

UNIVERSITY OF CALIFORNIA

Los Angeles

Dynamic Modeling
of the High Purity Oxygen
Activated Sludge Process

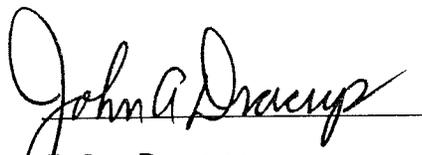
A thesis submitted in partial satisfaction of the
requirements for the degree Master of Science
in Civil Engineering

by

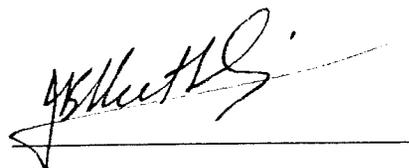
David Bryan Whipple

1989

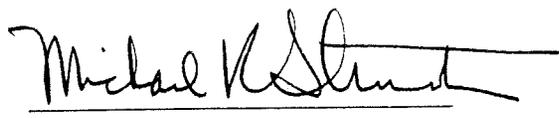
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1989

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ABSTRACT OF THE THESIS

Dynamic Modeling
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by

David Bryan Whipple

Master of Science in Civil Engineering
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Professor Michael K. Stenstrom, Chair

This thesis uses a dynamic model to quantify the capacity of the high purity oxygen activated sludge process. The Joint Water Pollution Control Plant in Carson California was used as an example plant. Data collected in May, 1984 during a full scale test of this facility were used to calibrate the dynamic mathematical model. Following calibration, the model was used to simulate process performance. Specifically, the model was used to determine the treatment capacity of the activated sludge reactors. The results of the computer

simulation indicate that the original design capacity can be exceeded by sixty percent (80 million gallons per day maximum) including a twenty percent sinusoidal diurnal flow fluctuation. However, those conditions were achieved during a simulation that included automatic oxygen flow control based on the fourth stage dissolved oxygen concentration. Under those conditions, the fourth stage dissolved oxygen concentration never declined below 3.0 mg/l. It was concluded that, although the Carson plant is currently under loaded, any increase in the influent wastewater flow rate must consider the resulting decreasing sludge age, and the possibility of increased instability from industrial waste.

I INTRODUCTION

During the past several years, the Environmental Protection Agency working under the Clean Water Act has begun to enforce the requirement that all sewage treatment conform to secondary effluent standards. The current favored technology for municipalities is the activated sludge process. The activated sludge process presents two operational options: aeration using air as the oxygen transfer fluid, or a contained vessel using high purity oxygen. The high purity process option presents two distinct advantages. The plant requires a significantly smaller geographic area than an air plant treating the same waste flow. Secondly, the high purity system uses covered reactors. The covered reactors may be advantageous in the control of volatile emissions.

In 1984 the County Sanitation Districts of Los Angeles County began operation of a high purity oxygen activated sludge plant in Carson California. The original plant provided advanced primary treatment for 360 million gallons per day (MGD) of combined industrial and domestic sewage. The secondary system comprised four treatment trains. Each train was designed to treat 50 MGD . A treatment train consists of four 1.315 million gallon complete mix reactors in series. Oxygen is transferred by three surface aerators per reactor. To

provide the required oxygen, the County built two 150 ton per day cryogenic oxygen plants. During May of 1984 the County tested the oxygen transfer capability of the secondary treatment system to verify the warranty requirements of the purchase contract. The test results indicated the plant had transferred more oxygen than required by the warranty.

During verification testing, the County collected a significant amount of operational performance data. This thesis uses the historical data provided by the County and applies a dynamic mathematical model to predict operational performance and plant capacity. The model was written in Fortran and CSMP III.¹ CSMP III is a mathematical computer program designed to solve differential equations.

The significance of such a predictive tool is its future application by municipalities and industry to determine if their current activated sludge plants have additional capacity. Additional capacity will be required in the future as the Environmental Protection Agency enforces the Clean Water Act. Additionally, predictive tools of this nature allow design engineers to determine future capitol investment as a function of projected required capacity.

II LITERATURE REVIEW

Early work in mathematical modeling of the activated sludge process involved the application of mass and microbial balances to steady state processes. The model of Mueller, Mulligan, and diToro² was based on those conditions. The model described the transfer of oxygen, nitrogen, and carbon dioxide between the gas and liquid phases, but did not account for nitrification. Therefore the total ammonia nitrogen concentration remained constant. Additionally, given the absence of nitrification and the assumption that all biologically produced CO₂ remains as CO₂, eliminated any significant alkalinity source or sink. The model was calibrated to an operating high purity oxygen process. The model was then applied to predict plant performance utilizing several sets of constant (time-invariant) feed conditions.

Gaudy, Srinivasaraghavan, and Saleh developed a steady state algorithm to account for the variabilities in the concentration of the biological solids through control of the return sludge concentration.³ The Monod growth equation was used to model substrate removal. Gaudy assigned effluent substrate concentration as the basis for plant efficiency evaluation. He concluded that system engineering variables had a greater impact on

process dynamics than changes in the biological constants.

The development of a true multicomponent mass transfer model of the gas-liquid interface was presented by McWhirter and Vahldieck.⁴ Initial development of the model included coupled equations. However, following the assignment of ideal conditions to the gas phase, and considering the dilute nature of the liquid phase concentrations the equations became non-interactive. Equations for the CO₂ gas/liquid equilibrium were based on the assumption that all non-ionized CO₂ was dissolved rather than in the form of carbonic acid. The equation for alkalinity was developed as a function of system pH and the mole fraction CO₂ in the gas phase. A complete set of equations were presented for gas/liquid component mass transfer. The gas purity predictions were then compared to an operating UNOX plant. The data indicate a very good fit.

Stenstrom and Andrews⁵ presented a development of mathematical process control strategies for dynamic activated sludge operations based on SCOUR, the Specific Oxygen Uptake Rate. The model included nitrification and demonstrated variable effluent quality (ammonia basis) as a function of the dynamic state. Various process control strategies were simulated in an effort

to maintain constant SCOUR demand irrespective of the time dependent influent parameters.

Hansen, Fiok, and Hovious of Union Carbide developed a statistical model of activated sludge process effluent performance based on linear dynamic modeling of specific operational parameters.⁶ The model was based on 21 months of data from an industrial waste water treatment plant. The model's operational predictive capability was directed toward effluent suspended solids, effluent soluble chemical oxygen demand, and effluent soluble biochemical oxygen demand. Additionally, the model was utilized to redefine operational strategies.

Cliff and Andrews used a structured model which divides the biomass into sections: active, inert, stored and stored particulate substrate.⁷ In their model, substrate removal was limited by its transport into the floc rather than the organisms metabolic rate. The substrate that was not immediately synthesized into active mass was stored for future use. Process simulations using the modified substrate utilization equations successfully predicted O₂ utilization time lag and attenuation of O₂ demand.

In 1986 Cliff and Andrews applied their model to a Houston treatment plant under semi steady state

conditions.⁸ All influent waste parameters were held constant except the influent flow rate and the influent biochemical oxygen demand. These two parameters were varied sinusoidally at a ratio of 2:1. The specific oxygen uptake rate had been determined at the Houston site in previous work.⁷ Following "calibration" they modeled the effects of variable bicarbonate alkalinity, and respiratory quotient on fourth stage pH and dissolved oxygen. Additionally, the effect of varying the gas/liquid volume ratio on the fourth stage dissolved oxygen concentration was simulated.

In 1988 Clifft and Andrews calibrated their dynamic model to a Houston waste water treatment plant.⁹ The biological reactions were not modeled theoretically. Rather, the oxygen uptake rates were measured directly in field experiments and inserted into the model as specific rates. The gas phase components included oxygen, nitrogen, carbon dioxide and argon. The model also accounted for gas leaks in the system. Although the leaks had no significant effect in the first two stages, the partial pressure of oxygen in the fourth stage was enhanced due to the leaks. The results of the dynamic modeling evidenced a very close fit between the model and the actual operating conditions. The resulting computer model provided an accurate predictive tool for varying operational conditions.

In 1989 Stenstrom, Kido, Shanks, and Mulkerin developed and applied a dynamic system model to resolve a process warranty dispute.¹⁰ This represented the application of theoretical modeling to actual process verification. The model was designed to determine the oxygen transfer rate under warranty conditions at the Sacramento Regional Water Treatment Plant. Additionally, if the transfer rate was insufficient, the model was to determine under what conditions the warranty specifications could be met. The model considered mass transfer of oxygen, nitrogen, and carbon dioxide in the gas phase. The biological kinetics were based on a modified Monod equation. The alkalinity was considered to be carbonaceous, plus the additional contribution from non-ionized ammonia. The resulting fit was excellent.

III MODEL DEVELOPMENT

The Mathematical model used in this simulation is based upon the work of several previous authors.^{2,4,8,9} Specifically, the model follows directly from the model presented by Stenstrom, Kido, and Mulkerin.¹⁰

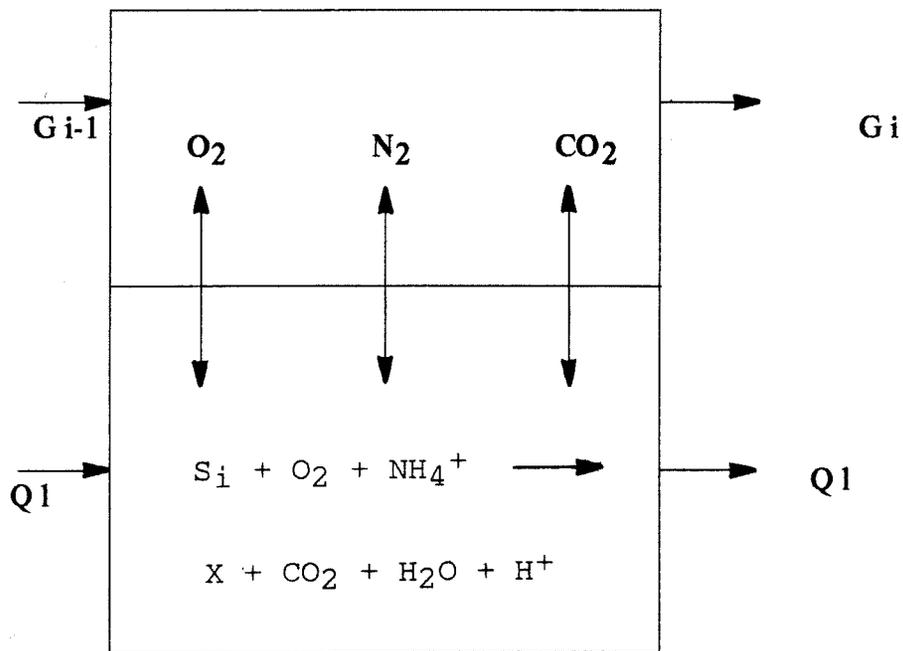


Figure 1

Mass transfer and the basic substrate reaction for Stage(i)

The following equations are used to mathematically represent a dynamic pure oxygen activated sludge process. Initially, all parameters have theoretical

values. During calibration, such parameters as the conversion factor for Biochemical Oxygen Demand (five day) to Biochemical Oxygen Demand (ultimate) are used to adjust the waste strength to match the operational process dynamics.

Mu: The Monod specific growth rate. This factor represents the growth rate of the microbiological population as a function of the substrate concentration available for consumption.¹⁰

Y: The yield coefficient. This parameter is a ratio of the mass of biologically active cells formed to the mass of substrate consumed.

Mu*X(1-Y)/Y: The total substrate converted to oxidation products during growth.

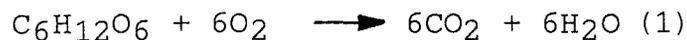
Mu*X(1-Y)*[]/Y:

[A]: Total oxygen consumed by substrate oxidation.



$$A = [\text{Kg O}_2/\text{Kg Substrate}] = 1.067$$

[YCO₂₁]: Total carbon dioxide produced during substrate oxidation.

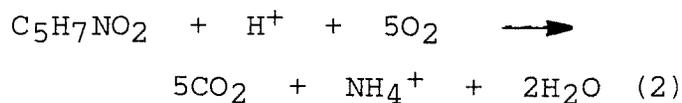


$$Y\text{CO}_{21} = [\text{Kg CO}_2/\text{Kg Substrate}] = 1.47$$

K_dX : Cells converted to oxidation products during decay.

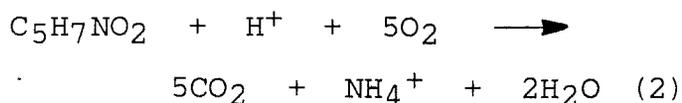
$K_dX[]$:

[B]: Oxygen consumed during cellular decay.



$$B = [\text{Kg O}_2/\text{Kg Cells}] = 1.42$$

[YCO_{22}]: Total carbon dioxide produced during cellular decay.



