XIO1)*YSB)*QO
        OUT11=(S3+N43*YSB)*QR
        OUT21=(S3+XTR+X1R+X2R+YSB*KN*(XAR+XIR))*QRO
        XM1=(IN1-OUT11-OUT21-OCRT)/CKG
        XMT1=INTGRL(XMTI1,XM1)
        OT1=OH1+ON1
        OT2=OH2+ON2
        OT3=OH3+ON3
        OTN=ON1+ON2+ON3
        OTH=OH1+OH2+OH3
        OCRH=OTH*V1
        OCRN=OTN*V1
        OCRT=OCRH+OCRN
*
*       OC,OCH AND OCN ARE IN KG.
        OC=MODINT(0.0,TRG24,1.0,OCRT/CKG)
        OCH=OC-OCN
        OCN=MODINT(0.0,TRG24,1.0,OCRN/CKG)
*
*       SLUDGE MASS AND RECYCLE CALCULATION
        MLSSRA=MODINT(0.0,TRG24,1.0,MLSSR)
*
*       SWR,VSWR,ESWR ARE IN GMS/HR AND MT1,MT2,MT3 ARE IN GMS.
        SWR=QRO*MLSSR
        VSWR=QRO*MLVSSR
        NVSWR=SWR-VSWR
        SWT=MODINT(0.0,TRG24,1.0,SWR)
        VSWT=MODINT(0.0,TRG24,1.0,VSWR)
        NVSWT=SWT-VSWT
        ESWR=(Q3-QR1)*XEFF
        EVSWR=ESWR*MLVSS/MLSS
        ENVSWR=ESWR-EVSWR
        ESWT=MODINT(0.0,TRG24,1.0,ESWR)
        EVSWT=MODINT(0.0,TRG24,1.0,EVSWR)
        ENVSWT=ESWT-EVSWT
        TSW=SWT+ESWT
        TSWR=SWR+ESWR
        TNVSW=TSW-TVSW
        TVSW=VSWT+EVSWT
        MT1=(XT1+X11+X21+XN1)*V1
        MT2=(XT2+X12+X22+XN2)*V2
        MT3=(XT3+X13+X23+XN3)*V3
        MTA=MT1+MT2+MT3
```

```
            MTNVA=XN1*V1+XN2*V2+XN3*V3
            MT=MTA+MXTS
            MTT=MODINT(0.0,TRG24,1.0,MT)
            CU=MLSSR
            BDPBN=BD1+BN1
            PRIMC1=IMPULS(0.0,4.0)
            QI=PPUMPF*INSW((HSPS-1.0),0.,1.)*PULSE(2.,PRIMC1)
            Q4MT1=MODINT(0.0,TRG24,1.0,Q4MT)
            QIIAV1=MODINT(0.0,TRG24,1.0,QIIIA)
            BDPBN1=MODINT(0.0,TRG24,1.0,BDPBN)
    NOSORT
    *       CALL DEBUG(1,DBTIME)
            S3C=S3
            SN3C=SN3
            XA3C=XA3
            XS3C=XS3
            XP3C=XP3
            XI3C=XI3
            XT3C=XT3
            XN3C=XN3
            X13C=X13
            X23C=X23
    TERMINAL
            OURTA=OC/T24
            Q4MTA=Q4MT1/T24
            QIIAV2=QIIAV1/T24
            BDPBN2=BDPBN1/T24
    PRINT S1,SN1,N41,N21,N31,XP1,XS1,XA1,XI1,XN1,X11,X21,XT1,...
          OH1,ON1,OT1,D1,S2,SN2,N42,N22,N32,XP2,XS2,XA2,XI2,XN2,X12,...
          X22,XT2,OH2,ON2,OT2,D2,S3,SN3,N43,N23,N33,XP3,XS3,...
          XA3,XI3,XN3,X13,X23,XT3,OH3,ON3,OT3,D3
    OUTPUT PI,QO,Q1,Q2,QR,QX,QRX,QRY,QRZ,QRO,QR2,QAI,QI,QII,QIIIA,...
           FA,OTH,OTN,OCRT,OCRN,OC,OCN,SWR,VSWR,NVSWR,SWT,ESWT,TSWR,...
           TSW,MTA,MTNVA,MXTS,MT,HRT,ORA,A2
    OUTPUT XPR,XAR,XSR,XIR,XTR,X1R,X2R,SAGE1,SAGE2,XEFF,RE,...
    SSOUT,XPO1,XIO1,XNO1,XEFFP1,BODEFF,FAC1,C(1-10),...
    BDO1,NBDO1,XNVO1,VD,OLR1,Q4MTA,TACID,BD1,BN1,XNCD1,PVSSD
    TIMER FINTIM=1.,DELT=0.02,PRDEL=1.0,OUTDEL=1.0,DELMIN=0.25E-10
    *FINISH FN=1.
    METHOD TRAPZ
            IF((FLAGC.LT.1.0).AND.FLAGO.GT.0.0) GO TO 601
            IF((FLAGC.GT.0.0).AND.FLAGO.GT.0.0) GO TO 601
            OCRT = QAV*(BOD5*1.5 + NH4*4.5)
    601     CALL COST(CCOST,OM,VOPC,OURTA,OCRT,BDPBN2,...
            QO,V,AREAP,BCAP,A3,AGT,QR1,QI,Q4MTA,QIIIA,VD,CKWH,COL,...
            CSD,DHR,HEAD,VOPC1,EFFG)
            IF(ILEVEL.GT.0) GO TO 145
            DO 605 I=1,NEF
    605     WEIGH(I)=1.
            DO 610 I=1,NCE
            ER(I,1)=(CCOST(I)/GAMMA)*FLAGC
            ER(I,2)=OM(I)*FLAGO
            ER(I,3)=0.0
```

```
610       CONTINUE
          ER(5,3)=VOPC*FLAGO
          ER(7,3)=(VOPC1+FVOPC1)*FLAGO
          DO 620 J=1,NEF
          SUM=0.0
          DO 625 I=1,NCE
625       SUM=SUM+ABS(ER(I,J))
620       ERP(J)=SUM*WEIGH(J)
          SUM=0.0
          DO 640 J=1,NEF
640       SUM=SUM+ERP(J)
*          WRITE(6,9191)
*9191      FORMAT(10X,'******CAPITAL COSTS *****')
*          WRITE(6,9192) (ER(I,1),I=1,NCE)
*9192      FORMAT(10X,5E15.5)
*          WRITE(6,9193)
*9193      FORMAT(/10X,'***** OPERATING COSTS *****')
*          WRITE(6,9194) (ER(I,2),I=1,NCE)
*9194      FORMAT(/10X,5E16.5)
*          WRITE(6,9195)
*9195      FORMAT(/10X,'**** VARIABLE OPERATING COSTS*****')
*          WRITE(6,9196) (ER(I,3),I=1,NCE)
*9196      FORMAT(/10X,5E17.5)
*
*         WRITE OUT THE SUM
          WRITE(6,1041) SUM
1041      FORMAT(' TOTAL ERROR = ',E17.6)
          ITER=ITER+1
          WRITE(6,1039) ITER
1039      FORMAT(/10X,'ITER=',I3)
*
*         CHECK FOR ABSOLUTE CONVERGENCE
          IF(SUM-EPS) 110,110,120
110       WRITE(6,1042)
1042      FORMAT(' EXECUTION TERMINATING DUE TO ABSOLUTE CONVERGENCE')
*
*         CHECK FOR ERROR IMPROVEMENT
          GO TO 500
120       IF(ABS(SUMOLD-SUM)-EPSI) 130,130,133
130       WRITE(6,1045) SUMOLD,SUM,ITER
1045      FORMAT(' EXECUTION STOPING DUE TO FAILURE TO IMPROVE ERROR',...
         /,' SUM OLD=',E17.6,5X,'SUM=',E17.6,'ITER=',I3)
          GO TO 500
*
* CHECK TO SEE IF THE MAXIMUM NUMBER OF ITERATIONS IS EXCEEDED
133       IF(ITMAX-ITER) 135,140,140
135       WRITE(6,1046) ITMAX,ITER
1046      FORMAT(' THE MAXIMUM NUMBER OF ITERATIONS IS EXCEEDED',...
         /,' ITMAX=',I4,5X,'ITER=',I4)
          GOTO 500
*
*         SAVE THE VALUE OF SUM FOR FUTURE ITERATIONS
140       SUMOLD=SUM
```

```
*
*         BEGIN PUTURBATIONS
          ILEVEL=1
          PSAVE=PAROLD(ILEVEL)
          PTURB=PAROLD(ILEVEL)*DP
          PAROLD(ILEVEL)=PAROLD(ILEVEL)-PTURB
          CALL RERUN
          GO TO 500
*
*         CALCULATE INFLUENCE COEFFICIENT
145       PAROLD(ILEVEL)=PSAVE
          DO 170 I=1,NCE
          CINF(1,ILEVEL,I)=FLAGC*(ER(I,1)-(CCOST(I)/GAMMA))/PTURB
          CINF(2,ILEVEL,I)=FLAGO*(ER(I,2)-OM(I))/PTURB
170       CINF(3,ILEVEL,I)=0.0
          CINF(3,ILEVEL,5)=FLAGO*(ER(5,3)-VOPC)/PTURB
          CINF(3,ILEVEL,7)=FLAGO*(ER(7,3)-(VOPC1+FVOPC1))/PTURB
          ILEVEL=ILEVEL+1
          IF(ILEVEL.GT.NP) GO TO 490
          PSAVE=PAROLD(ILEVEL)
          PTURB=PAROLD(ILEVEL)*DP
          PAROLD(ILEVEL)=PAROLD(ILEVEL)-PTURB
          CALL RERUN
          GO TO 500
490       WRITE(6,1213)
1213      FORMAT(//10X,'STARTING THE OPTIMIZATION PROCEDURE')
          CALL OPTIM5(PAROLD,PARL,PARU,WEIGH,CINF,ER,ERP,NP,NP2,NEF,...
             NCE,NCE,ITER,2,1)
*         DBTIME=0.0
          ILEVEL=0
          CALL RERUN
500       CONTINUE
END
STOP
          SUBROUTINE STEADY(SSI,BOD5,NH4,AREAPC,V,THETAC,THETAH,FLOW2,XR,
     1         AREAS,THETAD,VD,QII,MLSS,POFR,OFR,IFIRST)
C
          REAL KD,KS,KDN,KSN,MADPTH,MSR,MUH,MUHN,MCONT,NH4,NH4E,MLSS
C
C         STEADY STATE DESIGN OF ACTIVATED SLUDGE TREATMENT PLANT
          DATA BODE/20./
C
C         CONSTANTS FOR THE DESIGN OF ACTIVATED SLUDGE PLANT
          DATA KD/.06/,MUH/5.0/,YIELD/0.6/,KS/60.0/,BOD5BU/.68/,
     1FRACL/1.42/
C
C         CONSTANTS IN CASE OF NITRIFICATION
          DATA KDN/.005/,KSN/1.0/,MUHN/0.4/,NH4E/1.0/
C
          DATA VSBTS/.70/,MADPTH/5.0/,RSS/0.5/,RBOD5/.25/,
     1DTIME2/3.5/,DCLARP/10.0/,SPGSLG/1.03/,MCONT/.94/,
     2DTIMP1/2.0/,DCLAP/10.0/
          CONS=4.536E+05
```