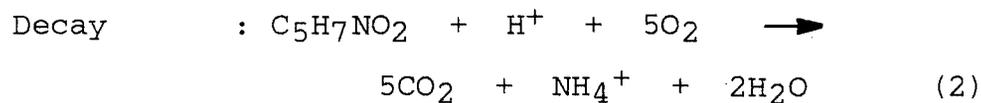
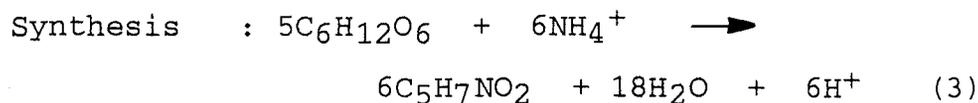
$$\text{YCO}_{22} = [\text{Kg CO}_2/\text{Kg Cells}] = 1.95$$

The K_{La} values were determined during a clean water test at the manufacturer's location. It is assumed that gas transfer occurs by two film theory and is liquid side limited. The wastewater is presumed to be of low ionic strength. Therefore the K_{La} for CO_2 and N_2 will be a function of the ratio of the molecular diffusivities of CO_2 and N_2 to oxygen.

BIOLOGICAL REACTIONS:

The equations used for the biological mass and substrate balances were based on a glucose model of growth and respiration.¹¹





Equations 1 to 3 are incorporated into the model in the mass balance equations.

Biological Solids:

$$\frac{dx}{dt} = \frac{Q_L}{V_L}[X_0 - X] + [\text{Mu} - K_d] \cdot X \quad (4)$$

Substrate:

$$\frac{ds}{dt} = \frac{Q_L}{V_L}[S_0 - S] - \frac{\text{Mu} \cdot X}{Y} \quad (5)$$

Where Q_L = Liquid Flow Rate

V_L = Reactor Volume

S_0 = Influent substrate concentration

S = Reactor substrate concentration

X_0 = Influent biological solids concentration

X = Reactor biological solids concentration

Modified Monod Growth Equation:

$$\text{Mu} = [(\text{Mu}_{\text{hat}} \cdot S) / (K_S + S)] / [\text{DO} / (\text{DO} + K_{\text{SDO}})] \quad (6)$$

The concentration of biological solids in the aeration tank at any time is a function of the flux plus the net growth. The net growth being the difference between μ (Monod specific growth rate) and K_d (decay rate).

The substrate serves as a food source for the biological solids.

MASS BALANCES:

Liquid Phase

Oxygen:

$$\frac{dO_2}{dt} = \frac{Q_L}{V} [C_{in} - C_{out}] + \alpha K_{La} [\text{Beta} \cdot C_{inf}^* - C] - \frac{A \cdot \mu \cdot X \cdot [1 - Y]}{Y} - B K_d \cdot X \quad (7)$$

Carbon Dioxide:

$$\frac{dDCD}{dt} = \frac{Q_L}{V_L} [DCD_o - DCD] + K_{KLaco2} [DCD_s - DCD] + \mu \cdot X \left[\frac{1 - Y}{Y} \right] \cdot Y_{co21} + K_d \cdot X \cdot Y_{co22} \quad (8)$$

Nitrogen:

$$\frac{dDN}{dt} = \frac{Q_L}{V_L} [DN_o - DN] + K_{LAN2} [DN_s - DN] \quad (9)$$

Gas Phase

Oxygen:

$$\frac{dO_2}{dt} = \frac{Q_{Go} O_{2o} - Q_G O_2}{V_G} - K_{LaO_2} [DO_s - DO] \frac{V_L}{V_G} \frac{1}{MW_{O_2}} \quad (10)$$

Carbon Dioxide:

$$\frac{dCO_2}{dt} = \frac{Q_{Go} CO_{2o} - Q_G CO_2}{V_G} - K_{LaDCD} [DCD_s - DCD] \frac{V_L}{V_G} \frac{1}{MW_{CO_2}} \quad (11)$$

Nitrogen:

$$\frac{dN_2}{dt} = \frac{Q_{Go} N_{2o} - Q_G N_2}{V_G} - K_{LaN_2} [DN_s - DN] \frac{V_L}{V_G} \frac{1}{MW_{N_2}} \quad (12)$$

Where: C_{in} = influent dissolved oxygen concentration

C_{out} = effluent dissolved oxygen concentration

C_{inf}^* = oxygen saturation concentration

C = dissolved oxygen concentration in reactor

DCD_o = influent dissolved carbon dioxide concentration.

DCD = dissolved carbon dioxide concentration in reactor.

DCD_s = dissolved carbon dioxide saturation concentration.

DN_o = influent dissolved nitrogen concentration.

DN = dissolved nitrogen concentration in reactor.

DN_s = dissolved nitrogen saturation concentration.

Q_{G0} = influent gas flow rate.

Q_G = effluent gas flow rate.

V_G = gas volume

O₂₀ = influent gas oxygen concentration

O₂ = reactor gas oxygen concentration

CO₂₀ = influent gas carbon dioxide concentration

CO₂ = reactor gas carbon dioxide concentration

N₂₀ = influent gas nitrogen concentration

N₂ = reactor gas nitrogen concentration

Gas Flow Forcing Function:

$$Q_G = K_{\text{flow}}[P_{\text{sp}} - P_t] \quad (13)$$

Partial Pressures:

$$P_{\text{CO}_2} = \text{CO}_2 \cdot RT \quad (14)$$

$$P_{\text{O}_2} = \text{O}_2 \cdot RT \quad (15)$$

$$P_{\text{N}_2} = \text{N}_2 \cdot RT \quad (16)$$

$$P_T = P_{\text{CO}_2} + P_{\text{O}_2} + P_{\text{N}_2} + P_{\text{H}_2\text{O}} \quad (17)$$

Saturation Concentrations:

H_e is the Henrys' Law constant. The model adjusts the constant as a function of the reactor liquid temperature.^{10,12}

$$DO_S = 5.5555 \cdot 10^4 [MWT_{O_2} / H_e O_2] \cdot P_{O_2} \cdot BETA \quad (18)$$

$$DCD_S = 5.5555 \cdot 10^4 [MWT_{CO_2} / H_e CO_2] \cdot P_{CO_2} \cdot BETA \quad (19)$$

$$DN_S = 5.5555 \cdot 10^4 [MWT_{N_2} / H_e N_2] \cdot P_{N_2} \cdot BETA \quad (20)$$

The alkalinity at the Joint Water Pollution Control Plant is assumed to be primarily carbonaceous in nature. The equation for alkalinity will include the contribution from ammonia.

$$ALK = \{HCO_3^-\} \cdot Activity_{HCO_3^-} + 2\{CO_3^{2-}\} \cdot Activity_{CO_3^{2-}} + \{OH^-\} \cdot Activity_{OH^-} + \{NH_3\} \cdot Activity_{NH_3} - \{H^+\} \cdot Activity_{H^+} \quad (21)$$

Following from the assumption that the wastewater is of low ionic strength, the activity coefficient will be assigned a value of 1.¹³

$$K_1 = [H^+] [HCO_3^-] / [H_2CO_3^*] \quad (22)$$

$$K_2 = [H^+] [CO_3^{2-}] / [HCO_3^-] \quad (23)$$

$$K_W = [H^+] [OH^-] \quad (24)$$

$$ALK = K_1 [H_2CO_3^*] / [H^+] + 2K_1K_2 [H_2CO_3^*] / [H^+]^2 + K_W / [H^+] - [H^+] + [NH_3] \quad (25)$$

$H_2CO_3^*$ is the total concentration of H_2CO_3 and the fraction of nonionized CO_2 that is dissolved. When the terms are combined the equation becomes cubic in $[H^+]$, and must be solved iteratively. The fraction of the total dissolved CO_2 that is nonionized can be expressed in the following form.

$$f_{CO_2} = [H_2CO_3^*] / [H_2CO_3^*] + [HCO_3^-] + [CO_3^{2-}] \quad (26)$$

$$= 1 / (1 + K_1 / [H^+] + K_1K_2 / [H^+]^2) \quad (27)$$

The concentration of dissolved CO_2 that is not ionized equals, $DCD * f_{CO_2}$.¹⁰

The fraction of the total ammonia that is NH_3 can be expressed in the following form.

$$f_{NH_3} = 1 / (1 + [H^+] K_{NH_3} / K_W) \quad (28)$$

The concentration of ammonia that is NH_3 equals, $[NH_3_{Total}] * f_{NH_3}$.

The final alkalinity equation is expressed as:

$$\text{ALK} = \frac{(K_1 [\text{H}_2\text{CO}_3^*] [\text{H}^+] + 2K_1K_2 [\text{H}_2\text{CO}_3^*] + K_W [\text{H}^+] - [\text{H}^+]^3 + [\text{H}^+]^2 [\text{NH}_3])}{[\text{H}^+]^2} \quad (29)$$

The program solves equation thirty iteratively to determine the pH.

$$0 = [\text{H}^+]^2 + [\text{H}^+] [\text{ALK} - \text{NH}_3] - K_W - (K_1 + 2K_1K_2/[\text{H}^+]) [\text{H}_2\text{CO}_3^*] \quad (30)$$

IV MODEL CALIBRATION

During an 8 day period in May of 1984 the County Sanitation Districts of Los Angeles County conducted a process water test at the Joint Water Pollution Control Plant in Carson California. The test was performed on reactor D, one of four parallel trains, of the recently completed high purity oxygen activated sludge plant. The test was to verify that the process could dissolve oxygen at the rate specified under the warranty conditions of the purchase contract. Those specifications are detailed in tables one and two. The results indicated that the process performed beyond expectations and easily achieved the warranty specifications.

The historical data collected during the verification test was used to calibrate a mathematical model to simulate process performance.

Certain fixed process parameters were required for the model. These included:

- 1) Physical Dimensions
- 2) K_{La}
- 3) Alpha Factors

TABLE 1 Warranty conditions

FLOW:	62.5 Million Gallons per Day
OXYGEN UPTAKE RATE:	5625 Lbs. per Day
AVERAGE CONCENTRATION OF DISSOLVED OXYGEN:	6 mg/l none less than 2 mg/l
POWER CONSUMPTION:	809 KWHr

TABLE 2 Operating conditions adjusted to warranty conditions for comparison.

FLOW:	62.41 Million Gallons per Day
OXYGEN UPTAKE RATE:	7600 Lbs. per Day
AVERAGE CONCENTRATION OF DISSOLVED OXYGEN:	14.5 mg/l
POWER CONSUMPTION:	600 KWHr

Table three presents the physical dimensions of the aeration basins.¹⁴ Although most primary effluent parameters are dynamic, the ammonia and alkalinity concentrations were considered to be static do to a lack of available data.

The K_{La} values were determined during clean water testing at the Mixco test facility in September and October of 1979. Table four contains the results of the K_{La} determination from the clean water test report, and the surface aerator placement at the Joint Water Pollution Control Plant.¹⁵

The actual tests were performed to simulate process conditions. The test tanks had the same liquid depth and 98% of the of the surface area per aerator.

The alpha factors were determined by analyzing the process water test data, and found to be 0.9 for all stages.

The data available for model calibration were historical. The data were collected for process warranty verification, as opposed to process modeling. Unfortunately, this situation presented several shortcomings. The Biochemical Oxygen Demand (five day) were collected at 24 hour intervals. For modeling, the

data should be collected at least every 4 hours to indicate fluctuations in waste strength. These fluctuations would be expected at a treatment facility with an influent that is a combination of domestic and industrial wastewater. The influent flow rate during the test period was 62.5 million gallons per day, which is the design peak capacity. There were no indications of any diurnal flow fluctuations during the test period. The dissolved oxygen concentration and head space gas purity data were collected at 3 hour intervals. Unfortunately, no carbon dioxide partial pressure or gas phase concentration data were included in the process verification report. The treatment plant laboratory data did not include influent alkalinity. Therefore, the process alkalinity was set to warranty conditions.

TABLE 3 Physical dimensions of the aeration basins.

UNITS PER TRAIN: 4
 LENGTH PER TRAIN: 250 ft.
 WIDTH PER TRAIN: 187.5 ft.
 WATER DEPTH: 15 ft.
 VOLUME PER TRAIN: 5.26 Million Gallons

TABLE 4 Oxygen transfer coefficient for the surface aerators.

STAGE	AERATOR	HP	K_{La20}
1	1 - 3	125	11.875
2	4 - 6	75	6.208
3	7 - 9	75	6.208
4a&b	10-12	75 & 125	7.767

CALIBRATING THE MODEL:

Calibrating any mathematical model to a dynamic system is a challenge unto itself. Fitting a model with data originally collected for another purpose can become quite an undertaking. The data available included:

1) dissolved oxygen concentration 2) partial pressure of oxygen 3) influent and effluent Biochemical Oxygen Demand 4) volatile suspended solids 5) gas and liquid flow rates 6) feed gas purity . It was decided to use the dissolved oxygen concentration and partial pressure data as the basis for the model fit.