```
      CONS1=CONS*0.03531
      CONS2=24.*7.48
      CONS3=10.76391
      BOD5IA=BOD5*RBOD5
      FLOW1=FLOW2*6340.1
      FLOW=FLOW1/1.E+06
C     FLOW2=FLOW*3785.4/24.
C
C     EFFLUENT BOD=INFLUENT BOD5 ESCAPING TREATMENT +BOD5 OF EFFLUENT
C     SUSPENDED SOLIDS
      BOD5EF=BOD5E*FRACB
      UBODL=BOD5EF*FRACL
      BOD5ES=UBODL*BOD5BU
C
C     INFLUENT SOLUBLE BOD ESCAPING TREATMENT
      SBODE=BOD5E-BOD5ES
C
C     EFFICIENCY BASED ON SOLUBLE BOD5
      TEFF=((BOD5-SBODE)/BOD5)*100.
C
C     OVERALL PLANT EFFICIENCY
      EOVER=((BOD5-BOD5E)/BOD5)*100.
      VOL=FLOW*THETAH/24.
      V=VOL*3785.4
      XV=MLSS*VOL*8.34
      SPROD=XV/THETAC
C
C     BY MATERIAL BALANCE IN THE CLARIFIER
      QR=FLOW*MLSS/(XR-MLSS)
      QW=VOL*MLSS/(THETAC*XR)
      FDM=FLOW*8.34*(BOD5-SBODE)/XV
C
C     O2 REQUIREMENT(WITHOUT CONSIDERING NITRIFICATION, IN TERMS OF COD)
C     O2 DEMAND IN = UNTREATED O2 DEMAND+OXIDIZED O2 DEMAND+O2 DEMAND
C     OF SLUDGE
      O2DH=(FLOW*8.34*(BOD5-SBODE)*1.47-SPROD*FRACL)*.4536
C
C     O2 DEMAND CONSIDERING NITRIFICATION(FOR THETAC>5 DAYS)
      O2DN=(FLOW*(BOD5-SBODE)*8.34*1.47+4.55*FLOW*8.34*(NH4-NH4E)-
     11.98*SPROD)*.4536
C
C     SECONDARY CLARIFIER
      AREA1=FLOW1/OFR
      AREAS=AREA1/CONS3
      XTSS=MLSS/VSBTS
      FLUX=(FLOW+QR)*XTSS*8.34/AREA1
C
C     ESTIMATE REQUIRED DEPTH FOR THICKENING
C     DETERMINE THE MASS OF SOLIDS IN THE AERATION BASIN
      ABSOLD=VOL*XTSS*8.34
      CSAV=(MLSS+XR)/(0.8*2.)
C
C     DEPTH OF SLUDGE ZONE IN THE SEDIMENTATION BASIN
```

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```
              MSSB=0.3*ABSOLD
              DEPTH1=(MSSB/(AREA1*CSAV))*CONS1
              PEAKQ=2.5*FLOW
              PKBOD=1.5*BOD5
              XV1=(YIELD*PEAKQ*(PKBOD-SBODE)*8.34)/(1.+KD*THETAC)
              QWXW=XV1
              TSOLID=QWXW+MSSB
              DEPTH2=(TSOLID/(AREA1*CSAV))*CONS1
              TRDPTH=MADPTH+DEPTH1+DEPTH2
              TRDPT=TRDPTH*.3048
              DTIME1=(AREA1*TRDPTH*CONS2)/FLOW1
       C
       C      ALTERNATE APPROACH
       C      ASSUMING DETENTION TIME=3.5HOURS
              VOL2=FLOW1*DTIME2/CONS2
              VOLS=VOL2/35.3147
              AREA2=VOL2/DCLARP
              AREAA=AREA2/CONS3
       C
       C      PRIMARY SEDIMENTATION TANK
              AREAP1=FLOW1/POFR
              AREAPC=AREAP1/CONS3
              FLUXP=(FLOW*8.34*SSI)/AREAP1
              MSR=RSS*SSI*FLOW*8.34
              VOLSLG=MSR/(SPGSLG*8.34*(1.-MCONT))
              DSISB=VOLSLG/(AREAP1*7.48)
              DEPTP=MADPTH+DSISB
              DTIMEP=AREAP1*DEPTP*CONS2/FLOW1
       C
       C      ALTERNATE APPROACH
              VOLP=FLOW1*DTIMP1/CONS2
              AREAP2=(VOLP/DCLARP)/CONS3
       C
       C      COMPUTE THE DIGESTER SOLID RETENTION TIME
       C
              IF(QII.LE.0.0) GO TO 123
              THETAD=VD/(QII*24.)
       123    IF(IFIRST.GT.1) GO TO 995
              WRITE(6,900)
       900    FORMAT(1H1,///20X,'STEADY STATE DESIGN OF ACTIVATED SLUDGE TREAT',
             1'MENT PLANT')
              WRITE(6,910) SSI,BOD5,NH4
       910    FORMAT(//20X,'INFLUENT SUSPENDED SOLIDS CONCENTRATION=',F8.2,
             1/20X,'INFLUENT BIOCHEMICAL OXYGEN DEMAND=',F8.2/20X,'INFLUENT ',
             2'AMMONIA CONCENTRATION(MG/L)=',F8.2)
              WRITE(6,920) MUH,KD,YIELD,KS,BOD5BU
       920    FORMAT(/20X,'SPECIFIC GROWTH RATE=',F10.5/20X,'DECAY COEFFICIENT='
             1,F10.5/20X,'YIELD COEFFICIENT=',F8.4/20X,'SATURATION COEFFICIENT',
             2'IN MG/L BOD5=',F8.4/20X,'BOD5/BODU=',F5.3)
              WRITE(6,930) RSS,RBOD5
       930    FORMAT(/20X,'REMOVAL OF SUSPENDED SOLIDS IN PRIMARY CLARIFIER=',
             1F5.2/20X,'REMOVAL OF BIOCHEMICAL OXYGEN DEMAND=',F8.4)
              WRITE(6,940) FLOW,FLOW2
```