Initial computer simulations used theoretical and average values for the biological parameters. Given that the Joint Water Pollution Control Plant receives an unknown portion of industrial waste in the secondary systems influent, the Biochemical Oxygen Demand (five day) to ultimate ratio was adjusted until the oxygen demand on a power weighted average basis matched the plants oxygen demand. μ and K_d were adjusted to distribute the load through the four tanks to match the oxygen partial pressure and dissolved oxygen concentrations. The alpha factor presented somewhat of a quandary. The values from steady-state analysis ranged from 0.904 to 1.051 depending upon which power weighted basis was used for calculation. Initially, a

value of 0.904 was used, but the resulting dissolved oxygen values were too low. The alpha value was then increased to 1.00. The fit improved, but the dissolved oxygen concentrations were still too low. Increasing the alpha factor above 1.00 could not be justified. The County Sanitation Districts of Los Angeles County used an in line flow totalizer to determine gas flow to the process, the accuracy of which is not known. Therefore, the oxygen gas feed rate to the process was increased until an acceptable fit was achieved. This required an increase of 8%.

The model's fit was good but not exceptional. The difference between the model's predicted dissolved oxygen concentration and oxygen partial pressure (P.P.) to the actual process data are presented in table five.

The error between the models predicted values, and the County's data are particularly evident in tanks 1 and 4. The oxygen purity in tank 1 was recorded at 87%. This value was suspect as it was about 10% greater than would be expected from this type of high purity plant. Unfortunately, no carbon dioxide partial pressure data were available. If the carbon dioxide concentration in the gas phase were known, the Y_{CO_2} coefficient [kg CO₂/kg substrate] could have been adjusted to fit the operational conditions, rather than using a

theoretical value. Given that the Joint Water Pollution Control Plant does treat industrial wastewater, in addition to domestic sewage, it is quite conceivable that the assigned value of Y_{CO_2} was too large. If a smaller coefficient had been used, the oxygen purities would have been greater, and the oxygen partial pressure depression would not have been as magnified in stage 4.

TABLE 5 Error in model prediction

TANK	D.O. ERROR mg/l	%	P.P. ERROR atm%	
1	1.25	11	0.1203	14
2	1.63	9	0.0538	7
3	0.94	5	0.0211	4
4	2.72	20	0.1068	25

V PLANT STUDIES

The dynamic model was applied to the Carson plant to determine its maximum treatment capacity. The Carson plant's history of stable performance and removal of the surface aerators blade tips to reduce the oxygen transfer coefficient was sufficient evidence to indicate the plant's capacity was significantly under utilized.

Two types of process simulations were preformed. The first modeled an increased wastewater flow rate with diurnal fluctuations. These fluctuations were based on a sinusoidal function whose amplitude was varied to achieve a predetermined flow variance. To determine if a more economical utilization of the plants' cryogenic oxygen capacity could be achieved, additional simulations were preformed with the oxygen feed rate based on the influent sewage flow rate and the dissolved oxygen concentration in stage four. The dissolved oxygen set point was 6.0 mg/l. This was based on the operational warranty conditions.

It was stipulated that the plants' capacity was exceeded if the dissolved oxygen concentration in tank four fell below 3.0 mg/L. This was based on the warranty condition that no dissolved oxygen would be below 2 mg/L. The 1.0 mg/L buffer was included to minimize the

effect of any oxygen production time lag resulting from unforeseen fluctuations in waste strength that might consume excessive amounts of oxygen in stage one. The operational parameters assigned to the model's influent variables were based on a seven day average during the verification period. These parameters included: 1) oxygen feed rate 2) feed gas purity 3) wastewater strength based on Biochemical Oxygen Demand {five day} 4) wastewater influent flow rate. The base influent parameters are presented in table six.

The first simulation was based on an operating strategy of constant influent wastewater flow rate and constant oxygen feed rate. The data are presented in Figure 2. At 90 MGD the stage four dissolved oxygen concentration did not drop below 3.0 mg/l. The initial part of the graph shows the initial condition of the transients. As the simulation proceeds, the process parameters reach steady-state condition.

TABLE 6 Steady state influent parameters for capacity simulation

Oxygen Feed Rate:	52.55 ton/day
Feed Gas Purity:	97%
Waste Strength:	127 (BOD5)
Influent Sewage Flow Rate:	62.5 MGD

FINAL STAGE D.O.
CONSTANT FLOW RATE

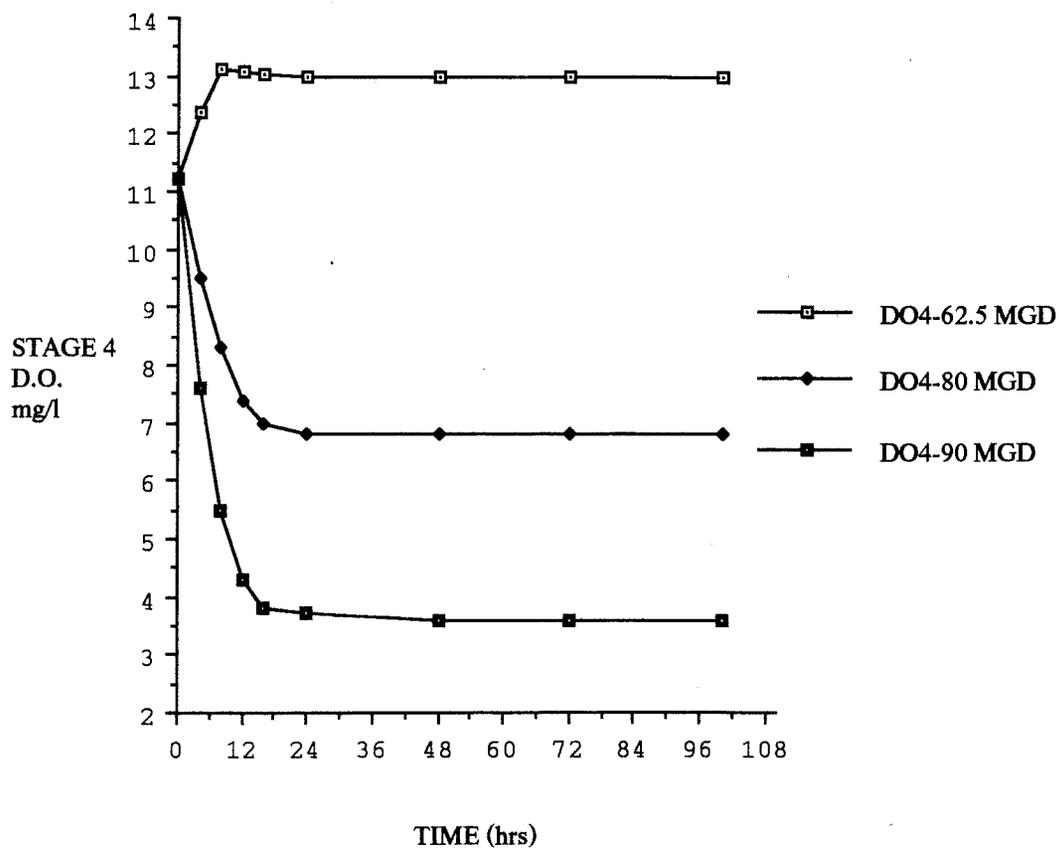


Figure 2 Final stage dissolved oxygen concentration, constant liquid and gas flow rates

FINAL STAGE D.O.
CONTROLLED GAS FLOW RATE

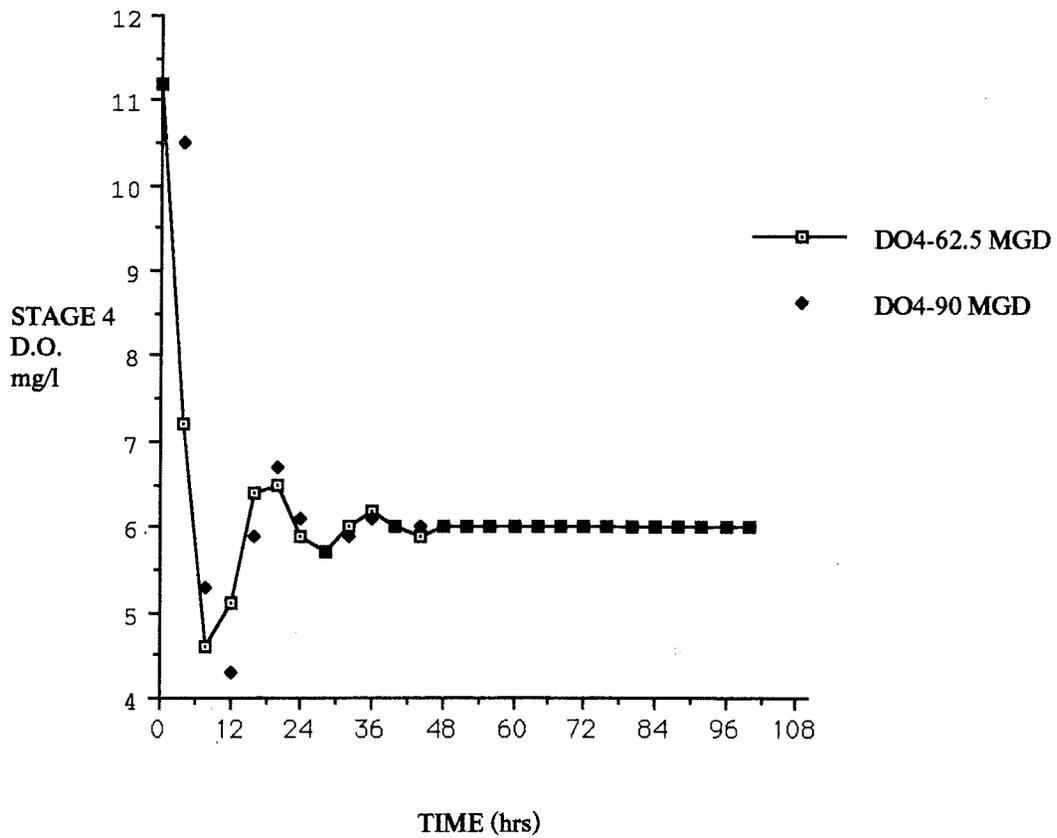


Figure 3 Final stage dissolved oxygen concentration, controlled gas flow rate.

INFLUENT GAS FEED RATE
CONSTANT WASTEWATER FLOW RATE

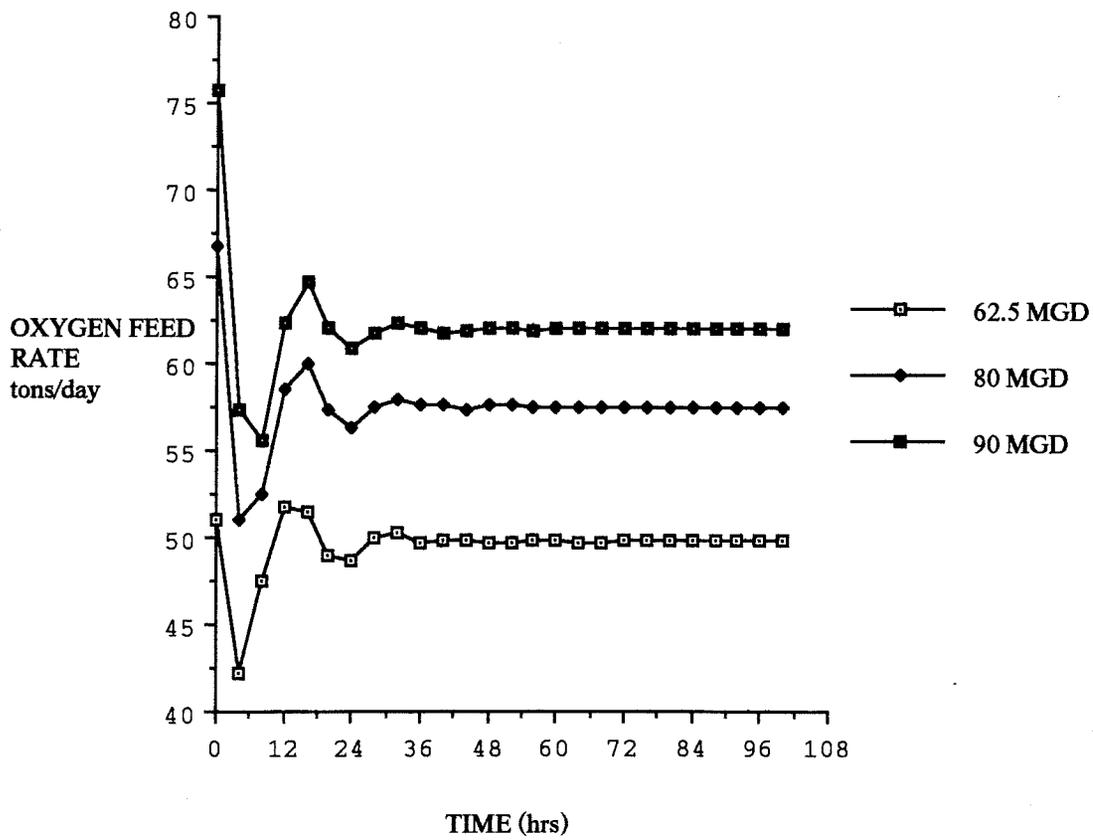


Figure 4 Influent gas feed rate, constant liquid feed rate.

The second simulation case was based upon a constant sewage influent rate while the oxygen feed rate was a function of the fourth stage dissolved oxygen concentration. Figure 3 presents the fourth stage dissolved oxygen concentration as a function of time. Steady state was achieved within 48 hours. Figure 4 shows the oxygen feed rate in tons per day as a function of time and influent wastewater flow rate. The maximum oxygen production rate of 75 tons per day-train was never exceeded by demand even at 90 MGD.

The third simulation involved a variable wastewater influent flow rate, while the oxygen feed rate was kept constant. This type of model simulates the behavior of a high purity plant with minimal or nonexistent turn down ability afforded by the oxygen plant. The magnitude of sinusoidal (diurnal) flow fluctuation was 16 and 32 percent. A third run set the influent sewage base rate to 80 MGD and 20 percent sinusoidal fluctuation. The data are presented in Figure 5. At no time did the dissolved oxygen concentration drop below 3.0 mg/l. However, when the fluctuation was increased to 40 percent, the model failed due to insufficient dissolved oxygen concentration.

The final simulation involved both diurnal fluctuation and a controlled variable oxygen feed rate. This case

represents process control, and real world feed conditions. Figure 6 presents the fourth stage dissolved oxygen concentration as a function of time for three cases of flow fluctuation. To determine the maximum plant capacity, the influent wastewater flow rate was steadily increased until the fourth stage dissolved oxygen concentration dropped below 3.0 mg/l. The maximum treatable capacity is 80 MGD with 20 percent diurnal fluctuation. However, the model predicts that 90 MGD could also be treated as the minimum dissolved oxygen concentration was 2.9 mg/l, only 0.1 mg/l below the cut off value. These data are presented in Figure 7.

The model was used to determine the required dynamic oxygen feed rate when the influent wastewater rate was 62.5 MGD with 16, 20, and 30 percent diurnal fluctuation. Figure 8 presents the required oxygen feed rate to maintain a dissolved oxygen concentration of 6.0 mg/L in tank four. At no time was the oxygen plants' capacity exceeded.

An example of a failure condition is presented in Figure 9. The gas flow rate was fixed, and the wastewater flow was 90 MGD with 20 percent diurnal fluctuation.

FINAL STAGE D.O.
 FIXED GAS : SINUSOIDAL WASTEWATER FEED RATE

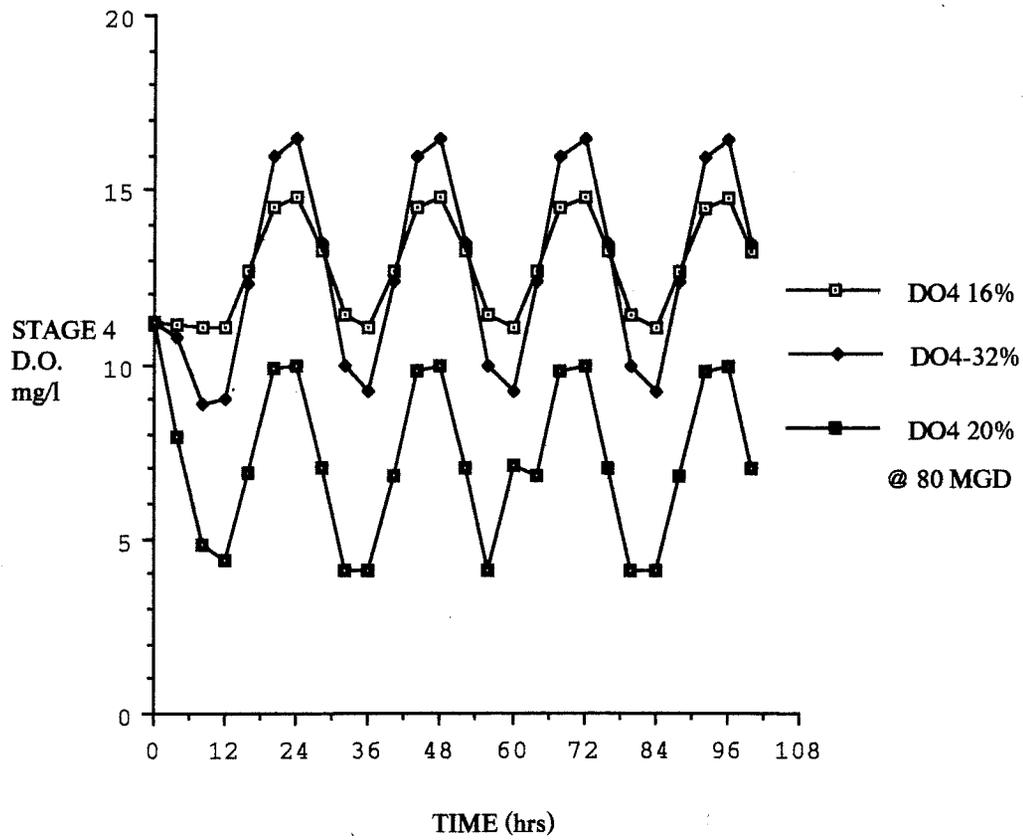


Figure 5 Final stage dissolved oxygen , fixed gas feed rate, sinusoidal liquid feed rate.

FINAL STAGE D.O.
 CONTROLLED GAS
 SINUSOIDAL WASTEWATER FEED RATE

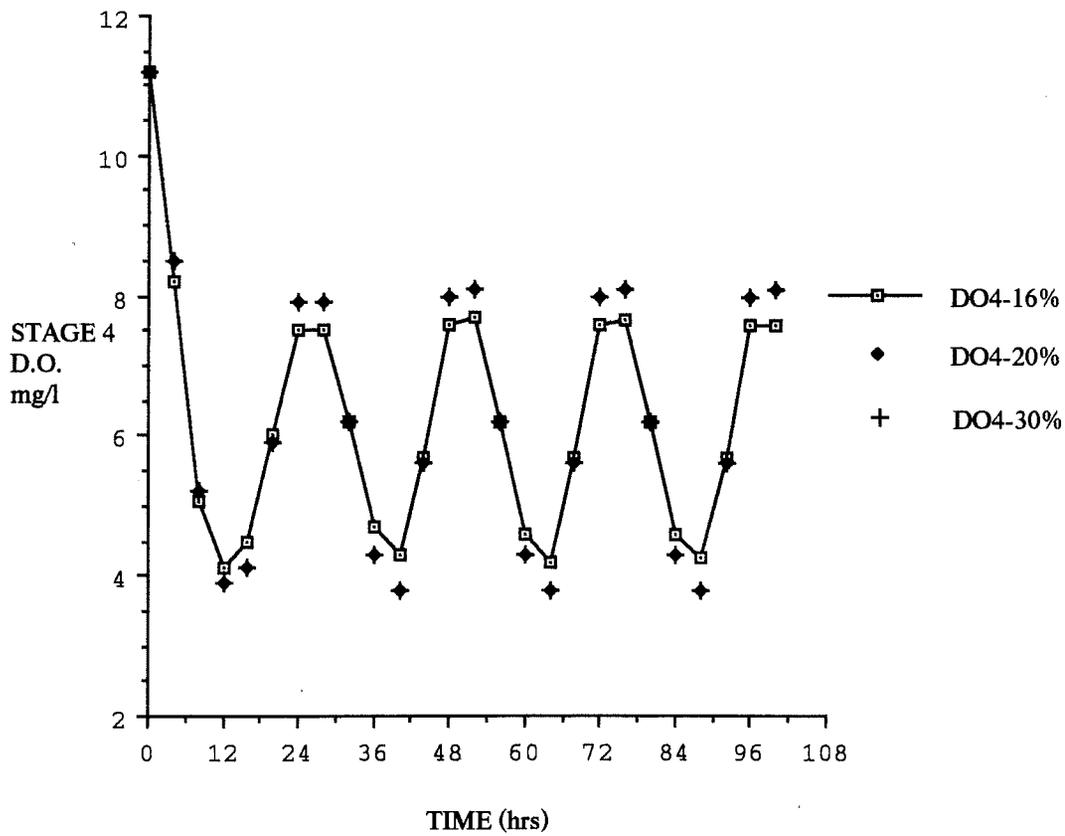


Figure 6 Final stage dissolved oxygen , controlled gas feed rate, sinusoidal liquid feed rate.

FINAL STAGE D.O.
 CONTROLLED GAS
 SINUSOIDAL WASTEWATER FEED RATE

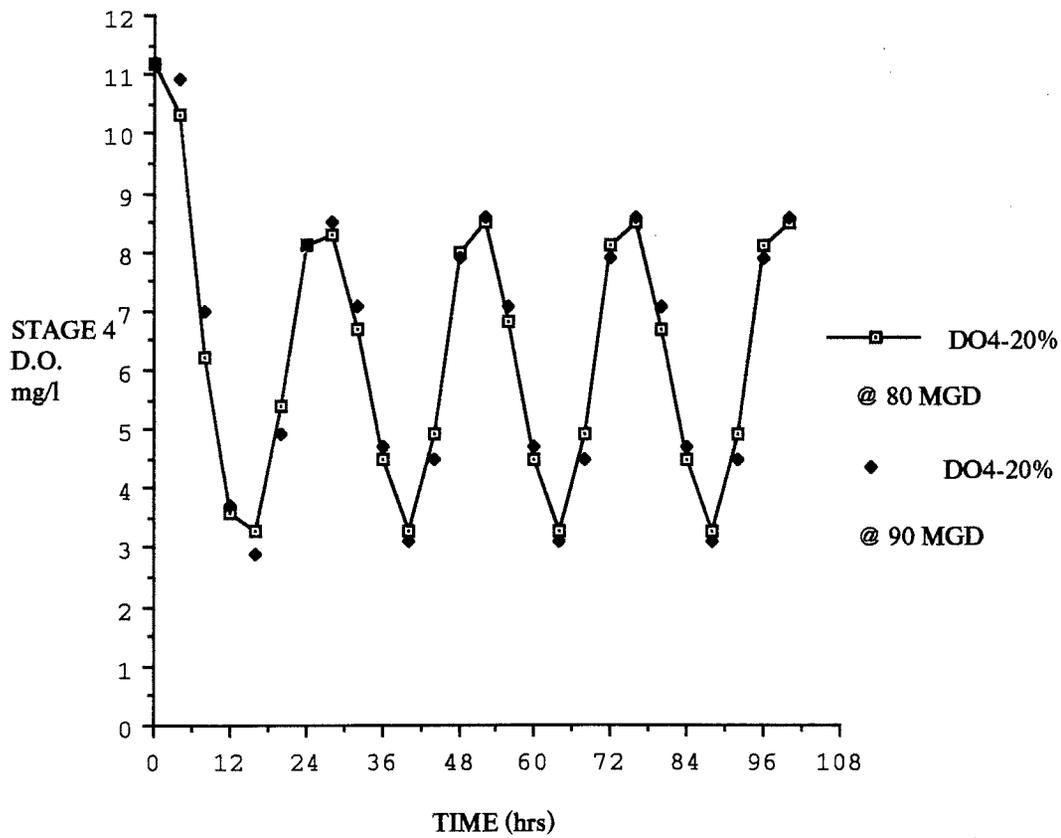


Figure 7 Final stage dissolved oxygen , controlled gas feed rate, sinusoidal liquid feed rate.