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940    FORMAT(/20X,'FLOW IN MGD=',F8.4/20X,'FLOW IN M**3/HR=',F8.4)
       WRITE(6,950)
950    FORMAT(//20X,'DESIGNED VALUES OF THE PRIMARY CLARIFIER')
       WRITE(6,960) AREAPC,FLUXP,POFR,DEPTP,DTIMEP
960    FORMAT(/20X,'AREA OF THE PRIMARY CLARIFIER IN M**2=',E13.5/20X,
      1'FLUX OF PRIMARY CLARIFIER(LB/FT**2.DAY)=',E13.5/20X,'OVERFLOW',
      2' RATE(GALLONS/FT**2.DAY)=',E15.5/20X,'DEPTH OF THE PRIMARY ',
      3'CLARIFIER(FEET)=',F8.4/20X,'DETENTION TIME(HOURS)=',F8.4)
       WRITE(6,970)
970    FORMAT(//20X,'ALTERNATE APPROACH(ASSUMED DETENTION TIME)')
       WRITE(6,980) AREAP2,DCLARP
980    FORMAT(/20X,'AREA OF THE PRIMARY CLARIFIER(M**2)=',E13.5/20X,
      1'DEPTH OF THE PRIMARY CLARIFIER(FEET)=',F7.4)
       WRITE(6,990)
990    FORMAT(//20X,'DESIGNED VALUES OF THE AERATION BASIN')
       WRITE(6,1000) V,QR,QW,MLSS,FDM,THETAH,THETAC,O2DH,O2DN
1000   FORMAT(//20X,'VOLUME OF THE AERATION BASIN(M**3)=',E13.5/20X,
      1'RECYCLE FLOW RATE(MGD)=',F8.4/20X,'WASTE FLOW RATE(MGD)=',F8.4/
      220X,'MICROBIAL CONCENTRATION IN THE AERATION BASIN(MG/L)=',E13.5/
      320X,'FOOD/MICRO-ORGANISM=',F8.4/20X,'HYDRAULIC DETENTION TIME(DA',
      4'YS)=',F8.4/20X,'SLUDGE RETENTION TIME(DAYS)=',F8.4/20X,'OXYGEN',
      5' DEMAND BY HETEROTROPHS(KG O2/DAY)=',E13.5/20X,'OXYGEN DEMAND ',
      6'IN CASE OF NITRIFICATION(KG O2/DAY)=',E13.5)
       WRITE(6,1005) XR
1005   FORMAT(20X,'RETURN MICROBIAL CONCENTRATION(MG/L)=',E13.5)
       WRITE(6,1010)
1010   FORMAT(//20X,'DESIGNED VALUES OF THE SECONDARY CLARIFIER')
       WRITE(6,1020) AREAS,FLUX,TRDPTH,DTIME1
1020   FORMAT(/20X,'AREA OF THE SECONDARY CLARIFIER(M**2)=',E13.5,/20X,
      1'FLUX IN LB/FT**2.DAY=',F8.4/20X,'TOTAL DEPTH OF THE SECONDARY ',
      2'CLARIFIER(FEET)=',F8.4/20X,'DETENTION TIME(HOURS)=',F8.4)
       WRITE(6,1030)
1030   FORMAT(//20X,'ALTERNATE APPROACH FOR SECONDARY CLARIFIER')
       WRITE(6,1040) VOLS,AREAA,DTIME2,QII,THETAD,VD
1040   FORMAT(/20X,'VOLUME OF SECONDARY CLARIFIER(M**3)=',E13.5/,
      120X,'AREA OF THE SECONDARY CLARIFIER(M**2)=',E13.5/20X,
      2'DETENTION TIME OF THE SECONDARY CLARIFIER(HOURS)=',F8.4/////20X,
      3 'DIGESTER INFLOW(M**3/HR)=',F8.4/20X,'DIGESTER DETENTION TIME=',
      4 F8.4/20X,'VOLUME OF THE DIGESTER(M**3)=',E13.5////)
995    RETURN
       END
       FUNCTION FMAX(ARRAY,N)
C
C
C      TO CALCULATE THE MAXIMUM OF NUMBERS
       DIMENSION ARRAY(1)
       FMAX=ARRAY(1)
       DO 10 I=2,N
       IF(ARRAY(I).LT.FMAX) GO TO 10
       FMAX=ARRAY(I)
10     CONTINUE
       RETURN
       END
```

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      FUNCTION TSS(TIME)
C
C
      DIMENSION A(5),B(5),C(5)
      DATA A/0.0,-6.96097E-02,-.176173,.14660,-9.67005E-02/,
     1 B/0.0,2.60089E-02,-.274343,4.09673E-02,2.49002E-02/,
     2 C/1.,2.,7.,14.,21./,F/3.73999E-02/
C      A(1)=-.154903,B(1)=0.127113
      TSS=1.0
      DO 10 I=1,5
      THETA=F*C(I)*TIME
10    TSS=TSS+A(I)*COS(THETA)+B(I)*SIN(THETA)
      RETURN
      END
      FUNCTION FLOW(TIME)
C
C
      DIMENSION A(5),B(5),C(5)
      DATA A/0.0,5.41989E-02,-.036769,-.052324,.0618556/,B/0.0,
     1 -1.3742E-03,2.57417E-02,-.201479,.155797/,C/1.,2.,5.,7.,14./,
     2 F/.0373999/
C      A(1)=.00294,B(1)=.0807689
C      DELETE THE FIRST TERM FOR ONE DAY PERIOD
      FLOW=1.0
      DO 10 I=1,5
      THETA=F*TIME*C(I)
10    FLOW=FLOW+A(I)*COS(THETA)+B(I)*SIN(THETA)
      RETURN
      END
      FUNCTION VBOD(TIME)
C
C
C      REMOVE THE FIRST TERM FOR ONE DAY PERIOD
C      A(1)=-1.36395E-01,B(1)=5.06542E-02
      DIMENSION A(5),B(5),C(5)
      DATA A/0.0,-8.15218E-02,-1.03362E-02,8.60951E-02,
     1-7.21783E-03/,B/0.0,1.236415E-01,-3.52977E-01,4.15623E-02,
     2-5.26710E-02/,C/1.,2.,7.,14.,21./,F/3.7399E-02/
      VBOD=1.0
      DO 10 I=1,5
      THETA=F*C(I)*TIME
10    VBOD=VBOD+A(I)*COS(THETA)+B(I)*SIN(THETA)
      RETURN
      END
      FUNCTION VSNH4(TIME)
C
C
      DIMENSION A(3),B(3),C(3)
      DATA A/-0.0794,0.0057,-0.0634/,B/-0.2996,-0.059,-0.0976/
      DATA C/1.,2.,3./,F/0.26179/
      VSNH4=1.0
      DO 10 I=1,3
      THETA=F*C(I)*TIME
```

```
10        VSNH4=VSNH4+A(I)*COS(THETA)+B(I)*SIN(THETA)
          RETURN
          END
           FUNCTION SVS(S)
C
C
C         SVS IS IN CMS/HR
          DATA A/.521753E-07/,B/.834793E-02/,D/-.103521E-01/,E/.419438E-02/
          C=S/1420.
          SVS=SQRT(231.37/(A+B*C+D*C**2+E*C**3))
          RETURN
          END
          SUBROUTINE PSD1(XEFFP,LENGTH,POFR,FLOW,HEIGHT,AREAPC,SSIN)
C
C         DETERMINATION OF EFFLUENT SOLIDS CONCENTRATION FROM PRIMARY
C         SEDIMENTATION TANK. EMPIRICAL EQUATIONS ARE DEVELOPED
C         USING THE SIMULATED DATA FORM THE ADVECTION-DIFFUSION
C         EQUATION OF PRIMARY SEDIMENTATION.
C
          REAL LENGTH
          DATA BO/10.898/,B1/-.0024733/,B2/.00861/,B3/.00849/,
        1 B4/.64623/,B5/-.95693E-03/,WIDTH/14.36/
C
C         FLOW IS IN M**3/HR
C         OVEL: PRIMARY CLARIFIER OVERFLOW RATE, M**3/M**2 DAY
C         WIDTH IS IN METERS, LENGTH IS IN CMS, AND HEIGHT IS IN METERS.
C         1 M**3/M**2/DAY = 24.5424 GALLONS/FT**2/DAY
C
          LENGTH=(AREAPC/WIDTH)*100.
          OVEL=POFR/24.5424
          HIGHT=HEIGHT*100.
          XEFFP=BO+B1*FLOW+B2*HIGHT+B3*LENGTH+B4*OVEL+B5*OVEL*OVEL
          RE=(SSIN-XEFFP)/SSIN
          IF(RE.GT.0.20) GO TO 10
          XEFFP=(1.-RE)*SSIN
10        RETURN
          END
          SUBROUTINE DIGST1(Q4MT,TACID,BD1,BN1,S1,XNCD1,PVSSD,SRT,OLR,
        1 OLR1,VD,QIIIA,XAR,XPR,XSR,X1R,X2R,CXTPU,XIR,XNR,XNVO1,BDO1,
        2 NBDO1,XTRDI,IFLAGD)
C
C
C         TOTAL ACIDS, BIODEGRADABLE SOLIDS, NON-BIO-
C         DEGRADABLE SOLIDS, SOLUBLE SUBSTRATE, NON-VOLATILE SOLIDS,
C         TOTAL FLOW OF CH4, AND % OF VOLATILE SOLIDS DESTRUCTION
C         ARE OBTAINED FROM THE DYNAMIC MATHEMATICAL MODEL OF
C         OF ANAEROBIC DIGESTION. EMIPRICAL EQUATIONS ARE DEVELOPED
C         FROM THE RESULTS OF DYNAMIC MATHEMATICAL MODEL.
C
          REAL MLSSR1,MLSSR2,NBDO1
          DIMENSION CCO(7),CCS1(7),CCS2(7),CCO2(7),CCO3(7)
          DATA CCO/35.91026,173.12294,318.82495,18312.2,31.731,12691.33,
        1 0.73391/,CCS1/0.0,-2.91355,0.0,-182.01,0.0,-185.76,0.0/,
```

```
      2 CCS2/0.0,0.0,0.0,1.25352,-0.01381,1.2852,0.0/,
      3 CCO2/-133.61868,0.0,46971.,0.0,0.0,0.0,-1.9068/,
      4 CCO3/-153.28,28760.1,86034.8,-19720.,8303.14,-20174.42,-4.301/
        DATA CONBD/0.7/,CONNB/0.30/,CONNV/0.21/,CONVF1/16018.7/
        DATA ADFLO/41.617/
        FACT1=QIIIA/ADFLO
        IF(IFLAGD.EQ.2) GO TO 10
        MLSSR1=XAR+XPR+XSR+X1R+X2R
        MLSSR2=MLSSR1+XIR+CXTPU+XNR
        BDO1=(XTRDI*(MLSSR1+CONBD*CXTPU))/MLSSR2
        NBDO1=XTRDI*((XIR+CONNB*CXTPU)/MLSSR2)
        XNVO1=XTRDI*((XNR+CONNV*CXTPU)/MLSSR2)
   10   IF(QIIIA.EQ.0.0) GO TO 110
        SRT=VD/(QIIIA*24.)
        VBNBI=NBDO1-XNVO1
        VSSIN=BDO1+VBNBI
C       OLR: ORGANIC LOADING RATE IN GRAMS/M**3 DAY
C       OLR1: ORGANIC LOADING RATE IN LBS/FT**3 DAY
        OLR=VSSIN*QIIIA*24./VD
        OLR1=OLR/CONVF1
        OLR2=OLR1*OLR1
        OLR3=OLR2*OLR1
        SRT2=SRT*SRT
        GO TO 120
  110   WRITE(6,1000)
 1000   FORMAT(/2X,' RUNNING AVERAGE OF UNDERFLOW FROM THICKENER=0.0')
  120   Q4MT=(CCO(1)+CCS1(1)*SRT+CCS2(1)*SRT2+CCO2(1)*OLR2
      1       +CCO3(1)*OLR3)*FACT1
        IF(Q4MT.LE.0.0) Q4MT=0.0
        TACID=CCO(2)+CCS1(2)*SRT+CCS2(2)*SRT2+CCO2(2)*OLR2
      1       +CCO3(2)*OLR3
        BD1=CCO(3)+CCS1(3)*SRT+CCS2(3)*SRT2+CCO2(3)*OLR2
      1       +CCO3(3)*OLR3
        BN1=CCO(4)+CCS1(4)*SRT+CCS2(4)*SRT2+CCO2(4)*OLR2
      1       +CCO3(4)*OLR3
        S1=CCO(5)+CCS1(5)*SRT+CCS2(5)*SRT2+CCO2(5)*OLR2
      1       +CCO3(5)*OLR3
        XNCD1=CCO(6)+CCS1(6)*SRT+CCS2(6)*SRT2+CCO2(6)*OLR2
      1       +CCO3(6)*OLR3
        IF(QIIIA.EQ.0.0) PVSSD=0.7
        PVSSD=CCO(7)+CCS1(7)*SRT+CCS2(7)*SRT2+CCO2(7)*OLR2
      1       +CCO3(7)*OLR3
        RETURN
        END
        SUBROUTINE SICOND(TSSI,BOD5,SRT,XAI1,XAI2,XAI3,XSI1,XSI2,XSI3,
      1XPI1,XPI2,XPI3,XII1,XII2,XII3,XNI1,XNI2,XNI3,X1I1,X1I2,X1I3,
      2X2I1,X2I2,X2I3,XTI1,V,THETAH)
C
C       EMPIRICAL EQUATIONS DEVELOPED USING THE SIMULATED DATA, CSMPIII.
C
        TSS=TSSI*0.40
        BOD=BOD5*0.55
        BOD2=BOD*BOD
```

```
         SRTT=SRT*TSS
         SRT2=SRT*SRT
         SRT3=SRT*SRT*SRT
         TXA=-1242397.+209788.625*SRT+16574.043*TSS-249.2727*SRT3
        1    +1200.9294*SRTT
         TXP=-1844901.+450681.9375*SRT+23641.293*TSS-436.2693*SRT3
        1    +3756.8967*SRTT
         TXI=1214202.+7254.95703*SRTT
         TXS=-95607.+13635.207*SRT+2881.7236*TSS-14.951*SRT3
        1    +58.41995*SRTT
         TXN=1220917.+4413.207*SRTT
         IF(SRT.LE.10.) GO TO 10
         TX1=-15437.7695+5950.82031*SRT
         TX2=-2294.85156+31.29755*SRT2+2.85385*SRTT
         GO TO 20
   10    TX1=0.0
         TX2=0.0
   20    TXT=-8428608.+1090400.*SRT+99631.125*TSS-1052.4563*SRT3
        1    -42.86723*BOD2+11677.16797*SRTT
         RECV=6./(V*THETAH)
         XAI1=TXA*RECV
         XPI1=TXP*RECV
         XSI1=TXS*RECV
         XII1=TXI*RECV
         XNI1=TXN*RECV
         X1I1=TX1*RECV
         X2I1=TX2*RECV
         XTI1=TXT*RECV
         XAI2=XAI1
         XAI3=XAI1
         XPI2=XPI1
         XPI3=XPI1
         XSI2=XSI1
         XSI3=XSI1
         XII2=XII1
         XII3=XII2
         XNI2=XNI1
         XNI3=XNI1
         X1I2=X1I1
         X1I3=X1I1
         X2I2=X2I1
         X2I3=X2I1
         RETURN
         END
         SUBROUTINE COST(CCOST,OM,VOPC,OURTA,OCRT,BDPBN2,
        1QO,V,AREAP,BCAP,A3,AGT,QR1,QI,Q4MT,QIIIA,VD,CKWH,COL,
        2CSD,DHR,HEAD,VOPC1,EFFG)
   C
   C     CCOST  : CAPITAL COST ($)
   C     OHRS   : OPERATION MAN-HOUR REQUIREMENT, MAN-HOUR/YEAR,
   C     XMHRS  : MAINTENANCE MAN-HOUR REQUIREMENTS, MAN-HOUR/YEAR,
   C     TMSU   : TOTAL MATERIAL AND SUPPLY COSTS($),
   C     EER    : ELECTRICAL ENERGY REQUIRED, KWH/YEAR,
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C     VOPC   : VARIABLE OPERATING COSTS($).
C     INDEX1 : CONSTRUCTION COST INDEX (UPDATING FROM 1969 TO 1984)
C     INDEX2 : MATERIAL AND SUPPLY COSTS INDEX( UPDATING FROM
C              1969 TO 1984
C
C
C     COST FUNCTIONS FOR UNIT PROCESSES
C
      DIMENSION P1(11),P2(11),P3(11),P4(11),P5(11),U1(11),U2(11),
     1 U3(11),U4(11),U5(11),R1(11),R2(11),R3(11),R4(11),R5(11),S1(11),
     2 S2(11),S3(11),S4(11),S5(11),T1(11),T2(11),T3(11),T4(11),T5(11),
     3 CCOST(11),X(11),OHRS(11),XMHRS(11),TOMMH(11),TMSU(11),EER(11),
     4 EERMS(11),EER1(11),OM(11)
      REAL INDEX1, INDEX2
C.
C             DATA FOR COST FUNCTIONS
C
      DATA P1/3.259716,3.716354,2.41438,4.14884,0.0,3.716354,7.679634,
     13.725902,3.481553,-1.4455,0.0/,P2/.619151,.389861,.175682,.713634,
     20.0,.389861,-1.949689,.39769,.377485,2.33858,0.0/,P3/0.0,.08456,
     33.084742,-.052596,0.0,.08456,.402561,.075742,.093349,-.382633,
     440.0/,P4/0.0,-.004718,-.00267,.0147487,0.0,-.004718,-.018211,
     5-.001977,-.006222,.025888,0.0/,P5/0.0,0.0,0.0,0.0,0.0,0.0,0.0,
     6-.000296,0.0,0.0,0.0/
      DATA U1/6.39872,5.846565,0.0,6.900586,0.0,5.846565,9.12925,
     15.846565,6.097269,4.36501,0.0/,U2/.230956,.258413,0.0,.323725,
     20.0,0.0,-1.816736,.254813,.253066,.7038535,0.0/,U3/.164959,
     3.113703,0.0,.059093,0.0,.113703,.373282,.113703,-.193659,
     4.0422545,0.0/,U4/-.014601,-.010942,0.0,-.004926,0.0,-.010942,
     5-.017429,-.010942,.078201,-.0019301,0.0/,U5/0.0,0.0,0.0,0.0,0.0,
     60.0,0.0,0.0,0.0,-.00668,0.0,0.0/
      DATA R1/5.846098,5.273419,0.0,6.169937,0.0,5.273419,8.566752,
     15.273419,5.911541,1.83957,0.0/,R2/.206513,.228329,0.0,.294853,
     20.0,.228329,-1.768137,.228329,-.013158,1.683691,0.0/,R3/.068842,
     3.122646,0.0,.175999,0.0,.122648,.363173,.122646,.076643,-.231481,
     40.0/,R4/.023824,-.011672,0.0,-.040947,0.0,-.011672,-.01662,
     5-.011672,0.0,.014133,0.0/,R5/-.00441,0.0,0.0,.0033,0.0,0.0,0.0,
     60.0,0.0,0.0,0.0/
      DATA S1/7.235657,5.669881,0.0,0.0,0.0,5.669881,8.702803,5.669881,
     15.051743,31.17094,.62138/,S2/.399935,.750799,0.0,0.0,0.0,.750799,
     2-1.182711,.750999,.30161,-15.22357,.482047/,S3/-.224979,0.0,0.0,
     30.0,0.0,0.0,.282691,0.0,.197183,3.07994,0.0/,S4/.110099,0.0,0.0,
     40.0,0.0,0.0,-.013672,0.0,-.017962,-.195488,0.0/,S5/-.011026,0.0,
     50.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0/
      DATA T1/6.30864,11.0736,0.0,0.0,-12.1285,5.97902,12.43648,
     1-12.5085,0.0,0.0,0.0/,T2/.234529,-1.25742,0.0,0.0,10.98686,
     2.377519,-2.089456,6.72116,0.0,0.0,0.0/,T3/-.0358436,.168361,
     30.0,0.0,-2.028497,.011379,.28,-.74406,0.0,0.0,0.0/,
     4T4/.008712,-.0046671,0.0,0.0,.171772,-.000841,-.0083527,
     5.0305456,0.0,0.0,0.0/,T5/0.0,0.0,0.0,0.0,-.0051743,0.0,0.0,
     60.0,0.0,0.0,0.0/
C
C     X(1) : FLOW THOROUGH THE SCREEN AND GRIT CHAMBER, MGD
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C     X(5) : OXYGEN REQUIREMENTS, LBS/DAY
C     OCRT : OXYGEN REQUIREMNETS, GMS/HR
C     BCAP : INITIAL FIRM BLOWER CAPACITY, 1000 CFM
C     X(9) : RECIRCULATION AND INTERMEDIATE PUMPING, MGD,
C     X(10): SLUDGE FLOW FROM THE PRIMARY SEDIMENTATION TANK, GPM
C     X(11): FLOW IN MGD (FOR TMSU OF AERATION TANK),
C     AREAP: SURFACE AREA OF THE PRIMARY SEDIMENTATION TANK, M**2
C     V    : VOLUME OF THE AERATION TANK, M**3
C     A3   : SURFACE AREA OF THE SECONDARY CLARIFIER, M**2
C     VD   : VOLUME OF THE DIGESTER, M**3
C     AGT  : SURFACE AREA OF THE GRAVITY THICKENER, M**2
C     QR1  : RECYCLE FLOW, M**3/HR
C     QI   : SLUDGE FLOW FROM THE PRIMARY SEDIMENTATION TANK, M**3/HR
C
      NCE=5
      CONST1=10.7639/1000.
      CONST2=35.3147/1000.
      CONST3=1.0E03*24./(3.785*1.0E06)
      CONST4=365.*24.
      CONST5=2000.*453.6
      INDEX1=3.9936
      INDEX2=2.9826
      BCAP=0.00232*OCRT/1000.
      X(1)=ALOG(QO*CONST3)
      X(2)=ALOG(AREAP*CONST1)
      X(3)=ALOG(V*CONST2)
      X(4)=ALOG(BCAP)
      X(5)=ALOG(OURTA*24.*1000./453.6)
      X(6)=ALOG(A3*CONST1)
      X(7)=ALOG(VD*CONST2)
      X(8)=ALOG(AGT*CONST1)
      X(9)=ALOG(QR1*CONST3)
      IF(QI.LE.1.0) GO TO 14
      X(10)=ALOG(QI*1.0E03/(3.785*60.))
14    X(11)=ALOG(QO*CONST3)
      EER(3)=0.0
      EER(4)=0.0
      EER(11)=0.
      TMSU(4)=0.0
      NC1=NCE+6
      DO 10 I=1,NC1
      IF(VD.LT.566.33.AND.I.EQ.7) GO TO 21
      CCOST(I)=(EXP(P1(I)+P2(I)*X(I)+P3(I)*X(I)*X(I)+P4(I)*(X(I)**3)
     1 +P5(I)*(X(I)**4))*1000.)*INDEX1
      GO TO 22
21    CCOST(7)=EXP(4.594215+.127244*X(7)-.004001*X(7)*X(7))*1000.
     1             *INDEX1
22    IF(I.EQ.3) GO TO 15
      IF(VD.LT.566.33.AND.I.EQ.7) GO TO 23
      OHRS(I)=EXP(U1(I)+U2(I)*X(I)+U3(I)*X(I)*X(I)+U4(I)*(X(I)**3)
     1 +U5(I)*(X(I)**4))
      XMHRS(I)=EXP(R1(I)+R2(I)*X(I)+R3(I)*X(I)*X(I)+R4(I)*(X(I)**3)
     1 +R5(I)*(X(I)**4))
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        TOMMH(I)=(OHRS(I)+XMHRS(I))*DHR
        IF(I.EQ.11) GO TO 110
        TMSU(I)=(EXP(S1(I)+S2(I)*X(I)+S3(I)*X(I)*X(I)+S4(I)*(X(I)**3)
       1 +S5(I)*(X(I)**4)))*INDEX2
        GO TO 25
23      OHRS(7)=EXP(6.163803+.166305*X(7)-.01247*X(7)*X(7))
        XMHRS(7)=EXP(5.726981+.113674*X(7))
        TOMMH(7)=(OHRS(7)+XMHRS(7))*DHR
        TMSU(7)=EXP(6.531623+.198417*X(7)+.02166*X(7)*X(7))*INDEX2
        GO TO 25
110     TMSU(I)=(EXP(S1(I)+S2(I)*X(I)+S3(I)*X(I)*X(I)+S4(I)*(X(I)**3)
       1 +S5(I)*(X(I)**4))*1000.)*INDEX2
        GO TO 95
25      IF(I.EQ.4) GO TO 95
        IF(I.EQ.9) GO TO 30
C       FOR THE CALULATION OF ELECTRICAL ENERGY REQUIRED, KWH/YR
C       DIGESTER VOLUME(FT**3) , MECHANICAL MIXING(1/2 HP
C       1000 FT**3), THICKENER AREA (FT**2), AND SECONDARY CLARIFIER
C       (FT**2)
        IF(I.EQ.6) X(I)=ALOG(A3*10.7639)
        IF(I.EQ.7) X(I)=ALOG(VD*35.3147)
        IF(I.EQ.8) X(I)=ALOG(AGT*10.7639)
        IF(I.EQ.10) GO TO 30
        EER(I)=EXP(T1(I)+T2(I)*X(I)+T3(I)*X(I)*X(I)+T4(I)*(X(I)**3)
       1 +T5(I)*(X(I)**4))*CKWH
        GO TO 95
30      IF(I.EQ.10) QR1=QI
        IF(QR1-1.44) 72,74,74
72      PEFF=0.7
        GO TO 80
74      IF(QR1-10.08) 76,78,78
76      PEFF=0.74
        GO TO 80
78      PEFF=0.83
C
C       YKWPY : KWH/YR
C
80      YKWPY=(QR1*1.0E06*62.4*1.03*HEAD*.7437*365.)/(7.48*24.*3600.
       1 *550.*PEFF)
        EER(I)=YKWPY*CKWH
        IF(I.GT.1) GO TO 95
        EERMS(I)=EXP(7.14972+.288558*X(I)-.078864*X(I)*X(I)+.014662*
       1 (X(I)**3))*CKWH
        EER1(I)=EER(I)+EERMS(I)
95      IF(I.EQ.5) OM(I)=(TOMMH(I)+TMSU(I))
        OM(I)=(TOMMH(I)+TMSU(I)+EER(I))
        IF(I.EQ.4) OM(I) = TOMMH(I)+TMSU(11)+EER(I)
        IF(I.EQ.5) GO TO 15
        IF(I.EQ.11) GO TO 15
        GO TO 10
15      OHRS(I)=0.0
        XMHRS(I)=0.
        TOMMH(I)=0.0
```

```
          TMSU(I)=0.0
10        CONTINUE
          CCOST(5)=0.0
          CCOST(11)=0.0
          OM(11) =0.0
          OM(3)=0.0
          X1=ALOG(QO*CONST3)
C
C         CAPITAL COST FOR ADMINISTRATION AND LABORATORY FACILITIES, $1000
C
          CCOSTA=EXP(3.55928+.350947*X1+.08306*X1*X1 -.009318*X1*X1*X1)
      1 *1000.
C         CLAND : COST OF TOTAL LAND REQUIRED.
C         COL   : COST OF LAND/ACRE
          CLAND=EXP(2.322414+.1879797*X1+.04151*X1*X1+.0023517*X1*X1*X1)
      1  *COL
          TCST1=0.0
          DO 200 I=1,NC1
200       TCST1=TCST1+CCOST(I)
          TCST=TCST1/1000.
C
C         TCST : TOTAL CONSTRUCTION COST, $1000
          X2=ALOG(TCST)
C
C         ECOST : ENGINEERING COST
          ECOST=EXP(.6654462+.44256*X2+.023343*X2*X2-.0001259*X2*X2*X2)
      1*1000.
C
C         TCOST : TOTAL CONSTRUCTION, ENGINEERING AND LAND COSTS
C         TCOST : ALL CONSTRUCTION COSTS+ECOST+CLAND
C         ADMNC : LEGAL, FISCAL AND ADMINISTRATION COSTS
C         CSLUDG : COST OF SLUDGE DISPOSAL
C
          TCOST=TCST1+ECOST+CLAND
          TCOST1=TCOST/1000.
          X3=ALOG(TCOST1)
          ADMNC=EXP(-1.23038+.313308*X3+.0691976*X3*X3-.004646*X3*X3*X3)
      1*1000.
C         ENERGY FROM GAS, BTU/FT**3
C         35.3147  :  CONVERSION FROM M**3 TO FT**3
C         2.9037* E-04 : CONVERSION FROM HP TO KWH (1./550*7.48*0.83)
C         0.83 IS THE EFFICIENCY
          WRITE(6,1000)
1000  FORMAT(//10X,'CAPITAL COSTS ($)')
          WRITE(6,1010) CCOST(1),CCOST(2),CCOST(3),CCOST(4),CCOST(6),
      1CCOST(7),CCOST(8),CCOST(9),CCOST(10)
1010  FORMAT(/5X,'PRIMARY TREATMENT(SCREENING, GRIT REMOVAL, AND',
      $' FLOW MEASUREMENTS)=',E15.5/5X,
      $'PRIMARY CLARIFIER=',48X,E15.5/5X,'AERATION TANK=',52X,E15.5/5X,
      $'DIFFUSERS=',56X,E15.5/5X,'SECONDARY CLARIFIER=',46X,E15.5/5X,
      $'DIGESTER=',57X,E15.5/5X,'THICKENER=',56X,E15.5/5X,
      $'RECIRCULATION AND MIXING PUMPS=',35X,E15.5/5X,
      $'SLUDGE PUMPS=',53X,E15.5)
```

```
          WRITE(6,1020)
1020   FORMAT(//10X,'OPERATION AND MAINTENANCE COSTS($/YR)')
          WRITE(6,1030) OM(1),OM(2),OM(4),OM(5),OM(6),OM(7),OM(8),
       $OM(9),OM(10)
1030   FORMAT(/5X,'PRIMARY TREATMENT=',48X,E15.5/5X,
       $'PRIMARY CLARIFIER=',48X,E15.5/5X,
       $'AERATION (EXCLUDING ENERGY COST)=',33X,E15.5/5X,
       $'DIFFUERS=',57X,E15.5/5X,'SECONDARY CLARIFIER=',46X,E15.5/5X,
       $'DIGESTER=',57X,E15.5/5X,'THICKENER=',56X,E15.5/5X,
       $'RECIRCULATION AND INTERMIDIATE PUMPING=',27X,E15.5/5X,
       $'SLUDGE PUMPING=',51X,E15.5)
          CQCH4=(Q4MT*35.3147*550.*2.9307*1.E-04*CKWH)*EFFG*CONST4
          IF(QIIIA.EQ.0.0) QIIIA=1.35
          CSLUDG=(QIIIA*BDPBN2*CSD*CONST4/CONST5)
          VOPC=EER(5)-CQCH4
          VOPC1=CSLUDG
          WRITE(6,1040)
1040   FORMAT(//10X,'VARIABLE OPERATING COSTS($/YR)')
          WRITE(6,1050) VOPC,CSLUDG,CQCH4
1050   FORMAT(/5X,'ENERGY COST (AERATION)=',43X,E15.5/5X,
       $'SLUDGE DISPOSAL COST=',45X,E15.5/5X,
       $'REVENUE FROM METHANE GAS=',41X,E15.5)
          TOTLC=0.0
          DO 11 I=1,NC1
11        TOTLC=TOTLC+CCOST(I)+OM(I)
          TOTALC=TOTLC+VOPC+VOPC1
          WRITE(6,1060) TOTALC
1060   FORMAT(///5X,'TOTAL COSTS/YR=',51X,E15.5//////////)
          RETURN
          END
          SUBROUTINE OPTIM5(PARO,PARL,PARU,PADJ,C,ER,ERM,ND,ND2,NE,M,
       1 MM,MITER,IN,NN)
C.. THIS SUBROUTINE IS THE MAIN CALL TO THE OPTIMIZATION PROGRAMS.
C.. THE PARAMETERS IN THE CALL TO OPTIM ARE :
C        PARO = OLD VALUE OF THE PARMETERS ESTIMATES
C        PARL = LOWER CONSTRAINTS ON THE PARAMETERS
C        PARU = UPPER CONSTRAINTS ON THE PARAMETERS
C        PADJ = WEIGHTING FACTOR FOR EACH ERROR FUNCTION
C        PAR1 = NEW VALUE OF THE PARAMETER ESTIMATES
C        CC   = INFLUENCE COEFFICIENT ARRAY
C        ER   = ARRAY CONTAINING MODEL RESIDUALS AT ALL OBSERVATIONS
C        ERM  = UNWEIGHTED MODEL SUM OF SQUARES ERROR, BY ERROR FUNCTION
C        ND   = NUMBER OF PARAMETERS TO BE ESTIMATED
C        ND2  = ND*2
C        ND5  = 5*ND
C        ND5P1 = ND5+1
C        NE   = NUMBER OF ERROR FUNCTIONS
C        M    = NUMBER OF OBSERVATIONS
C        MM   = MAXIMUM NUMBER OF OBSERVATIONS
C        MITER= MODEL ITERATION NUMBER
C        ITERM= NUMBER OF ITERATIONS ALLOWED FOR THE QUADRATIC AND
C                PATTERN SEARCH ROUTINES
C        IN   = METHOD OF SEARCH 1 = LINEAR REGRESSION (NO CONSTRAINTS)
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C                2 = PATTERN SEARCH, AND 3 = QUADRATIC PROGRAMING
C          NN  = TYPE OF WEIGHTING MATRIX: 1 = IDENTITY MATRIX
C                2 = INVERSE OF COVARIANCE MATRIX OF ERRORS
C.. THE FOLLOWING ARRAYS ARE USED FOR THE PARAMETER CORRELATION
C   SUBROUTINE AND ARE DIMENSIONED IN THIS SUBROUTINE IN ORDER
C   TO AVOID DIMENSIONS IN THE CALLING PROGRAM
C   ARRAYS COVAR, HESS, AND CORR ARE DIMENSIONED (ND,ND,NE)
C   ARRAYS INDEX(NE),FACTOR(NE)
C   ARRAY LL(ND) (USED TWICE, IN THE OPTIMIZATION AND CORRELATION
C   PGMS). THE FOLLOWING GROUP OF ARRAYS USE DYNAMIC ALLOCATION
C   ARRAYS PARO,PARL,PADU,AND PARJ ARE DIMENSIONED IN THE
C   MAIN PROGRAM AT ND
        DIMENSION PARO(ND),PARL(ND),PARU(ND),PADJ(ND)
C.. ARRAY C IS THE INFLUENCE COEFFICIENT ARRAY AND IS DIMENSIONED
C.. NE BY ND BY MM IN THE MAIN PGM
        DIMENSION C(NE,ND,MM)
C.. ARRAY ER IS THE ERROR ARRAY AND IS DIMENSIONED MM BY NE IN THE MAIN
C   PGM. ERM IS THE UNWEIGHTED MODEL ERROR.
        DIMENSION ER(MM,NE),ERM(NE)
C************************************************************************
C.. THE NEXT GROUP OF ARRAYS MUST BE DIMENSIONED USING NUMERIC CONSTANTS
C   THOSE ARRAYS ARE USED BY THE OPTIMIZATION PROGRAMS
C.. ARRAYS PAR1, CQD,DD,LL AND BB MUST BE DIMENSIONED ND
        DIMENSION PAR1(5),CQD(5),DD(5),LL(5),BB(5),IPARM(5)
C.. ARRAYS CQC AND CC MUST BE DIMENIONED ND BY ND
        DIMENSION CQC(5,5),CC(5,5)
C..    ARRAY AA MUST BE DIMENSIONED ND BY ND2
        DIMENSION AA(5,10)
C.. ARRAYS QQ AND QA MUST BE DIMENIONED AT NE BY NE
        DIMENSION QQ(3,3),QA(3,3)
C.. ARRAY D MUST BE DIMENSIONED NE BY MM
        DIMENSION D(3,11)
C.. ARRAY WA6,IWA7 AND WA9 MUST BE DIMENSIONED ND2
        DIMENSION WA6(10),IWA7(10),WA9(10)
C.. ARRAY IWA8 MUST BE DIMENSIONED ND5 (ND5=5*ND)
        DIMENSION IWA8(25)
C.. ARRAY WA2,WA3,WA4 AND WA5 MUST BE DIMENSIONED ND5P1 (ND5P1=5*ND+1)
        DIMENSION WA2(26),WA3(26),WA4(26),WA5(26)
C.. ARRAY WA1 MUST BE DIMENSIONED ND2 BY ND5P1
        DIMENSION WA1(10,26)
C.. ARRAYS COVAR, HESS, COR MUST BE DIMENSIONED ND BY ND BY NE
        DIMENSION HESS(5,5,3),COVAR(5,5,3),COR(5,5,3)
C.. ARRAYS INDEX AND FACTOR  MUST BE DIMENSIONED NE
        DIMENSION FACTOR(3),INDEX(3)
C..    ARRAYS CENTER AND EROBFU MUST BE DIMENSIONED ND+1
        DIMENSION CENTER(6),EROBFU(6)
C..    ARRAY PARMS MUST BE DIMENSION ND BY ND+1
        DIMENSION PARMS(5,6)
        COMMON /DBUG/ IDEBG
        COMMON /IOPT/NROPT,NWOPT
        COMMON /IOSRC/NRISRC,NWISRC
        COMMON /IOCOR/NRICOR,NWICR
        COMMON /IOPRT/NRIPRT,NWIPRT
```

```
        DATA JUMP /0/
C*********************************************************************
C..     DETECT THE FIRST CALL TO THE SUBROUTINE AND WRITE A HEADING
        IF (JUMP) 10,10,160
10      JUMP=1
        NROPT=5
        NWOPT=6
        NWISRC=6
        NRISRC=5
        NWIPRC=6
        NRIPRC=5
        NWICOR=6
        NRICOR=5
        NREAD=5
        NWRITE=6
        WRITE(NWRITE,1000)
1000    FORMAT('1INFLUENCE COEFFICIENT OPTIMIZATION PROCEDURE BEGINNING')
        IF(IN.GT.0.AND.IN.LT.4) GOTO 20
        WRITE(NWRITE,1010) IN
1010    FORMAT(' *** ERROR *** METHOD CODE OUT OF RANGE *** ERROR ***',
     1/,'IN=',I5,/,' EXECUTION TERMINATING ')
        STOP 10
20      IF(NN.GT.0.AND.NN.LT.3) GOTO 30
        WRITE(NWRITE,1020) NN
1020    FORMAT(' *** ERROR *** WEIGHTING CODE OUT OF RANGE *** ERROR ***',
     1/,' NN=',I5,/,' EXECUTION TERMINATING')
        STOP 20
C.. WRITE OUT THE HEADINGS
30      GOTO(40,50,60),IN
40      WRITE(NWRITE,1030)
1030    FORMAT(' NORMAL EQUATION SOLUTION SELECTED (NO CONSTRAINTS)')
        GOTO 70
50      WRITE(NWRITE,1040)
1040    FORMAT(' CONSTRAINED PATTERN SEARCH METHOD SELECTED')
        GOTO 70
60      WRITE(NWRITE,1050)
1050    FORMAT(' QUADRATIC PROGRAMING (WOLF ALGORITHM) SELECETED')
70      GOTO (80,90),NN
80      WRITE(NWRITE,1060)
1060    FORMAT(' IDENTITY ERROR WEIGHTING MATRIX SELECTED')
        GOTO 100
90      WRITE(NWRITE,1070)
1070    FORMAT('0INVERSE OF THE ERROR COVARIANCE MATRIX SELECTED')
C.. CALCULATE THE MAXIMUM NUMBER OF ITERATIONS FOR THE INFLUENCE
C    OPTIMIZATION
100     ITERM=20
C.. IF THE PATTERN SERARCH IS SELECTED RECALCULTATE ITERM
        IF(IN.EQ.2) ITERM=ND*150
C.. WRITE OUT THE REST OF THE SUMMARY
        WRITE(NWRITE,1080) ND,NE,M,ITERM
1080    FORMAT(///,' NUMBER OF PARAMETERS=            ',I5,
     1/,         ' NUMBER OF ERROR FUNCTIONS        ',I5,
     2/,         ' NUMBER OF DATA POINTS=           ',I5,
```

```
               3/,               ' MAXIMUM NUMBER OF ITERATIONS',
               4/,                 ' FOR THE INFLUENCE OPTIMIZATION= ',I5,//)
C.. SKIP CHECKING FOR CONSTRAINTS IF THE METHOD CODE = 1
C   (UNCONSTRAINED LINEAR REGRESSION)
         IF(IN.EQ.1) GOTO 140
C.. CHECK TO MAKE SURE THAT THE LOWER CONTRAINTS ARE LESS THAN
C   THE UPPER CONSTRAINTS; OTHERWISE AN INFINITE LOOP WILL BE
C   GENERATED IN THE OPTIMIZATION ROUTINES
         DO 110 I=1,ND
         IF(PARL(I).GE.PARU(I)) GOTO 120
110      CONTINUE
         GOTO 124
120      WRITE(NWRITE,1090) PARL(I), I, PARU(I)
1090     FORMAT(///,' ***** ERROR *****',/, ' THE LOWER CONTRAINT(',
      1E17.6,' ) FOR PARMATER NO.',I2,' IS GREATER THAN OR EQUAL TO',
      2' THE UPPER CONSTRAINT(',E17.6,' )')
C..      CHECK TO MAKE SURE THE INITIAL PARAMETER SET IS FEASIBLE
124      DO 130 I=1,ND
         IF(PARO(I)-PARL(I)) 127,125,125
125      IF(PARO(I)-PARU(I)) 130,130,127
127      WRITE(6,1100) I,PARL(I),PARU(I),PARO(I)
1100     FORMAT(' **** ERROR ****',/,' PARAMETER NO.',I3,' IS EITHER LESS',
      1' THAN THE LOWER CONSTRAINT (',E17.6,')',/,' OR GREATER THAN THE '
      2,' UPPER CONSTRAINT(',E17.6,')',/,' PARMETER=',E17.6)
         STOP 50
130      CONTINUE
         WRITE(6,1102)
1102     FORMAT(//,
      1'                        CONSTRAINTS SUMMARY',/,
      2' PARAMETER NUMBER  LOWER LIMIT    STARTING VALUE    UPPER LIMIT',
      3/,1X,63('-'))
         DO 128 I=1,ND
128      WRITE(6,1103) I,PARL(I),PARO(I),PARU(I)
1103     FORMAT(8X,I2,3(3X,E12.5))
C.. THIS CALL TO CORDUM IS FOR DYNAMIC ARRAY ALLOCATION
140      CALL CORDUM(ERM,C,HESS,COVAR,COR,CC,FACTOR,INDEX,LL,IPARM,
      1ND,NE,M,MM)
C.. THE PAR1 ARRAY REQUIRES INITILIZATION AND IS CHECKED IN SUBROUTINE
C   WOLFE
         DO 150 I=1,ND
150      PAR1(I)=PARO(I)
         ND5=ND2+ND2+ND
         ND5P1=ND5+1
         NDP1=ND+1
160      CONTINUE
C.. WRITE OUT THE MODEL ERROR
         SUM =0.
         DO 170 I=1,NE
170      SUM=SUM+ERM(I)
         WRITE(NWRITE,1110) MITER,((I,ERM(I)),I=1,NE)
1110     FORMAT('0UNWEIGHTED MODEL SUM OF SQUARE ERRORS FOR MODEL ITERAT',
      1'ION NUMBER ',I2,/,'0ERROR FUNCTION',7X,'ERROR',
      210(/,7X,I2,6X,E12.5))
```

```
      WRITE(NWRITE,1120) SUM
1120  FORMAT(' TOTAL ERROR=   ',E12.5)
      CALL TRANSF(C,ER,PARO,PARL,PARU,PADJ,QQ,QA,LL,D,CQC,CQD,AA,BB,CC,
     1DD,EE,NE,ND,ND2,M,MM,IN,NN)
      GO TO (180,190,200),IN
180   CALL LREGRE(CC,DD,EE,PAR1,LL,CQC,ND)
      GO TO 210
C.. THIS ENTRY IS TO THE PATTERN SEARCH BECAUSE WOLFE FAILS
C.. THE NUMBER OF ITERATIONS MUST BE INCREASED AND RESET
185   ITERMS=ITERM
      ITERM=200*ND
190   CALL PATSRC(PARL,PARU,PARO,PAR1,PADJ,C,ER,QA,FACTOR,ND,NDP1,NE,MM,
     1ITERM,M,PARMS,EROBFU,CENTER,EE)
      IF(IFAULT.GT.0) ITERM=ITERMS
      GO TO 210
200   CALL WOLFE(PARL,PAR1,AA,BB,CC,DD,EE,WA1,WA2,WA3,WA4,WA5,WA6,IWA7,
     1 IWA8,WA9,ND,ND,ND2,ND5,ND5P1,ITERM,IDEBG,IFAULT)
C.. CHECK FOR NON-CONVERGENCE OF THE WOLFE ALGORITHM AND CHANGE
C   TO PATTERN SEARCH FOR THIS ITERATION ONLY IF UNCONVERGED
      IF(IFAULT.GT.0) GOTO 185
210   WRITE(NWRITE,1130) (I,I=1,ND)
      WRITE(NWRITE,1140) (PAR1(I),I=1,ND)
      WRITE(NWRITE,1150) EE
1130  FORMAT(/,' NEW PARAMETER ESTIMATES',/,10(5X,I2,5X),/)
1140  FORMAT(1X,8E12.5)
1150  FORMAT(/,' LINEARIZED OBJECTIVE VALUE=',E13.5,/)
C.. REPLACE THE NEW PARAMETERS IN THE OLD PARAMETER ARRAY
      DO 220 I=1,ND
220   PARO(I)=PAR1(I)
      RETURN
      END
      SUBROUTINE CORDUM(ER,C,HESS,COVAR,COR,ARED,FACTOR,INDEX,LL,IPARM,
     1ND,NE,M,MM)
C.. THIS ENTRY IS USED TO SET-UP THE DYNAMIC DIMENSION ALLOCATIONS
      DIMENSION COVAR(ND,ND,NE),HESS(ND,ND,NE),COR(ND,ND,NE),LL(ND),
     1ARED(ND,ND),IPARM(ND),INDEX(NE),FACTOR(NE),ER(NE),C(NE,ND,MM)
      COMMON /DBUG/ IDEBUG
      COMMON /IOCOR/NREAD,NWRITE
      RETURN
      ENTRY  CORREL(ER,C,ND,NE,M,MM)
C.. CALCULATE HESSIAN MATRIX OF THE ESTIMATES OF PARAMETERS FOR EACH
C   CONCENTRATION PROFILE FUNCTION
      IFIN=0
      NEO=NE
5     DO 200 II=1,NEO
      INDEX(II)=0
      FACTOR(II)=0.
      DO 10 L=1,ND
      LL(L)=0
      DO 10 K=1,ND
      COR(K,L,II)=0.
      COVAR(K,L,II)=0.
10    HESS(K,L,II)=0.0
```

```
          DO 20 J=1,M
          DO 20 K=1,ND
          DO 20 L=K,ND
   20     HESS(K,L,II)=HESS(K,L,II)+C(II,K,J)*C(II,L,J)
          DO 30 I=2,ND
          I1=I-1
          DO 30 J=1,I1
   30     HESS(I,J,II)=HESS(J,I,II)
          IF(IDEBUG) 60,60,40
C.. WRITE OUT THE HESSIAN MATRIX IF IDEBUG IS TURNED ON
C.. FIRST INITIALIZE THE ARRAY CONTAINING THE PARAMETER NUMBERS
   40     DO 50 I=1,ND
   50     IPARM(I)=I
          WRITE(NWRITE,1000) II
 1000     FORMAT(///,' HESSIAN MATRIX FOR ERROR PROFILE NO ',I2,///)
          CALL PRINTA(HESS,IPARM,II,ND,ND,NE)
C..   CALCULATE COVARIANCE AND CORRELATION MATRIX OF THE ESTIMATES OF
C     PARAMETERS FOR EACH CONCENTRATION PROFILE FUNCTION
   60     DO 70 I=1,ND
   70     COVAR(I,I,II)=1.0
          CALL RNKRED(HESS,ARED,LL,IPARM,ND,NE,II,IRANK)
          CALL LUPPDC(ARED,LL,IRANK,ND,ND,INDEX(II))
C.. CHECK FOR SINGULARITY AND END PROCESSING IF SINGULAR
          IF(INDEX(II)-1) 90,80,80
C.. SINGULAR HESSIAN MATRIX
   80     WRITE(NWRITE,1010) II
 1010     FORMAT('OTHE HESSIAN MATRIX FOR CONCENTRATION  PROFILE ',I2,
         1' IS SINGULAR',/,' PROCESSING STOPPING FOR THIS PROFILE')
C.. WRITE OUT THE HESSIAN MATRIX IF IDEBUG IS NOT TURNED ON
          IF(IDEBUG)200,85,200
   85     WRITE(NWRITE,1000) II
          CALL PRINTA(HESS,IPARM,II,IRANK,ND,NE)
          GOTO 200
   90     DO 100 J=1,IRANK
  100     CALL LUPPSB(ARED,COVAR(1,J,II),LL,IRANK,ND,ND)
C.. NOTE THAT THE NE/NEO IN THE NEXT LINE KEEPS THE DATA POINT COUNT
C     CORRECT FOR THE COMPOSITE ANALYSIS WHICH FOLLOWS LATER.
          FACTOR(II)=ER(II)/((NE/NEO)*M-ND)
          DO 110 I=1,ND
          DO 110 J=1,ND
  110     COVAR(J,I,II)=FACTOR(II)*COVAR(J,I,II)
          WRITE(NWRITE,1020) II
 1020     FORMAT(///,' THE COVARIANCE MATRIX OF THE ESTIMATES OF PARAMETERS'
         1,' FOR CONCENTRATION PROFILE',I3,/)
          CALL PRINTA(COVAR,IPARM,II,IRANK,ND,NE)
C..   CALCULATE CORRELATION MATRIX OF THE ESTIMATES OF PARAMETERS FOR
C     EACH CONCENTRATION PROFILE FUNCTION
          DO 120 I=1,IRANK
          DO 120 J=1,IRANK
          TERM=COVAR(I,I,II)*COVAR(J,J,II)
  120     COR(I,J,II)=COVAR(I,J,II)/(SQRT(ABS(TERM)))
          WRITE(NWRITE,1030) II
 1030     FORMAT(///,' THE CORRELATION MATRIX OF THE ESTIMATES OF',
```