INFLUENT GAS FEED RATE
SINUSOIDAL WASTEWATER FEED RATE

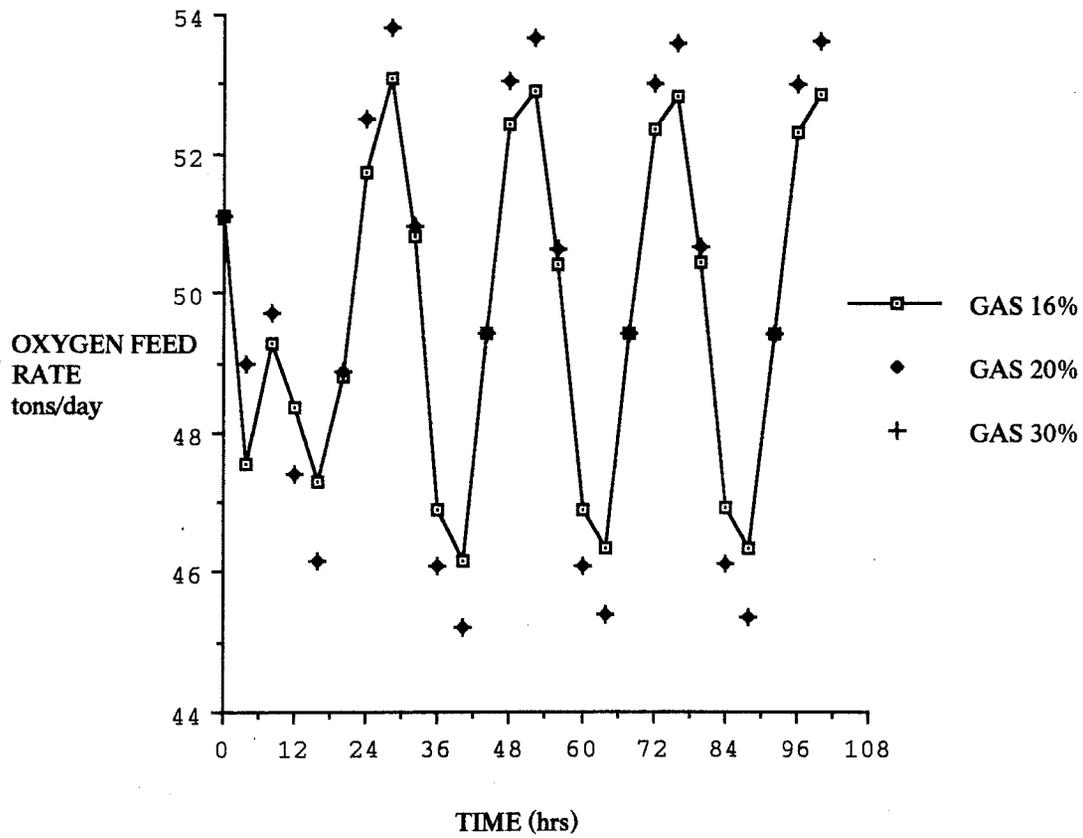


Figure 8 Influent gas feed rate with sinusoidal liquid feed rate.

STAGE 4 D.O.
BELOW MINIMUM

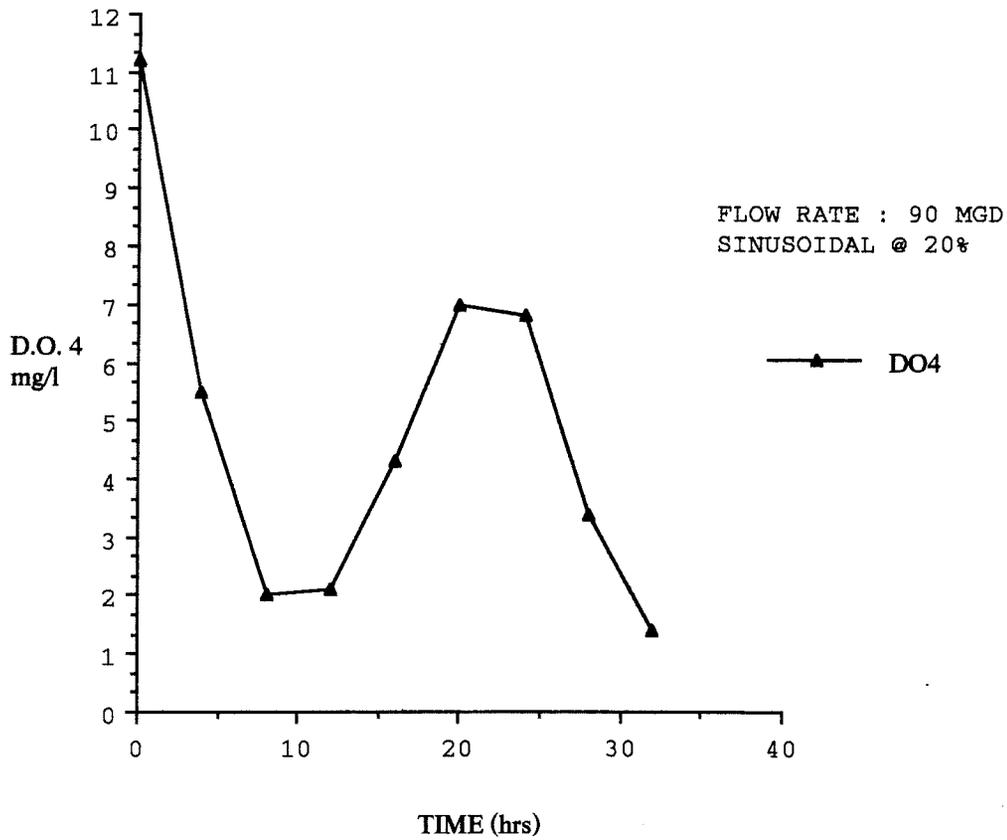


Figure 9 Final stage dissolved oxygen below the established minimum.

STAGE 4 D.O. FOR VARIABLE
AND FIXED GAS FLOW

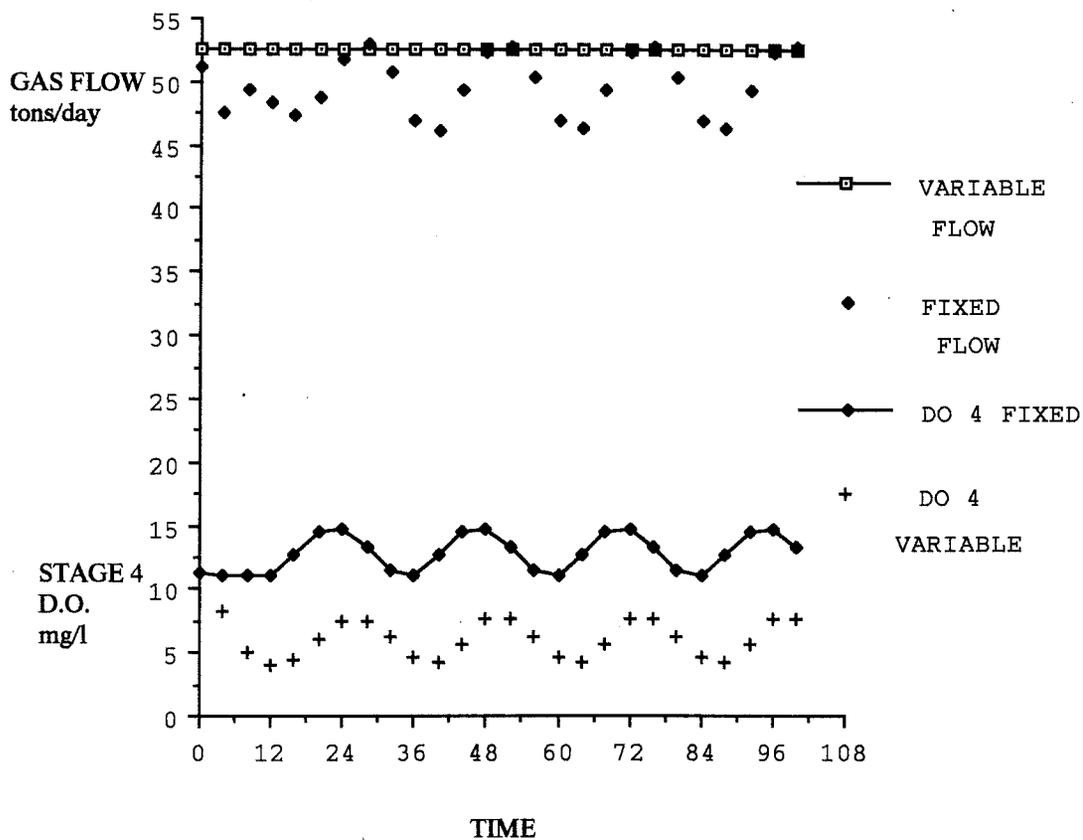


Figure 10 Final stage dissolved oxygen for variable and fixed gas flow.

To determine if any reduction in oxygen usage could be realized through flow control, the operating condition of 62.5 MGD with 16 percent diurnal fluctuation was selected. The standard feed condition used 54.18 tons of oxygen per day, while the flow controlled system used 49.71 tons of oxygen per day. A savings of 4.47 tons of oxygen per day. The data are presented in Figure 10.

VI CONCLUSIONS

The application of a dynamic mathematical model to the County Sanitation District of Los Angeles Counties' high purity oxygen activated sludge treatment plant produced two distinct conclusions: 1) The computer model's applicability is a function of the quality and quantity of the calibration data. 2) The Carson plant is significantly under loaded.

The computer model was stable and flexible during the simulations. However, any model is only as strong as its weakest link. In this case, that link is the calibration data. The calibration data were originally collected during a warranty verification experiment of the oxygen transfer capability, shortly after the initial start up. For modeling, the Biochemical Oxygen Demand samples should have been taken every four hours. The dissolved oxygen concentration, oxygen and carbon dioxide partial pressure, and influent gas and wastewater flow rates should have been collected hourly. Had the data been acquired more frequently, the model's calibration would have been better, although, the fit was good.

The conclusions based upon simulation results about the operation of the Carson plant are straightforward. The

plant is operating significantly below capacity as a function of oxygen transfer capability. The plant has a design load capacity of 50 MGD, with peak flow capacity of 62.5 MGD. The warranty conditions were specified for the peak operational conditions. The data from the simulations indicate that each stage could treat as much as 90 MGD under ideal constant flow conditions. Each stage has a capacity of 80 MGD with the inclusion of sinusoidal diurnal flow, if the oxygen feed rate is coupled to the fourth stage dissolved oxygen concentration, and influent sewage flow rate. Although, as the influent flow rate increases, the predicted sludge age decreases. To maintain a sludge with good settling characteristics, a balance must be struck between capacity and stability. The conclusions drawn from the simulation data are strictly based on oxygen transfer capability, and Biochemical Oxygen Demand (five-day) removal. Process hydraulics and secondary clarifier performance are untested. Actual operational conditions may significantly restrict any increase in treatment capacity. Additionally, the model does not account for sludge production, which may also limit any increased treatment rate.

The plants current under loading provides the County with a situation wherein the plant has an extensive degree of industrial waste shock capacity. A stable

plant does not provide the impetus to drastic operational change. However, a new operational strategy might be to balance the ratio of flow to capacity against industrial waste shock stability as a function of the industrial waste feed fraction.

Finally, older cryogenic oxygen production plants have limited ability to modulate oxygen production. Therefore, if flow control is instituted, the plant could operate at the average rate of the sinusoidal demand curve. During the decreasing demand portion of the curve, the excess oxygen could be stored for use during the peak portion of the curve, which would reduce the overall operating costs.

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APPENDIX

A : MODEL PARAMETERS

B : COMPUTER PROGRAM LISTING

SECTION A:

Model Parameters

Muhat	=	0.25 hr ⁻¹
Y	=	0.62
Y _{O21}	=	1.07
Y _{O22}	=	1.42
Y _{NH31}	=	0.039
Y _{NH32}	=	0.1239
K _{SDO}	=	2.5 g/M ³
K _S	=	50 g/M ³
Y _{CO21}	=	1.37
Y _{CO22}	=	1.95
K _D	=	0.0127 hr ⁻¹
BETA	=	0.985
K _{LaCO2}	=	0.836K _{LaO2}
K _{LaN2}	=	0.943K _{LaO2}
THETA	=	1.024
BOD5TOU	=	0.52

SECTION B:

Computer Program Listing

MACRO

XJ, SJ, DOJ, DN2J, DCDJ, HIJ, FCDJ, QGJ, PCO2J, PO2J, PN2J, CO2J, N2J, O2J, ...
DNH3J, ALKJ=REACT (THETAJ, XOJ, SOJ, DOOJ, DN2OJ, DCDOJ, HIOJ, QGOJ, CO2OJ, .
..
N2OJ, O2OJ, ICXJ, ICSJ, ICDOJ, ICDN2J, ICDCDJ, ICCO2J, ICO2J, ICN2J, CKLAOJ,
...

VLJ, TPRESJ, TPRESI, DNH3OJ, ALKOJ)

***** LIQUID PHASE MASS BALANCES *****

* CORRECT FLOW FOR PRESSURE CHANGE

QGNJ=QGOJ*TPRESJ/TPRESI

* MICROBIAL MASS BALANCE

$DXDT = (XOJ - XJ) / THETAJ + (MUJ - KD * O2LIM) * XJ$

$XJ = INTGRL(ICXJ, DXDT)$

* ORGANISM GROWTH RATE

$MUJ = MUHAT * SJ * DOJ / ((SJ + KS) * (DOJ + KSDO))$

* COMMENT OUT THE ABOVE EXPRESSION FOR MU AND SUBSTITUTE WITH THE

* FOLLOWING EXPRESSION WHICH IS MORE CONVENIENT FOR PERFORMANCE

CALCS.

$O2LIM = (DOJ / KSDO) / (1. + (DOJ / KSDO))$

$MUJ = MUHAT * SJ / (SJ + KS) * O2LIM$

* SUBSTRATE BALANCE

$DSDT = (SOJ - SJ) / THETAJ - MUJ * XJ / Y$

$SJ = INTGRL(ICSJ, DSDT)$

* AMMONIA BALANCE

$DNH3RJ = (YNH32 * KD * O2LIM + YNH31 * MUJ / Y - YNH32 * MUJ) * XJ$

$DDNH3J = (DNH3OJ - DNH3J) / THETAJ + DNH3RJ$

$DNH3J = INTGRL(ICNH3J, DDNH3J)$

* CALCULATE THE ALKALINITY INCREASE FROM AMMONIA INCREASE

$ALKJ = ALKOJ + (DNH3J - DNH3OJ) / 14.E+03$

* SET THE MASS TRANSFER COEFFICIENTS FOR NITROGEN AND CARBON

DIOXIDE

* TO THE SOME FRACTION OF THE VALUE FOR OXYGEN

$CKLANJ = CKLAOJ * FKLAN2$

$CKLACJ = CKLAOJ * FKLACO$

* DISSOLVED OXYGEN

$O2UPJ = MUJ * XJ * YPO21 + KD * XJ * YO22 * O2LIM$

```

DODT= (DOOJ - DOJ)/THETAJ + SDOJ - O2UPJ
DOJ = INTGRL(ICDOJ,DODT)
* DISSOLVED NITROGEN
DN2DT=(DN2OJ - DN2J)/THETAJ +SDN2J
DN2J = INTGRL(ICDN2J,DN2DT)
* DISSOLVED CO2
*DCDR=MUJ*XJ*YPCO21 + KD*XJ*YCO22*O2LIM
DCDRJ=O2UPJ*1.375
DCDDT=(DCDOJ-DCDJ)/THETAJ+SDCDJ + DCDRJ
DCDJ = INTGRL(ICDCDJ,DCDDT)
***** GAS SATURATION CONCENTRATIONS *****
* OXYGEN
DOSJ=PO2J/HEO2
* NITROGEN
DN2SJ=PN2J/HEN2
* CARBON DIOXIDE
DCDSJ=PCO2J/HECO2
***** PH AND FRACTION OF DISSOLVED CARBON DIOXIDE WHICH IS
*
          H2CO3 (USE FUNCTIONS TO SIMPLIFY)
FCDJ =FCO2 (HIJ,CK1,CK2)
HIJ=PHCAL (ALKJ,DCDJ,DNH3J,CK1,CK2,CKW,CKNH3)
***** GAS SIDE BALANCES*****
* STRIPPING RATES
* CO2
SDCDJ=CKLACJ*(DCDSJ - DCDJ*FCDJ)
* DO
SDOJ =CKLAOJ*(DOSJ - DOJ)
* NITROGEN
SDN2J =CKLANJ*(DN2SJ - DN2J)
* VOLUMETRIC GAS PRODUCTION
  QGJ=LIMIT(0.,10000.,(KFLOW*((VPH2O+PCO2J+PO2J+PN2J)-TPRESJ)))
* CO2 BALANCE
CO2DT = (QGNJ*CO2OJ - QGJ*CO2J)/VG -SDCDJ*VLJ/(VG*MWCO2)
CO2J = INTGRL(ICCO2J,CO2DT)
* N2 BALANCE
N2DT = (QGNJ*N2OJ - QGJ*N2J)/VG -SDN2J*VLJ/(VG*MWN2)

```

N2J = INTGRL(ICN2J,N2DT)

* O2 BALANCE

O2DT = (QGNJ*O2OJ - QGJ*O2J)/VG - SDOJ*VLJ/(VG*MWO2)

O2J =INTGRL(ICO2J,O2DT)

* PARTIAL PRESSURES

* CO2

PCO2J = CO2J*RT

* N2

PN2J = N2J*RT

* O2

PO2J = O2J*RT

ENDMAC

INITIAL

* THIS SECTION DESCRIBES THE INITIAL CONDITIONS AND INPUTS TO THE
* REACTORS.

** FIRST THE BIOX PARAMETERS

PARAM MUHAT=0.250, Y=0.62, YO21=1.07, YO22=1.42, YB5TOU=0.52

PARAM YNH31=0.039, YNH32=0.1239

PARAM KSDO=2.50, KS=50., YCO21=1.37, YCO22=1.95, KD=0.01270, NPRINT=2

* PARAMETERS FOR SLUDGE RECYCLE

PARAM ALKR=5.76E-03, DCDR=120., DN2R=10.

PARAM DTIME1=0., DTIME2=100.0, OFFSET=0., O2LAG=0

PARAM MWCO2=44.009, MWN2=28.013, MWO2=31.998, R=8.2056E-05

* ALPHA AND BETA FACTORS; EFFECTIVE SATURATION DEPT

***** MODIFY FOR COUNTY *****

PARAM

ALPHA1=1.000, ALPHA2=1.000, ALPHA3=1.000, ALPHA4=1.000, BETA=0.985

PARAM CFCONV=0.58858

* RATIOS OF NITROGEN AND CO2 KLA'S TO OXYGEN

PARAM FKLACO=0.836, FKLAN2=0.943, BKLA1=11.875

* CSD'S KLAS FROM CLEAN WATER TANK TEST

PARAM BKLA2=6.208, BKLA3=6.208, BKLA4=7.767

* FIT O2 FEED RATE TO MATCH ORIGINAL OPERATIONAL PERFORMANCE

PARAM O2ERR=1.08

* OPERATIONAL SIMULATION AND OPTIMIZATION PARAMETERS

```

PARAM MGDMOD=1.0
PARAM FPMOD=1.0
PARAM KLAMOD=1.0
PARAM BOOST=0.0
FEDFLX=(1+BOOST*SIN(0.2618*TIME))
PARAM DOSP=6.0,KERR=1.0,KINTER=1.0
DOERR=(DOSP-DO4)
GASMOD=DOERR*KERR+KINTER*INTGRL(0.0,DOERR)
* SET THE CONTROLLER PARAMETERS
PARAM RSETS=0.,RSETI=0.0,SRTSP=7.,RO2GP=0.,RO2GI=0.0
* TOTAL PRESSURES. LET THEM VARY BY 2 INCHES
PARAM TPRES1=1.006,TPRES2=1.0045,TPRES0=1.006
PARAM TPRES3=1.0030,TPRES4=1.0015
** INITIAL CONDITIONS
PARAM ICS1=120.,ICDO1=11.0,ICNH3J=24.0
PARAM ICS2=90.,ICDO2=16.4
PARAM ICS3=60.,ICDO3=16.3
PARAM ICS4=30.,ICDO4=11.2
* INITIAL PURITY PROFILES IN FRACTIONS (SAME AS PARTIAL PRESSURE)
PARAM FPO21=.905,FPO22=0.7202,FPO23=0.5888,FPO24=0.4106
PARAM FPCO21=0.01,FPCO22=0.01,FPCO23=0.01,FPCO24=0.01
PARAM ICPH1=7.5,ICPH2=7.5,ICPH3=7.5,ICPH4=7.5
* INLET GAS PURITY (% O2) AND OXYGEN FLOW IN TONS PER DAY.
PARAM ZWSCFM=0.056
* CHECK INTO CSD'S WATTAGE DRAW PER STAGE
PARAM ZWM1=286.0,ZWM2=183.0,ZWM3=176.0,ZWM4=207.0
** INFLUENT PARAMETERS
PARAM BOD5IN=153.,PHO=7.6,DOO=0.,DNH3I=13.5,XPEFF=0.
PARAM ACACO3=275.
PARAM QMGDA=63.,QRRAT=0.35,NBASIN=1
QMGDI=QMGDA*MGDMOD
* LIQUID VOLUMES
PARAM VLCF1=175781.,VLCF2=175781.,VLCF3=175781.,VLCF4=175781.
* GAS VOLUMES
PARAM KFLOW=80000.
PARAM VGCF1=58594.,VGCF2=58594.,VGCF3=58594.,VGCF4=58594.

```

* HEAD SPACE VOLUME

FIXED NPRINT

** NOW THE FUNCTIONS FOR ION PRODUCTS OF WATER, CARBONIC ACID,

*AMMONIA,

* AND VAPOR PRESSURE OF WATER.

FUNCTION

FPKW=(0.,14.944), (5.,14.734), (10.,14.535), (15.,14.346),...

(20.,14.167), (25.,13.996), (30.,13.833), (35.,13.680), (40.,13.535),..

..

(50.,13.262)

* AMMONIA

FUNCTION FPKNH3=(0.,10.081), (5.,9.904), (15.,9.564), (20.,9.4),...

(25.,9.245), (30.,9.093), (35.,8.947), (40.,8.805), (50.,8.539)

* CARBON DIOXIDE PK1

FUNCTION

FPK1=(0.,6.58), (10.,6.46), (15.,6.42), (20.,6.38), (25.,6.35),...

(30.,6.34), (35.,6.332), (40.,6.325), (45.,6.3215), (50.,6.320)

* CARBON DIOXIDE PK2

FUNCTION FPK2=(0.,10.63), (10.,10.49), (15.,10.43), (25.,10.33),...

(40.,10.22), (50.,10.17)

* VAPOR PRESSURE OF H2O IN MM HG

FUNCTION FVPH2O=(0.,4.579), (5.,6.543), (10.,9.209), (15.,12.788),...

(20.,17.535), (25.,23.756), (30.,31.824), (35.,41.175),...

(40.,55.324), (50.,92.51)

* SET THE MEASURED VARIABLES FOR THE INITIAL SECTION

** LOAD CARSON DATA INTO FILES FOR COMPARISON TO MODEL

PO21D=GDATA (TIME,1)

PO22D=GDATA (TIME,2)

PO23D=GDATA (TIME,3)

PO24D=GDATA (TIME,4)

DO1D=GDATA (TIME,5)

DO2D=GDATA (TIME,6)

DO3D=GDATA (TIME,7)

DO4D=GDATA (TIME,8)

FPURO2=GDATA (TIME,9) *FPMOD

```

*      TGASM1=GDATA (TIME, 10)
*      TGASMU=TGASM1*O2ERR
      TGASMU=0.9*QMGD+GASMOD
      QMGD=GDATA (TIME, 11) *MGDMOD*FEDFLX
      TEMP=AFGEN (TEMPF, TIME)
      BOD5IN=GDATA (TIME, 12)
      BOD5OD=GDATA (TIME, 13)
      XSETA=GDATA (TIME, 18) -OFFSET
**  LATER USE OFFSET TO  ADJUST MODEL WASTE RATE TO MATCH MLVSS
*****  CALCULATE THE CONSTANTS
      PK1=NLFGEN (FPK1, TEMP)
      CK1=1./ (10**PK1)
      PK2=NLFGEN (FPK2, TEMP)
      CK2=1./ (10**PK2)
      PKNH3=PKW-NLFGEN (FPKNH3, TEMP)
      CKNH3=1./ (10**PKNH3)
      PKW=NLFGEN (FPKW, TEMP)
      CKW=1./ (10**PKW)
*  WATER VAPOR PRESSURE (CONVERT TO ATMOSPHERES)
      VPH2O=NLFGEN (FVPH2O, TEMP) /760.
*****  HENRY'S LAW CONSTANTS.
*  OXYGEN (* 10 E-04 )
FUNCTION FHO2=(0.,2.5410), (5.,2.903), (10.,3.279), (15.,3.66), ...
      (20.,4.052), (25.,4.434), (30.,4.869), (35.,5.07), (40.,5.35)
*  NITROG (* 10E-04 )
FUNCTION
FHN2=(0.,5.29), (5.,5.97), (10.,6.68), (15.,7.38), (20.,8.04), ...
      (25.,8.65), (30.,9.24), (35.,9.85), (40.,10.4), (50.,1.13)
*  CARBON DIOXIDE (* 10 E-03 )
FUNCTION FHCO2=(0.,0.728), (5.,0.876), (10.,1.04), (15.,1.22), ...
      (20.,1.42), (25.,1.64), (30.,1.86), (35.,2.09), (40.,2.33), (50.,2.83)
*****  CALCULATE THE CONSTANTS INCLUDING THE MW OF EACH SPECIES AND
**
***  THE MOLE FRACTION OF WATER
      HEO2=NLFGEN (FHO2, TEMP) / (55555.*MWO2*1.E-04*BETA)