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                 1' PARAMETERS FOR CONCENTRATION PROFILE',I3,/)
                 CALL PRINTA(COR,IPARM,II,IRANK,ND,NE)
     200    CONTINUE
                 IF(IFIN.GT.0.OR.NE.EQ.1) GOTO 240
                 IFIN=1
       C.. ADD UP THE INFLUENCE COEFFICIENT MATRIX BY ERROR FUNCTIONS
       C    AND THE ERROR VECTOR TO CALCULATE A COMPOSITE CORRELATION
       C    AND COVARIANCE MATRIX
                 DO 220 J=1,ND
                 DO 220 K=1,M
                 SUM=0.
                 DO 210 I=1,NE
     210    SUM=SUM+C(I,J,K)
     220    C(1,J,K)=SUM/NE
       C.. ADD UP THE ERROR VECTOR
                 DO 230 I=2,NE
     230    ER(1)=ER(1)+ER(I)
       C.. NOW SET THE DO LOOP COUNTER FOR ERROR FUNCTIONS TO 1
       C    NEO IS ALSO USED IN THE FACTOR CALCULATIONS.
                 NEO=1
       C.. WRITE OUT A HEADER TO INDICATE THAT THE COMPOSITE ERROR FUNCTION
       C    IS BEING EVALUATED
                 WRITE(NWRITE,1040)
     1040   FORMAT(//,' ****************COMPOSITE ANALYSIS BEGINNING********'
                 1,'**********')
                 GOTO  5
     240    CONTINUE
                 RETURN
                 END
                 SUBROUTINE COVARI(X,Y,Q,M)
                 DIMENSION X(M),Y(M)
                 SUMX=0.0
                 SUMY=0.0
                 K=0
                 DO 100 I=1,M
                 IF(X(I).EQ.0.0.OR.Y(I).EQ.0.0) GO TO 100
                 SUMX=SUMX+X(I)
                 SUMY=SUMY+Y(I)
                 K=K+1
       100  CONTINUE
                 SUMX=SUMX/K
                 SUMY=SUMY/K
                 Q=0.0
                 DO 200 I=1,M
                 IF(X(I).EQ.0.0.OR.Y(I).EQ.0.0) GO TO 200
                 Q=Q+(X(I)-SUMX)*(Y(I)-SUMY)
       200  CONTINUE
                 Q=Q/K
                 RETURN
                 END
                 FUNCTION ERRFNK(ER,C,QA,PARO,PAR1,FAC,ND,NE,MM,NPOINT)
       C.. THIS FUNCTION EVALUATES THE INFLUENCE COEFFICIENT MATRIX
       C    FOR THE PATTERN SEARCH ROUTINE.
```

```
       DIMENSION ER(MM,NE),C(NE,ND,MM),PARO(ND),PAR1(ND),FAC(NE),
      1QA(NE,NE)
C.. INITIALIZE THE ERRFNK AND FAC ARRAYS TO ZERO
       ERRFNK=0.
C.. CALCUALTE THE RELATIONSHIP "E X INV COV X E TRANSPOSE"
C    FOR EACH ERROR POINT. THE TOTAL IS SUMMED USING THE
C    FUNCTION NAME
       DO 40 K=1,NPOINT
C.. FIRST CALCULATE THE ERROR VECTOR AT EACH OBSERVATION
       DO 25 I=1,NE
       SUM=0.
       DO 20 J=1,ND
20     SUM=SUM+(PAR1(J)-PARO(J))*C(I,J,K)
25     FAC(I)=ER(K,I)+SUM
C.. NEXT MULTIPLY THE ERROR AND INVERSE COVARIANCE MATRICES
C    USING THE INTERMEDIATE VARIABLE SUM FOR STORAGE
       DO 40 I=1,NE
       SUM=0.
       DO 30 J=1,NE
30     SUM=SUM+QA(J,I)*FAC(J)
40     ERRFNK=ERRFNK+SQRT(SUM*FAC(I))
       RETURN
       END
       SUBROUTINE LREGRE(CC,DD,EE,P1,L,CQ,ND)
       DIMENSION CC(ND,ND),DD(ND),P1(ND),L(ND),CQ(ND,ND),TEM1(1),TEM2(1)
       DO 100 I=1,ND
       P1(I)=DD(I)
       DO 100 J=1,ND
  100 CQ(J,I)=CC(J,I)
       CALL LUPPDC(CQ,L,ND,ND,ND,INDEX)
       CALL LUPPSB(CQ,P1,L,ND,ND,ND)
       CALL MULTIQ(P1,CC,P1,TEM1,1,ND,ND,1)
       CALL MULTIP(P1,DD,TEM2,1,ND,1,1,ND,1)
       EE=EE+TEM1(1)-2.0*TEM2(1)
       RETURN
       END
       SUBROUTINE LUPPDC(A,L,N,ND1,ND2,INDEX)
       DIMENSION A(ND2,ND1),L(ND1)
C**
C**    DECOMPOSITION WITH PARTIAL PIVOTING A=LU
C**
       DO 50 J=1,N
       J1=J-1
       AJJ=0.0
       DO 30 I=1,N
       I1=MIN0(I-1,J1)
       AIJ=A(I,J)
       IF(I1.LE.0) GO TO 15
       DO 10 K=1,I1
   10 AIJ=AIJ-A(I,K)*A(K,J)
C**
   15 IF(I.GE.J) GO TO 20
       A(I,J)=AIJ/A(I,I)
```