```

```

HEN2=NLFGEN(FHN2,TEMP)/(55555.*MWN2*1.E-04*BETA)
HECO2=NLFGEN(FHCO2,TEMP)/(55555.*MWCO2*1.E-03*BETA)
***** GAS TRANSFER COEFFICIENTS
* FIRST STAGE
* FUNCTION FKLA1 PREVIOUSLY A FUNCTION OF GAS RECIRCULATION RATES
*** TEMPERATURE FOR THE FIRST TEST
FUNCTION
TEMPF=(0.,27.0),(8.,27.0),(32.,27.0),(56.,27.0),(80.,27.0),...
(104.,27.0),(128.,27.0),(152.,27.0),(168.,27.0),(200.,27.0),...
(300.,27.0),(408.,27.0)
**** CALCULATE THE COEFFICIENTS
* CALCULATE THE VALUE OF R * T
RT=R*(TEMP+273.15)
* CALCULATE THE INLET HYDROGEN ION CONCENTRATION FROM PHO
HIO=1./(10**PHO)
* CALCULATE THE INLET AMMONIA CONCENTRATION IN G/MOLES
* NH3I=CNH3I/14.E+03
* CONVERT THE VOLUMES TO M**3 AND CALCULATE THETAS. FOR THE
Q=QMGDI*1.E+06*0.003875/(24.*NBASIN)
QR=QRRAT*Q
QT=Q+QR
XR=XSETA*QT/QR
VL1=VLCF1*0.02832
VL2=VLCF2*0.02832
VL3=VLCF3*0.02832
VL4=VLCF4*0.02832
VG=VGCF1*0.02832
THETA1=VL1/(Q+QR)
THETA2=VL2/(Q+QR)
THETA3=VL3/(Q+QR)
THETA4=VL4/(Q+QR)
ALKI=ACACO3/(50.E+03)
* CALCULATE THE INITIAL PARTIAL NITROGEN PRESSURE BY DIFFERENCE
* INDICATED AS %
FPN21=TPRES1-VPH20-FPO21-FPCO21
FPN22=TPRES2-VPH20-FPO22-FPCO22

```

FPN23=TPRES3 - VPH20 - FPO23 - FPCO23

FPN24=TPRES4 - VPH20 - FPO24 - FPCO24

- * INITIAL GAS HEADSPACE CONCENTRATIONS FROM ABOVE CONVERTED TO MOLES

ICO21=TPRES1*FPO21/RT

ICN21=TPRES1*FPN21/RT

ICCO21=TPRES1*FPCO21/RT

ICO22=TPRES2*FPO22/RT

ICN22=TPRES2*FPN22/RT

ICCO22=TPRES2*FPCO22/RT

ICO23=TPRES3*FPO23/RT

ICN23=TPRES3*FPN23/RT

ICCO23=TPRES3*FPCO23/RT

ICO24=TPRES4*FPO24/RT

ICN24=TPRES4*FPN24/RT

ICCO24=TPRES4*FPCO24/RT

- * INITIAL MLVSS CONCENTRATIONS

ICXS=XR*QR/(QR+Q)

ICX1=ICXS

ICX2=ICXS

ICX3=ICXS

ICX4=ICXS

- * CALCULATE THE INLET DISSOLVED GAS CONCENTRATIONS

DN2I=0.791/HEN2

DOI=0.

DCDI=(ALKI - (DNH3I/14.E+03)/(1. + HIO * CKNH3/CKW)) *

MWCO2*1.E+03

- * INITIAL PH CALCULATIONS

HI1=10**(-ICPH1)

HI2=10**(-ICPH2)

HI3=10**(-ICPH3)

HI4=10**(-ICPH4)

- * INITIAL CONDITIONS FOR DISSOLVED GASSES. CALCULATE FROM

- * PARTIAL PRESSURES. ASSUME SATURATION

ICDCD1=TPRES1*FPCO21/(HECO2*FCO2(HI1,CK1,CK2))

ICDN21=TPRES1*FPN21/HEN2

```

ICDCD2=TPRES2*FPCO22/(HECO2*FCO2(HI2,CK1,CK2))
ICDN22=TPRES2*FPN22/HEN2
ICDCD3=TPRES3*FPCO23/(HECO2*FCO2(HI3,CK1,CK2))
ICDN23=TPRES3*FPN23/HEN2
ICDCD4=TPRES4*FPCO24/(HECO2*FCO2(HI4,CK1,CK2))
ICDN24=TPRES4*FPN24/HEN2
* CALCULATE THE INLET VOLUMETRIC GAS FLOW RATE
TGASB=TGASMU*2000./(24.*NBASIN)
QGO=TGASB*RT*454./(MWO2*(TPRES1-VPH20))+TGASB*(1.-...
FPURO2)/FPURO2*RT*454./(MWN2*(TPRES1-VPH20))
O2O=(TPRES1-VPH20)*FPURO2/RT
N2O=(TPRES1-VPH20)*(1.-FPURO2)/RT
QGOCF=QGO*CFCONV
CO2O=0.
* CALCULATE THE FOLLOWING COMBINATIONS OF PARAMETERS TO IMPROVE
* SPEED.
YPO21=(1.-Y)*YO21/Y
YPCO21=(1.-Y)*YCO21/Y
YPNH31=YNH32-YNH31
* CONVERSION FACTOR FOR GLOBAL BALANCES
CFTON=NBASIN*24./(454.*2000.)
* CALCULATE THE LEAK FLOWS
** QLK1= NOT FOR CSD
SOI=BOD5IN/YB5TOU
* CALCULATE INITIAL CONDITIONS FOR SRT AND FMR
SODIFF=(Q+QR)*(SOI-ICS4)*CFTON
SMASS=NBASIN*(ICX1*VL1+ICX2*VL2+ICX3*VL3+ICX4*VL4)/9.098E+05
XMDIFF=LIMIT(0.004,1000.,((ICX4*(Q+QR)-QR*XR)*CFTON))
*****
DYNAMIC
NOSORT
CALL DEBUG(NPRINT,DTIME1)
CALL DEBUG(NPRINT,DTIME2)
SORT
PROCEDURE DO1D,DO2D,DO3D,DO4D,PO21D,...
PO22D,PO23D,PO24D,TGASM1,FPURO2,TEMP,BOD5IN=INDATA(TIME)

```

```

*      IF (KEEP.NE.1) GOTO 90
      PO21D=GDATA (TIME, 1)
      PO22D=GDATA (TIME, 2)
      PO23D=GDATA (TIME, 3)
      PO24D=GDATA (TIME, 4)
      DO1D=GDATA (TIME, 5)
      DO2D=GDATA (TIME, 6)
      DO3D=GDATA (TIME, 7)
      DO4D=GDATA (TIME, 8)
      FPURO2=GDATA (TIME, 9) *FPMOD
*      TGASM1=GDATA ( (TIME-O2LAG) , 10) *O2ERR
      TGASM1=0.9*QMGD+GASMOD
      QMGD=GDATA (TIME, 11) *MGDMOD*FEDFLX
      TEMP=AFGEN (TEMPF, TIME)
      BOD5IN=GDATA (TIME, 12)
      BOD5OD=GDATA (TIME, 13)
      XSETA=GDATA (TIME, 18) -OFFSET
90     CONTINUE
ENDPROCEDURE
      DOERR= (DOSP-DO4)
      GASMOD=DOERR*KERR+KINTER*INTGRL (0.0, DOERR)
      TFAC=1.024** (TEMP-20.)
      RT=R* (TEMP+273.15)
      TGASB=TGASMU *2000./ (24.*NBASIN)
      QGO=TGASB*RT*454./ (MWO2* (TPRES1-VPH2O) )+TGASB* (1.- ...
      FPURO2) /FPURO2 *RT*454./ (MWN2* (TPRES1-VPH2O) )
      O2O= (TPRES1-VPH2O) *FPURO2/RT
      N2O= (TPRES1-VPH2O) * (1.-FPURO2) /RT
      QGOA=QGO
* INFLUENT PARAMTERS
      FEDFLX= (1+BOOST*SIN (0.2618*TIME) )
      Q=QMGD*1.E+06*0.003875/ (24.*NBASIN)
*      QR=QRRAT*Q
      QT=Q+QR
      THETA1=VL1/ (Q+QR)
      THETA2=VL2/ (Q+QR)

```

```

THETA3=VL3 / (Q+QR)
THETA4=VL4 / (Q+QR)
SOI=BOD5IN/YB5TOU
DCDI=(ALKI - (DNH3I/14.E+03)) / (1. + HIO * CKNH3/CKW) *
MWCO2*1.E+03
* CALCULATE THE RESULTS OF MIXING RECYCLE AND INFLUENT FLOWS. MOVE
* IT TO THE DYNAMIC SECTION FOR TIME VARYING FLOW RATE.
PROCEDURE SO, DNH3O, ALKO, DCDO, DN2O, SOA, XOA = INPUT (Q, QR, QT)
XO=(Q*XPEFF+QR*XR) / QT
SO=(Q*SOI+QR*S4) / QT
DNH3O=(Q*DNH3I+QR*DNH31) / QT
ALKO=(Q*ALKI+QR*ALKR) / QT
DCDO=(Q*DCDI+QR*DCDR) / QT
DN2O=(Q*DN2I+QR*DN2R) / QT
XOA=XO
SOA=SO
ENDPROCEDURE
* CKLA2L=NLFGEN(FKLA2, GAS2) --- KLA AS A FUNCTION OF GAS
* RECIRCULATION RATIO NOT APPLICABLE TO CARSON
CKLA1=BKLA1*TFAC*ALPHA1*KLAMOD
CKLA2=BKLA2*TFAC*ALPHA2*KLAMOD
CKLA3=BKLA3*TFAC*ALPHA3*KLAMOD
CKLA4=BKLA4*TFAC*ALPHA4*KLAMOD
X1, S1, DO1, DN21, DCD1, HI1, FCD1, QG1, PCO21, PO21, PN21, CO21, N21, O21, ...
DNH31, ALK1=REACT (THETA1, XOA, SOA, DOO, DN2O, DCDO, HIO, QGOA, CO2O, N2O, ...
.
O2O, ICX1, ICS1, ICDO1, ICDN21, ICDCD1, ICCO21, ICO21, ICN21, CKLA1, ...
VL1, TPRES1, TPRES0, DNH3O, ALKO)
* MIX THE FLOWS FOR SLUDGE REAERATION. PROCEDURE DROPPED FOR CSD
** STAGE #2 **
X2, S2, DO2, DN22, DCD2, HI2, FCD2, QG2, PCO22, PO22, PN22, CO22, N22, O22, ...
DNH32, ALK2=REACT (THETA2, X1, S1, DO1, DN21, DCD1, HI1, QG1, CO21, N21, ...
O21, ICX2, ICS2, ICDO2, ICDN22, ICDCD2, ICCO22, ICO22, ICN22, CKLA2, ...
VL2, TPRES2, TPRES1, DNH31, ALK1)
** STAGE #3 **
X3, S3, DO3, DN23, DCD3, HI3, FCD3, QG3, PCO23, PO23, PN23, CO23, N23, O23, ...

```

DNH33, ALK3=REACT (THETA3, X2, S2, DO2, DN22, DCD2, HI2, QG2, CO22, N22, . . .
O22, ICX3, ICS3, ICDO3, ICDN23, ICDCD3, ICCO23, ICO23, ICN23, CKLA3, . . .
VL3, TPRES3, TPRES2, DNH32, ALK2)

** STAGE #4 **

X4, S4, DO4, DN24, DCD4, HI4, FCD4, QG4, PCO24, PO24, PN24, CO24, N24, O24, . . .
DNH34, ALK4=REACT (THETA4, X3, S3, DO3, DN23, DCD3, HI3, QG3, CO23, N23, . . .
O23, ICX4, ICS4, ICDO4, ICDN24, ICDCD4, ICCO24, ICO24, ICN24, CKLA4, . . .
VL4, TPRES4, TPRES3, DNH33, ALK3)

BOD5OC=S4*YB5TOU

PH1=-ALOG10 (LIMIT (1.E-14, 1., HI1))

PH2=-ALOG10 (LIMIT (1.E-14, 1., HI2))

PH3=-ALOG10 (LIMIT (1.E-14, 1., HI3))

PH4=-ALOG10 (LIMIT (1.E-14, 1., HI4))

SR=S4

NOSORT

* THIS SECTION CONTROLS THE SLUDGE AGE
* CONSIG=INSW ((TIME-3.) , 0. , (SRTSP-SRT))
* XSET1=RSETS* (CONSIG) +RSETI*INTGRL (0. , CONSIG) +XSETA
XSET=LIMIT (500. , 3200. , XSETA)
XR=QT/QR*XSET
* CONP=LIMIT (0. , 1.0, PUTILU)

TGASMU=TGASM1

SORT

* CALCULATE THE GLOBAL BALANCE INFORMATION AFTER STEADY-STATE
* HAS BEEN REACHED. MOVE THIS SECTION TO TERMINAL TO INCREASE
SPEED.