```fortran
      GO TO 30
   20 A(I,J)=AIJ
      IF(AJJ.GE.ABS(AIJ)) GO TO 30
      M=I
      AJJ=ABS(AIJ)
   30 CONTINUE
C**
      IF(AJJ.EQ.0.0) GO TO 55
      L(J)=M
      IF(M.EQ.J) GO TO 50
      DO 40 I=1,N
      AIJ=A(M,I)
      A(M,I)=A(J,I)
   40   A(J,I)=AIJ
   50   CONTINUE
C.. SUCCESSFUL CALL. RETURN INDEX CODE = 0 TO INIDCATE SUCCESS
      INDEX=0
      RETURN
C.. SINGULAR MATRIX. RETURN INDEX CODE = 1 TO INDICATE SINGULARITY
   55   INDEX=1
      RETURN
      END
      SUBROUTINE LUPPSB(A,B,L,N,ND1,ND2)
      DIMENSION A(ND2,ND1),B(ND1),L(ND1)
C**
C**   AX=B  :   LUX=B
C**   FORWARD SUBSTITUTION LY=B
C**
      DO 70 I=1,N
      I1=I-1
      M=L(I)
      BI=B(M)
      B(M)=B(I)
      IF(I1.LE.0) GO TO 70
      DO 60 K=1,I1
   60 BI=BI-A(I,K)*B(K)
   70 B(I)=BI/A(I,I)
C**
C**   BACKWARD SUBSTITUTION UX=Y
C**
      N1=N-1
      DO 90 IN=1,N1
      I=N-IN
      I1=I+1
      BI=B(I)
      DO 80 K=I1,N
   80 BI=BI-A(I,K)*B(K)
   90 B(I)=BI
      RETURN
      END
      SUBROUTINE MULTIP(A,B,C,N,M,L,NA,NB,NC)
      DIMENSION A(NA,M),B(NB,L),C(NC,L)
      DO 100 I=1,N
```

```
          DO 100 J=1,L
          C(I,J)=0.0
          DO 100 K=1,M
   100    C(I,J)=C(I,J)+A(I,K)*B(K,J)
          RETURN
          END
          SUBROUTINE MULTIQ(A,B,C,D,MA,MB,MC,MD)
          DIMENSION A(MB,MA),B(MB,MC),C(MC,MD),D(MA,MD)
          DO 100 I=1,MA
          DO 100 J=1,MD
          D(I,J)=0.0
          DO 100 K=1,MB
          DO 100 N=1,MC
   100    D(I,J)=D(I,J)+A(K,I)*B(K,N)*C(N,J)
          RETURN
          END
          SUBROUTINE PATSRC(PARL,PARU,PARO,PAR1,W,C,ER,QA,FAC,ND,NDP1,
         1NE,MM,ITERM,NPOINT,PARMS,EROBFU,CENTER,EE)
C.. THIS SUBROUTINE DETERMINES THE OPTIMAL SET OF PARAMETERS FOR THE
C    INFLUENCE COEFFICIENT ERROR FUNCTIONS USING THE COMPLEX METHOD
C    OF BOX. IT WILL ALWAYS CONVERGE FOR THE QUADRATIC OBJECTIVE
C    FUNCTION.
          DIMENSION PARMS(ND,NDP1),PARL(ND),PARU(ND),PARO(ND),PAR1(ND),
         1C(NE,ND,MM),ER(MM,NE),QA(NE,NE),EROBFU(NDP1),W(NE),CENTER(NDP1),
         2FAC(NE)
          COMMON /IOSRC/NREAD,NWRITE
          DATA EPS/1.0E-03/,ISEED/68457/
C.. MULTIPLY THE INVERSE OF THE COVARIANCE MATRIX (QA) AND THE WEIGHTING
C    MATRIX, W TO OBTAIN AN OVERALL WEIGHTING MATRIX.  IF INVERSE
C    COVARIANCE WEIGHT IS NOT DESIRED, QA IS THE ASSIGNED WEIGHING
C    MATRIX
C.. CONSTRUCT AN INITIAL COMPLEX OF POINTS USING THE OLD VALUES
C    OF THE PARAMETERS AND A CLUSTER OF RANDOMLY GENERATED PARAMETERS
C    AROUND THE OLD SET. ASSUME THAT THE INITIAL SET OF PARAMETERS IS
C    FEASIBLE.
          DO 10 I=1,ND
          PAR1(I)=PARO(I)
   10     PARMS(I,1)=PARO(I)
          EROBFU(1)=ERRFNK(ER,C,QA,PARO,PAR1,FAC,ND,NE,MM,NPOINT)
          DO 35 INDEX=2,NDP1
          DO 30 I=1,ND
          ICOUNT=0
   20     PAR1(I)=PARO(I)*(1.+(0.5-RANDU(ISEED))/10.)
C.. CHECK TO SEE IF THE RANDOMLY GENERATED PARAMETER IS OUTSIDE THE
C    FEASIBLE REGION
          ICOUNT=ICOUNT+1
          IF(ICOUNT-2000) 25,21,21
   21     WRITE(6,1000) ICOUNT,I
   1000   FORMAT(' **** ERROR ****',//,' AN ENDLESS LOOP HAS OCCURRED IN',
         1' PATSRC (ICOUNT=',I6,')',//,' CHECK THE CONSTRAINTS AND INITIAL'
         2,' PARAMETER SET FOR PARAMETER NO.',I2)
          GOTO 230
   25     IF(PAR1(I).LT.PARL(I)) GOTO 20
```

```
            IF(PAR1(I).GT.PARU(I)) GOTO 20
30      CONTINUE
C.. EVALUATE THE OBJECTIVE FUNCTION
        EROBFU(INDEX)=ERRFNK(ER,C,QA,PAR0,PAR1,FAC,ND,NE,MM,NPOINT)
        DO 31 I=1,ND
31      PARMS(I,INDEX)=PAR1(I)
35      CONTINUE
C..     SET THE ITERATION COUNTER TO ZERO
        ITER=0
        IRTRN=0
C.. LOOP POINT: THE PROGRAM LOOPS BACK TO THIS POINT AFTER SUCCESSFULLY
C   GENERATING A NEW VERTEX.
C.. CHECK FOR TERMINATION
40      ALPHA=1.3
C.. DETERMINE IF THE ITERATIONS ARE EXCESSIVE
        IF(ITER.GT.ITERM) GOTO 110
C.. DETERMINE IF THE COMPLEX HAS COLAPSED, IF SO TERMINATE
        VART=0.
        DO 46 I=1,ND
        SUM1=0.
        SUM2=0.
        DO 44 J=1,NDP1
        SUM1=SUM1+PARMS(I,J)**2
44      SUM2=SUM2+PARMS(I,J)
        VAR=(SUM1-(SUM2**2)/NDP1)/(NDP1-1)
46      VART=VART+VAR
        IF(VART.LE.EPS) GOTO 200
C.. DETERMINE THE TWO WORST VALUES
        IWORST=1
        DO 50 INDEX=2,NDP1
50      IF(EROBFU(INDEX).GE.EROBFU(IWORST)) IWORST=INDEX
C.. CALCULATE THE CENTROID OF THE REMAINING POINTS NEGLECTING THE
C   REJECTED POINT.
        DO 70 I=1,ND
        SUM=0.
        DO 60 J=1,NDP1
        IF(J.EQ.IWORST) GOTO 60
        SUM=SUM+PARMS(I,J)
60      CONTINUE
70      CENTER(I)=SUM/(NDP1-1)
C.. PROJECT FROM THE REJECTED POINT THROUGH THE CENTROID TO
C   THE NEW TRIAL POINT ALPHA TIMES THE DISTANCE FROM THE
C   REJECTED POINT TO THE CENTROID
75      DO 80 I=1,ND
80      PAR1(I)=ALPHA*(CENTER(I)-PARMS(I,IWORST))+CENTER(I)
C.. CHECK TO MAKE SURE THE NEW VERTEX  SATISFIES ALL THE CONSTRAINTS
        DO 90 I=1,ND
        IF(PAR1(I).LT.PARL(I)) GOTO 100
        IF(PAR1(I).GT.PARU(I)) GOTO 100
90      CONTINUE
C.. NOW CHECK THE ERROR FUNCTION TO SEE IF THE NEW SET OF PARAMETERS
C   IMPROVES THE OBJECTIVE VALUE.
        ERRNEW=ERRFNK(ER,C,QA,PAR0,PAR1,FAC,ND,NE,MM,NPOINT)
```

```fortran
      ITER=ITER+1
      IF(ERRNEW.GT.EROBFU(IWORST)) GOTO 100
C.. IMPROVEMENT. SAVE THE RESULTS
      EROBFU(IWORST)=ERRNEW
      DO 95 I=1,ND
95    PARMS(I,IWORST)=PAR1(I)
      GOTO 40
C.. NO IMPROVEMENT OR CONSTRAINT VIOLATION
100   ALPHA=ALPHA*0.5
      IF(ALPHA.LE.0.002) GOTO 130
      IRTRN=IRTRN+1
C.. CHECK FOR EXCESSIVE ITERATIONS
      IF(ITER.GT.ITERM) GOTO 110
      GOTO 75
C.. TERMINATION DUE TO EXECSSIVE ITERATIONS
110   WRITE(NWRITE,1010) ITER
1010  FORMAT(' PATTERN SEARCH ENDING WITH EXCESSIVE ITERATIONS',
     1/,' ITER=',I6)
C.. WRITE OUT THE PARAMETER SET TO SHOW HOW CLOSE IT CAME TO
C   CONVERGENCE
      WRITE(NWRITE,1020)
1020  FORMAT(66X,' PARAMETERS')
      WRITE(NWRITE,1030) (I,I=1,ND)
1030  FORMAT(1X,'VERTEX NO.',6X,'ERROR',6X,6(6X,I2,7X),/,1X,7(6X,I2,7X))
      DO 120 J=1,NDP1
120   WRITE(NWRITE,1040) J,EROBFU(J),(PARMS(I,J),I=1,ND)
1040  FORMAT(6X,I2,6X,7E15.6,/,14X,7E15.6)
      GOTO 200
C.. TERMINATION DUE TO AN EXCESSIVE NUMBER OF RETURNS TO THE CENTROID
130   WRITE(NWRITE,1050) ALPHA,ITER
1050  FORMAT(' PATTERN SEARCH ENDING WITH EXCESSIVE RETURNS TO THE',
     1' CENTROID',/,' ALPHA=',E17.6,5X,'ITER=',I6)
      WRITE(NWRITE,1020)
      WRITE(NWRITE,1030) (I,I=1,ND)
      DO 121 J=1,NDP1
121   WRITE(NWRITE,1040) J,EROBFU(J),(PARMS(I,J),I=1,ND)
C.. NORMAL TERMINATION
C.. FIND THE BEST PARAMETER SET AND RETURN IT IN PAR1
200   IBEST=1
      DO 210 I=2,NDP1
210   IF(EROBFU(I).LT.EROBFU(IBEST)) IBEST=I
      DO 220 I=1,ND
220   PAR1(I)=PARMS(I,IBEST)
      EE=EROBFU(IBEST)
      RETURN
230   WRITE(6,1060) ((I,PARL(I),PARU(I),PAR0(I)),I=1,ND)
1060  FORMAT(//,' PARM NO.',I3,' LOWER LIMIT=',E12.6,' UPPER LIMIT=',
     1E12.6,' ACTUAL VALUE=',E12.6)
      STOP 45
      END
      SUBROUTINE PRINTA(A,IPARM,II,IRANK,ND,NE)
      DIMENSION A(ND,ND,NE),IPARM(ND)
      COMMON /IOPRT/NREAD,NWRITE
```

```fortran
      WRITE(NWRITE,1000) (IPARM(J),J=1,IRANK)
      DO 10 I=1,IRANK
10    WRITE(NWRITE,1010) IPARM(I),(A(I,JA,II),JA=1,IRANK)
1000  FORMAT(1H0,10I12)
1010  FORMAT(1X,I5,10E12.5)
      RETURN
      END
      SUBROUTINE RNKRED(A,B,LL,IPARM,ND,NE,II,ISI)
C.. THIS SUBROUTINE TESTS FOR PARAMETER INDEPENDENCE, REDUCES
C   RANK IF NECESSARY, AND STORES THE RESULT IN TWO DIMENSIONAL
C   ARRAY FOR LATER PROCESSING.
C   IF THE ERROR FUNCTION IS COMPLETELY INDEPENDENT OF THE PARAMETER
C   THE DIAGONAL OF THE HESSIAN MATRIX WILL BE ZERO.
C   THIS SUBROUTINE USES THIS INFORMATION TO DETERMINE INDEPENDENCE
C   AND REDUCE RANK.
      DIMENSION A(ND,ND,NE),B(ND,ND),LL(ND),IPARM(ND)
      COMMON/IOCOR/NREAD,NWRITE
      DATA FAC/1.D-25/
C.. SET IDETEC TO 0 AND USE IT LATER TO DETERMINE IF RANK REDUCTIONS
C   HAVE BEEN MADE
C.. FIND THE MAXIMUM DIAGONAL VALUE TO USE TO COMPARE THE OTHER DIAGONAL
C   VALUES TO FIND THE "RELATIVE" ZEROS.
      BIG=A(1,1,II)
      DO 10 I=2,ND
10    IF(BIG.LT.A(I,I,II)) BIG=A(I,I,II)
      EPS=FAC*BIG
C.. NUMBERS LESS THAN EPS ARE "RELATIVE" ZERO
C.. DETERMINE THE RELATIVE ZERO DIAGONALS.
      DO 20 I=1,ND
C.. ALSO USE THIS DO LOOP TO ZERO THE IPARM ARRAY
      IPARM(I)=0
      LL(I)=0
20    IF(A(I,I,II).LT.EPS) LL(I)=I
C.. REDUCE THE RANK OF THE MATRIX BY ELIMINATING THE ROWS AND COLUMNS
C   CORRESPONDING TO LL VALUES.
C.. SET THE B ARRAY TO ZERO. IT WAS USED PREVIOUSLY IN THE QUADRATIC
C   PROGRAM SUBROUTINE
      DO 25 I=1,ND
      DO 25 J=1,ND
25    B(I,J)=0.0
C.. REDUCE THE RANK
      ISI=0
      DO 60 I=1,ND
      IF(I-LL(I)) 30,60,30
30    ISI=ISI+1
      IPARM(ISI)=I
      ISJ=0
      DO 50 J=1,ND
      IF(J-LL(J)) 40,50,40
40    ISJ=ISJ+1
      B(ISI,ISJ)=A(I,J,II)
50    CONTINUE
60    CONTINUE
```

```
C.. SKIP THE WRITES IF NO RANK REDUCTIONS ARE MADE
         IF(ISJ.EQ.ND) GOTO 80
C.. WRITE OUT THE RANK REDUCTIONS
         WRITE(NWRITE,1000) II,ISI
1000  FORMAT('OTHE HESSIAN MATRIX RANK FOR CONCENTRATION PROFILE',I2,
     1' HAS BEEN REDUCED TO ',I2,/,' PARAMETERS NUMBER ',/)
         DO 70 I=1,ND
70       IF(LL(I).GT.0) WRITE(NWRITE,1010) LL(I)
1010  FORMAT(1X,I2)
         WRITE(NWRITE,1020)
1020  FORMAT(' HAVE BEEN ELIMINATED')
80       RETURN
         END
         SUBROUTINE TRANSF(C,E,PO,PL,PU,PA,QQ,QA,L,D,CQC,CQD,AA,BB,CC,DD,
     1 EE,NE,ND,ND2,M,MM,IN,NN)
         DIMENSION C(NE,ND,M),E(MM,NE)    ,PO(ND)     ,PL(ND)     ,PU(ND)     ,
     1              QQ(NE,NE) ,QA(NE,NE) ,L(ND)       ,D(NE,M)    ,CQC(ND,ND),
     2              CQD(ND)    ,AA(ND,ND2),BB(ND)      ,CC(ND,ND) ,DD(ND)     ,
     3              PA(ND)     ,TEM1(1)    ,TEM2(1)
         COMMON /IOSRC/NREAD,NWRITE
C**   COMPUTE COVARIANCE MATRIX QQ
         DO 110 J=1,NE
         DO 100 I=1,NE
  100 QA(I,J)=0.0
  110 QA(J,J)=PA(J)
C.. SKIP THE NEXT SECTION IF INVERSE COVARIANCE IS NOT DESIRED,
C    LEAVING QA AS THE WEIGHTING MATRIX
         IF(NN.EQ.1) GO TO 265
         DO 120 I=1,NE
         DO 120 J=I,NE
120      CALL COVARI(E(1,I),E(1,J),QQ(I,J),M)
         DO 150 I=2,NE
         K=I-1
         DO 150 J=1,K
150      QQ(I,J)=QQ(J,I)
C**   COMPUTE INVERSE OF COVARIANCE MATRIX QQ
         CALL LUPPDC(QQ,L,NE,NE,NE,INDEX)
         DO 250 J=1,NE
250      CALL LUPPSB(QQ,QA(1,J),L,NE,NE,NE)
C.. WRITE OUT THE COVARIANCE MATRIX
         WRITE(NWRITE,1000) (J, J=1,NE)
1000  FORMAT(' INVERSE COVARIANCE WEIGHTING MATRIX',/,1X,10I12)
         DO 260 I=1,NE
260      WRITE(NWRITE,1010) I,(QA(I,J),J=1,NE)
1010  FORMAT(1X,I5,10E12.5)
C**   COMPUTE MATRIX D(NE,M)
265      DO 300 I=1,M
         CALL MULTIP(C(1,1,I),PO,D(1,I),NE,ND,1,NE,ND,NE)
         DO 300 J=1,NE
  300 D(J,I)=D(J,I)-E(I,J)
C**   COMPUTE MATRIX CC(ND,ND), DD(ND), AND EE
         DO 350 I=1,ND
         DD(I)=0.0
```

```
              DO 350 J=1,ND
      350 CC(J,I)=0.0
              EE=0.0
              DO 450 I=1,M
C*        COMPUTE MATRIX CQC(ND,ND), CQD(ND), AND DQD
              CALL MULTIQ(C(1,1,I),QA,C(1,1,I),CQC,ND,NE,NE,ND)
              CALL MULTIQ(C(1,1,I),QA,D(1,I),CQD,ND,NE,NE,1)
              CALL MULTIQ(D(1,I),QA,D(1,I),DQD,1,NE,NE,1)
              EE=EE+DQD
              DO 400 J=1,ND
              DD(J)=DD(J)+CQD(J)
              DO 400 K=1,ND
      400 CC(K,J)=CC(K,J)+CQC(K,J)
      450 CONTINUE
              GO TO (650,650,500),IN
C**       TRANSFER OF LOWER LIMIT CONDITIONS
      500 CALL MULTIQ(PL,CC,PL,TEM1,1,ND,ND,1)
              CALL MULTIP(PL,DD,TEM2,1,ND,1,1,ND,1)
              EE=EE+TEM1(1)-2.0*TEM2(1)
              CALL MULTIP(CC,PL,CQD,ND,ND,1,ND,ND,ND)
              DO 550 J=1,ND
      550 DD(J)=2.0*(CQD(J)-DD(J))
              DO 600 I=1,ND
      600 BB(I)=PU(I)-PL(I)
              DO 640 J=1,ND
              K=J+ND
              DO 620 I=1,ND
              AA(I,J)=0.0
      620 AA(I,K)=0.0
              AA(J,J)=1.0
      640 AA(J,K)=1.0
      650 RETURN
              END
              SUBROUTINE WOLFE(XL,XX,A,B,C,P,OBJ,T,COST,DIFF,TT,PRFIT,RATIO,IB,
          1 III,OPP,N,M,MN,NZ,NC,ITMAX,MTR,IFAULT)
C*******************************************************************************
C*                                                                            *
C*        QUADRATIC PROGRAM BY THE WOLFE METHOD.                              *
C*        MINIMIZES OBJECTIVE FUNCTION (Z)                                    *
C*            Z = P(J) * X(J) + X(I) * C(I,J) * X(J) + OBJ                    *
C*        THE CONSTRAINTS ARE                                                 *
C*            A(I,J) * X(J) .LE. B(I)                                         *
C*            ALL X(J) .GT. 0.0                                              *
C*        XX(J)=X(J)+XL(J)                                                   *
C*                                                                            *
C*******************************************************************************
              DIMENSION A(M,MN),B(M),C(N,N),P(N),T(MN,NC),COST(NC),DIFF(NC),
          1 TT(NC),PRFIT(NC),RATIO(MN),IB(MN),III(NZ),OPP(MN),XL(N),XX(N)
              COMMON /IOSRC/ NREAD,NWRITE
              IFAULT=0
              IF (MTR) 350, 350, 351
      351 WRITE (NWRITE,123)
      123 FORMAT ('ON,M,ITERATION LIMIT,TRACE IN ORDER')
```

```fortran
      DO 350 J=1,ND
  350 CC(J,I)=0.0
      EE=0.0
      DO 450 I=1,M
C*    COMPUTE MATRIX CQC(ND,ND), CQD(ND), AND DQD
      CALL MULTIQ(C(1,1,I),QA,C(1,1,I),CQC,ND,NE,NE,ND)
      CALL MULTIQ(C(1,1,I),QA,D(1,I),CQD,ND,NE,NE,1)
      CALL MULTIQ(D(1,I),QA,D(1,I),DQD,1,NE,NE,1)
      EE=EE+DQD
      DO 400 J=1,ND
      DD(J)=DD(J)+CQD(J)
      DO 400 K=1,ND
  400 CC(K,J)=CC(K,J)+CQC(K,J)
  450 CONTINUE
      GO TO (650,650,500),IN
C**   TRANSFER OF LOWER LIMIT CONDITIONS
  500 CALL MULTIQ(PL,CC,PL,TEM1,1,ND,ND,1)
      CALL MULTIP(PL,DD,TEM2,1,ND,1,1,ND,1)
      EE=EE+TEM1(1)-2.0*TEM2(1)
      CALL MULTIP(CC,PL,CQD,ND,ND,1,ND,ND,ND)
      DO 550 J=1,ND
  550 DD(J)=2.0*(CQD(J)-DD(J))
      DO 600 I=1,ND
  600 BB(I)=PU(I)-PL(I)
      DO 640 J=1,ND
      K=J+ND
      DO 620 I=1,ND
      AA(I,J)=0.0
  620 AA(I,K)=0.0
      AA(J,J)=1.0
  640 AA(J,K)=1.0
  650 RETURN
      END
      SUBROUTINE WOLFE(XL,XX,A,B,C,P,OBJ,T,COST,DIFF,TT,PRFIT,RATIO,IB,
     1 III,OPP,N,M,MN,NZ,NC,ITMAX,MTR,IFAULT)
C*******************************************************************
C*                                                                *
C*    QUADRATIC PROGRAM BY THE WOLFE METHOD.                      *
C*    MINIMIZES OBJECTIVE FUNCTION (Z)                            *
C*        Z = P(J) * X(J) + X(I) * C(I,J) * X(J) + OBJ            *
C*    THE CONSTRAINTS ARE                                         *
C*        A(I,J) * X(J) .LE. B(I)                                 *
C*        ALL X(J) .GT. 0.0                                       *
C*    XX(J)=X(J)+XL(J)                                            *
C*                                                                *
C*******************************************************************
      DIMENSION A(M,MN),B(M),C(N,N),P(N),T(MN,NC),COST(NC),DIFF(NC),
     1 TT(NC),PRFIT(NC),RATIO(MN),IB(MN),III(NZ),OPP(MN),XL(N),XX(N)
      COMMON /IOSRC/ NREAD,NWRITE
      IFAULT=0
      IF (MTR) 350, 350, 351
  351 WRITE (NWRITE,123)
  123 FORMAT ('ON,M,ITERATION LIMIT,TRACE IN ORDER')
```

```
      WRITE(NWRITE,300) N, M, ITMAX, MTR
      WRITE ( NWRITE,124)
  124 FORMAT ('1  A MATRIX')
      DO 225 I = 1, M
      WRITE (NWRITE, 100) (A(I,J), J = 1, N)
  225 CONTINUE
      WRITE (NWRITE, 125)
  125 FORMAT ('1  B VECTOR (CONSTRAINTS)')
      WRITE(NWRITE,100)(B(J),J=1,M)
      WRITE (NWRITE, 126)
  126 FORMAT ('1  C MATRIX (OBJ. FCT.)')
      DO 230 I = 1, N
      WRITE (NWRITE, 100) (C(I,J), J = 1, N)
  230 CONTINUE
      WRITE (NWRITE, 127)
  127 FORMAT ('1  P VECTOR (COST COEFF.)')
      WRITE(NWRITE,100)(P(I),I=1,N)
  350 MP1=M+1
      MM1=M-1
      NP1=N+1
      NP2=N+2
      MNM1=MN-1
      MNP1=MN+1
      MNP2=MN+2
      NV=MN+N
      NVP1=NV+1
      NVP2=NV+2
      NY=NV+M
      NYP1=NY+1
      NYP2=NY+2
      NZP2=NZ+2
      DO 180 I=1,MN
      DO 180 J=1,NC
  180 T(I,J)=0.0
      DO 182 I=1,M
  182 T(I,1)=B(I)
      DO 183 I=MP1,MN
      J=I-M
  183 T(I,1)=-P(J)
      DO 184 I=1,M
      DO 184 J=1,N
      JP1=J+1
  184 T(I,JP1)=A(I,J)
      DO 185 I=1,N
      DO 185 J=1,N
      IPM=I+M
      JP1 = J + 1
  185 T(IPM,JP1)=2.*C(I,J)
      DO 186 I=MP1,MN
      IMM=I-M
      DO 186 J=NP2,MNP1
      JMN=J-N-1
  186 T(I,J) = A(JMN,IMM)
```

```
          DO 187 I=1,MN
          IJ = I + NVP1
          DO 187 J = NYP2, NC
          IF(J-IJ)187,179,187
 179   T(I,J)=1.
 187   CONTINUE
          DO 188 I = MP1, MN
          IJ = I - M + MNP1
          DO 188 J = MNP2, NC
          IF(J-IJ)188,178,188
 178   T(I,J)=-1.
 188   CONTINUE
          DO 208 I=1,MN
          OPP(I) = T(I,1)
 208   CONTINUE
          DO 340 J=1,NZ
 340   COST(J)=0.0
          DO 189 I=1,M
          J=NP1+I
 189   COST(J)=T(I,1)
          DO 190 J=NYP2,NC
 190   COST(J)=1.E+70
          NN=NZ-MN
          DO 25 KK=1,NZ
  25   III(KK)=KK
          DO 1 I = 1, MN
   1   IB(I)=NN+I
          K=0
C      ITERATION START
  19   K=K+1
          DO 2 J=1,NC
   2   PRFIT(J)=0.
          DO 3 J=1,NC
          SUM=0.
          DO 4 I = 1, MN
          JJ=IB(I)+1
   4   SUM=SUM+COST(JJ)*T(I,J)
          PRFIT(J)=SUM
   3   DIFF(J)=COST(J)-PRFIT(J)
          IF(MTR)555,666,555
 555   WRITE(NWRITE,111)K
C      PRINT TABLE IF DESIRED.
          WRITE(NWRITE,102)(COST(J),J=2,NC)
          WRITE(NWRITE,103)(III(KK),KK=1,NZ)
          DO 26 I=1,MN
          JJ=IB(I)+1
  26   WRITE(NWRITE,104)COST(JJ),(T(I,J),J=1,NC)
          WRITE(NWRITE,105)(PRFIT(J),J=1,NC)
          WRITE(NWRITE,106)(DIFF(J),J=2,NC)
C      FIND THE PIVOT ELEMENT --- T(IPR,IPC)
 666   IPC=0
          TEST=0.
C      FIND THE VARIABLE WITH THE LARGEST PROFIT
```

```
          DO 5 I=2,NC
  235 IF ( DIFF(I) - TEST) 6, 5, 5
    6 TEST=DIFF(I)
          IPC=I
    5 CONTINUE
          IF(IPC)99,99,7
    7 KCK=0
          DO 8 I=1,MN
          IF(T(I,IPC))32,32,20
   20 RATIO(I) = T(I,1) / T(I,IPC)
          GO TO 8
   32 KCK=KCK+1
          IF(KCK-MN)21,31,21
   21 RATIO(I)=1.E20
    8    CONTINUE
C        REMOVE LIMITING VARIABLE
          DO 9 I=1,MN
          IF(RATIO(I))9,10,10
   10 IF(RATIO(I).GT.10000.)RATIO(I)=10000.
          TEST=RATIO(I)
          IPR=I
          GO TO 11
    9 CONTINUE
   11 DO 12 I = 1, MN
          IF(TEST-RATIO(I))12,12,13
   13 TEST=RATIO(I)
          IPR=I
   12 CONTINUE
C        START PIVOTING AND INTRODUCING NEW VARIABLE INTO SOLUTION
          PIVOT=T(IPR,IPC)
C.. THE NEXT STATEMENT WAS ADDED BY MKS ON 8/21/83 TO TEST FOR
C    PIVOT=0 AND EXIT THROUGH THE NORMAL EXIT IF PIVOT=0.
          IF(PIVOT.EQ.0.) GOTO 9998
          DO 15 J=1,NC
   15 T(IPR,J)=T(IPR,J)/PIVOT
          DO 171 I=1,MN
          IF(I-IPR)17,171,17
   17 DO 18 J=1,NC
   18 TT(J)=T(IPR,J)*T(I,IPC)/T(IPR,IPC)
          DO 172 J=1,NC
  172 T(I,J)=T(I,J)-TT(J)
  171 CONTINUE
          COST(IPR)=COST(IPC)
          IB(IPR)=IPC-1
C        TRACE OUTPUT IF DESIRED.
          IF(MTR-1)205,205,86
   86 WRITE(NWRITE,114)
          DO 87 I=1,MN
   87 WRITE (NWRITE,300) I, IB(I)
          WRITE(NWRITE,119)
          WRITE(NWRITE,121)IPR,IPC,KCK
          WRITE(NWRITE,120)
          WRITE(NWRITE,100)TEST,PIVOT,DIFF(IPC)
```

```
      WRITE(NWRITE,117)
      DO 88 I=1,MN
   88 WRITE (NWRITE,302) I, RATIO(I)
C     RECOMPUTE COSTS
  205 DO 176 J=1,NYP1
  176 COST(J)=0.
      DO 197 I=1,MN
      IF(IB(I)-MN)192,192,195
  192 JJ=IB(I)+MNP1
      GO TO 198
  195 IF(IB(I)-NY)196,196,197
  196 JJ=IB(I)-MNM1
      GO TO 198
  198 COST(JJ)=T(I,1)
  197 CONTINUE
      IF(K - ITMAX) 19, 830, 830
C.. THIS WRITE STATEMENT INCLUDED TO ACCOMODATE THE MODIFICATIONS
C   MADE FOR UNBOUNDED SOLUTIONS AND PIVOT=0.
 9998 WRITE(6,1001)
 1001 FORMAT(' PIVOT =0.')
      IFAULT=1
      GOTO 999
   99 DO 200 I=1,N
      IF(XX(I).LE.0.0) XX(I)=XL(I)
  200 CONTINUE
      SUM=0.
      DO 201 I=1,MN
      IN=IB(I)
      IF(IN.GT.N)GO TO 201
      XX(IN)=XL(IN)+T(I,1)
      SUM=SUM+P(IN)*T(I,1)
  201 CONTINUE
      FRST=SUM
      SUM=0.
      DO 202 I=1,MN
      DO 202 J=1,MN
      IN=IB(I)
      IF(IN.GT.N)GO TO 202
      JN=IB(J)
      IF(JN.GT.N)GO TO 202
      SUM=SUM+C(IN,JN)*T(I,1)*T(J,1)
  202 CONTINUE
      SCND=SUM
      OBJ=FRST+SCND+OBJ
      WRITE(NWRITE,107) OBJ
      WRITE(NWRITE,118)N,NP1,MN
      WRITE(NWRITE,122)MNP1,NY,NYP1,NZ
      WRITE(NWRITE,108)
      WRITE (NWRITE,128)
      DO 28 I=1,MN
      IF ( T( I,1)) 27, 28, 27
   27 WRITE(NWRITE,110)IB(I),T(I,1)
   28 CONTINUE
```

```fortran
      WRITE(NWRITE,109)
      WRITE(NWRITE,115)
      DO 53 I=1,MN
      IF (OPP(I)) 52, 53, 52
   52 WRITE (NWRITE,113) I, OPP(I)
   53 CONTINUE
      WRITE(NWRITE,116)
      GO TO 999
   31 WRITE(NWRITE,112)
      IFAULT=1
      GO TO 999
  100 FORMAT (1X,10F10.3)
  102 FORMAT(/18X,'C(J)',3X,9(1X,F8.3,1X)/(14X,10(F9.2,1X)))
  103 FORMAT (6X,'C(I)',3X,'T(I)',10(4X,I2,4X)/(17X,10(4X,I2,4X)))
  104 FORMAT(2X,F8.2,2X,F11.2,1X,9(1X,F8.2,1X)/(14X,10(1X,F8.2,1X)))
  105 FORMAT(//5X,'Z(J)',3X,F11.2,1X,9(F9.2,1X)/14X,10(F9.2,1X))
  106 FORMAT(//5X,'C-Z',6X,10(F9.2,1X)/14X,10(F9.2,1X))
  107 FORMAT (//9X,'THE MINIMUM VALUE OF Z IS=',E16.8)
  108 FORMAT (//9X,'THE OPTIMUM POINTS ARE PRINTED BELOW ')
  109 FORMAT (//9X,'THE REST OF THE VARIABLES ARE EQUAL TO ZERO')
  128 FORMAT(//,6X,'  I' ,8X,'X(I)'//)
  110 FORMAT (9X,I2,1X,4X,E16.8)
  111 FORMAT ('1',4X,'TABLE',3X,I3)
  112 FORMAT (13X,'THE OBJECTIVE FUNCTION IS UNBOUNDED.')
  113 FORMAT (9X,'C-Z(', I2, 1X,')=', E16.8)
  114 FORMAT (//3X,'IB(I)')
  115 FORMAT (//9X,'THE OPPORTUNITY COSTS ARE'/)
  116 FORMAT (//9X,'THE REST OF THE OPPORTUNITY COSTS ARE ZERO')
  117 FORMAT (5X,'RATIO(I)')
  118 FORMAT (//4X,'NUMBERS 1 THROUGH',I3,' ARE ORDINARY VARIABLES'
     1,' NUMBERS',I3,' THROUGH',I3,' ARE LAGRANGIANS.')
  119 FORMAT (8X,'IPR',7X,'IPC',7X,'KCK')
  120 FORMAT (7X,'TEST',7X,'PIVOT',6X,'DIFF(IPC)')
  121 FORMAT(8I10)
  122 FORMAT (/4X,'NUMBERS',I3,' THROUGH ',I3,' ARE SLACKS, NUMBERS ',
     1I3,' THROUGH',I3,' ARE GRADIENTS.')
  300 FORMAT (4I10)
  302 FORMAT (3X,I4,F20.6)
  830 WRITE(NWRITE,831)
  831 FORMAT(1X,'ITERATION LIMIT EXCEEDED')
      IFAULT=1
  999 RETURN
      END
      FUNCTION RANDU(ISEED)
C.. THIS FUNCTION GENERATES A RANDOM NUMBER BETWEEN 0. AND 1.0
C   'WHITE' PROBABILITY
      IY=ISEED*65539
      IF(IY) 10,10,20
   10 IY=IY+2147483647 +1
   20 RANDU=IY
      RANDU=RANDU*0.4656613D-09
      ISEED=IY
      ISEED=IDFIX(FLOAT(ISEED)*RANDU)
```

```
RETURN
END
FUNCTION IDFIX(A)
IDFIX=A
RETURN
END
```