MLSS= (X1+X2+X3+X4) /4

XMDIFF=LIMIT (0.004, 1000. , ((X4* (Q+QR) -QR*XR) *CFTON))

SODIFF= (Q+QR) * (SO-S4) *CFTON

N2MIN= (QGO*N2O*MWN2+Q*DN2I+QR*DN2R) *CFTON

O2MIN=QGO*O2O*MWO2*CFTON

CO2MIN= (CO2O*MWCO2+Q*DCDI+QR*DCDR) *CFTON

O2MOUT= (QG4*O24*MWO2+ (Q+QR) *DO4) *CFTON

CO2MOU= (QG4*CO21*MWCO2+ (Q+QR) *DCD1) *CFTON

N2MOUT= (QG4*N21*MWN2+ (Q+QR) *DN24) *CFTON

```

O2UTIL=O2MIN-O2MOUT
PUTIL=O2UTIL/O2MIN
O2MOUC=QG4*O24*MWO2*CFTON
O2UTIU=O2MIN-O2MOUC
PUTILU=O2UTIU/O2MIN
O2CONS=O2UTIL/SODIFF
CO2PRO=(CO2MOU-CO2MIN)/SODIFF
CO2CHK=SODIFF*(1.-Y)*YCO21+(SODIFF*Y-XMDIFF)*YCO22
SMASS=NBASIN*(X1*VL1+X2*VL2+X3*VL3+X4*VL4)/9.098E+05
ERRDO1=ABS(DO1-DO1D)
ERRDO2=ABS(DO2-DO2D)
ERRDO3=ABS(DO3-DO3D)
ERRDO4=ABS(DO4-DO4D)
ERRPO1=ABS(PO21-PO21D)
ERRPO2=ABS(PO22-PO22D)
ERRPO3=ABS(PO23-PO23D)
ERRPO4=ABS(PO24-PO24D)
ERRDOT=ERRDO1+ERRDO2+ERRDO3+ERRDO4
ERRPOT=ERRPO1+ERRPO2+ERRPO3+ERRPO4
IERRDO=INTGRL(0.,ERRDOT)
IERRPO=INTGRL(0.,ERRPOT)
* ENERGY CALCULATIONS
*   MIXERS -- USE THE POWERS MEASURED IN THE GILBERT REPORT
ZWMIX=NBASIN*(ZWM1+ZWM2+ZWM3+ZWM4)
*   GAST=(GAS1)*NBASIN
*   ZWBLOW=ZWSCFM*GAST
    ZWALL=ZWBLOW+ZWMIX
*   ZWS1=NBASIN*(ZWM1)
* POWER WEIGHTED DO, PURITY, AND ALPHA
DOAVI=INTGRL(0.,((DO1*ZWM1+DO2*ZWM2+DO3*ZWM3+DO4*ZWM4)/ZWALL))
PO2AVI=INTGRL(0.,((PO21*ZWM1+PO22*ZWM2+PO23*ZWM3+PO24*ZWM4)/ZWALL)
)
ALPHA1=INTGRL(0.,((ALPHA1*ZWM1+ALPHA2*ZWM2+ALPHA3*ZWM3+ALPHA4*...
ZWM4)/ZWALL))
* O2 CONSUMPTION BY STAGE
O2COI1=INTGRL(0.,(QGOA*O2O-QG1*O21)*CFTON*MWO2)

```

```

O2COI2=INTGRL(0., (QG1*O21-QG2*O22) *CFTON*MWO2)
O2COI3=INTGRL(0., (QG2*O22-QG3*O23) *CFTON*MWO2)
O2COI4=INTGRL(0., (QG3*O23-QG4*O24) *CFTON*MWO2)
O2COI5=INTGRL(0., (QGOA*O2O-QG4*O24) *CFTON*MWO2)
* O2 PURITY AVERAGE
PUTAVI=INTGRL(0., PUTILU)
DO1I=INTGRL(0., DO1)
DO2I=INTGRL(0., DO2)
DO3I=INTGRL(0., DO3)
DO4I=INTGRL(0., DO4)
PO21I=INTGRL(0., PO21)
PO22I=INTGRL(0., PO22)
PO23I=INTGRL(0., PO23)
PO24I=INTGRL(0., PO24)
ENDT=TIME
NOSORT
FMR=YB5TOU*(SODIFF/SMASS)
SRT=LIMIT(0., 100., (SMASS/XMDIFF))
TERMINAL
* POWER WEIGHTED DO, PURITY, AND ALPHA
DOAVG=DOAVI/ENDT
PO2AVG=PO2AVI/ENDT
ALPHAA=ALPHAI/ENDT
* O2 CONSUMPTION BY STAGE
O2CON1=O2COI1/ENDT
O2CON2=O2COI2/ENDT
O2CON3=O2COI3/ENDT
O2CON4=O2COI4/ENDT
* O2 TOTAL CONSUMPTION
O2CON5=O2COI5/ENDT
* O2 PURITY AS A FUNCTION OF TIME
PUTAVE=PUTAVI/ENDT
DO1A=DO1I/ENDT
DO2A=DO2I/ENDT
DO3A=DO3I/ENDT
DO4A=DO4I/ENDT

```

```

PO21A=PO21I/ENDT
PO22A=PO22I/ENDT
PO23A=PO23I/ENDT
PO24A=PO24I/ENDT
* WRITE OUT THE RESULTS WITH FORTRAN WRITES
      WRITE (6,1004)
1004  FORMAT(' STAGE   RECIRCULATION   DO   PO2   O2 UPTAKE   PH
KW')
      WRITE (6,1005)
1005  FORMAT(' (NO)   (SCFM / STAGE) (MG/L)   (FRAC)   (TON/DAY) ')
      WRITE (6,1010) GAS1, DO1A, PO21A, O2CON1, PH1, ZWM1
      WRITE (6,1020) GAS2, DO2A, PO22A, O2CON2, PH2, ZWM2
      WRITE (6,1030) GAS3, DO3A, PO23A, O2CON3, PH3, ZWM3
      WRITE (6,1040) GAS4, DO4A, PO24A, O2CON4, PH4, ZWM4
      WRITE (6,1050) GAST, DOAVG, PO2AVG, O2CON5, ZWALL
1010  FORMAT(1X, '  1  ', 8X, F5.0, 4X, F6.2, 4X, F5.2, F8.1, 4X, F3.1, F6.0)
1020  FORMAT(1X, '  2  ', 8X, F5.0, 4X, F6.2, 4X, F5.2, F8.1, 4X, F3.1, F6.0)
1030  FORMAT(1X, '  3  ', 8X, F5.0, 4X, F6.2, 4X, F5.2, F8.1, 4X, F3.1, F6.0)
1040  FORMAT(1X, '  4  ', 8X, F5.0, 4X, F6.2, 4X, F5.2, F8.1, 4X, F3.1, F6.0)
1050  FORMAT(/, '   T  ', 6X, F7.0, 4X, F6.2, 4X, F5.2, F8.1, 6X, F7.0)
      WRITE (6,1060) PUTAVE, ALPHA, NBASIN
1060  FORMAT(/, ' FRACTION OXYGEN UTILIZATION=', F5.3, /, ...
        /, ' POWER WEIGHTED ALPHA FACTOR=', F5.3, /, ...
        /, ' NUMBER OF BASINS IN SERVICE=', F4.0, ///)
      WRITE (6,1070)
1070  FORMAT('1')
METHOD STIFF
PRINT
X1, S1, DNH31, DO1, DN21, DCD1, PH1, ALK1, FCD1, QG1, PCO21, PO21, PN21, ...
X2, S2, DNH32, DO2, DN22, DCD2, PH2, ALK2, FCD2, QG2, PCO22, PO22, PN22, ...
X3, S3, DNH33, DO3, DN23, DCD3, PH3, ALK3, FCD3, QG3, PCO23, PO23, PN23, ...
X4, S4, DNH34, DO4, DN24, DCD4, PH4, ALK4, FCD4, QG4, PCO24, PO24, PN24, ...
XR, XSET, SRT, FMR
OUTPUT
QMGD, BOD5IN, BOD5OD, BOD5OC, DO1, DO1D, DO2, DO2D, DO3, DO3D, DO4, ...
DO4D, PO21, PO21D, PO22, PO22D, PO23, PO23D, PO24, PO24D, S1, S4, MLSS, ...

```

```

FMR, SRT, PUTIL, O2CONS, XMDIFF, ERRDO1, ERRDO2, ERRDO3, ERRDO4, ERRDOT, ...
IERRDO, ERRPO1, ERRPO2, ERRPO3, ERRPO4, ERRPOT, IERRPO, PUTILU
OUTPUT DO1, DO2, DO3, DO4, DO1D, DO2D, DO3D, DO4D, TGASM1
OUTPUT PO21, PO22, PO23, PO24, PO21D, PO22D, PO23D, PO24D, QGO
TIMER FINTIM=100.0, PRDEL=24., OUTDEL=4., DELMIN=1.68E-06
END
STOP

```

```

FUNCTION SDIV(A,B)

```

```

C.. THIS FUNCTION GIVES YOU A "SAFE" DIVISION

```

```

SDIV=-1.

```

```

IF (ABS(B) .GT. 1.E-20) SDIV=A/B

```

```

RETURN

```

```

END

```

```

FUNCTION PHCAL (ALK, CO2, CNH3, CK1, CK2, CKW, CKNH3)

```

```

C.. THIS FUNCTION CALCULATES THE PH OF A DILUTE SOLUTION IN A
CLOSED

```

```

C BIOX REACTOR. THE CALCULATION IS IMPLICIT

```

```

REAL*8 DK1, DK2, DCO2, DPH, DNH3, DALK, B, C, ZGESS, DKNH3

```

```

C.. SET THE FIRST GUESS EQUAL TO THE OLD PH

```

```

ZGESS=1.D-06

```

```

C.. CONVERT THE SINGLE PRECISION ARGS TO DOUBLE PRECISION

```

```

DK1=CK1

```

```

DK2=CK2

```

```

DKW=CKW

```

```

C.. ALSO CONVERT CO2 AND NH3 TO MOLAR CONCENTRATION.

```

```

DCO2=CO2/44009.

```

```

DALK=ALK

```

```

DKNH3=CKNH3

```

```

DNH3=CNH3/14.E+03

```

```

C.. QUADRATIC COEFFICIENTS

```

```

B=DALK-DNH3/(1.+DPH*DKNH3/DKW)

```

```

ITER=0

```

```

10 C=-DKW-(DK1+2.D0*DK1*DK2/ZGESS)*DCO2

```

```

C.. CALC THE PH

```

```

DPH=(-B+DSQRT(B**2-4.D0*C))/2.D+00

```

```

IF (DABS(DPH-ZGESS) .GT. 1.D-12) GOTO 20

```

C.. NORMAL CONVERGENCE

PHCAL=DPH

RETURN

20 IF(ITER.GT.10) GOTO 30

ZGESS=DPH

B=DALK-DNH3/(1.+DPH*DKNH3/DKW)

ITER=ITER+1

GOTO 10

C.. NO CONVERGENCE

30 WRITE(6,1000) ZGESS,DPH,ITER

1000 FORMAT(' NON CONVERGENCE IN PH CALCULATION.',/,

1 1X,' EXECUTION STOPPING',/,,' FINAL GUESS FOR PH =',D17.6,

2 /,,' FINAL CALC FOR PH =',D17.6,/,,' ITERATION NUMBER=',I5)

PHCAL=DPH

RETURN

END

FUNCTION FCO2(PH,CK1,CK2)

C.. THIS FUNCTION CALCULATES THE FRACTION OF THE TOTAL CARBON

WHICH

C IS IN THE H2CO3 FORM.

REAL*8 DK1,DK2,DPH

C.. CONVERT TO DOUBLE PRECISION FOR THE CALCULATION

DK1=CK1

DK2=CK2

DPH=PH

FCO2=1.D+0/((DPH*DK1*DK2/DPH+DK1)/DPH+1.D0)

RETURN

END

FUNCTION GDATA(TIM,ITYPE)

REAL*4 MLFGEN,MLSS(10)

DIMENSION TIME(85),TF1(85),TF2(85),TF3(85),TF4(85),

1GP1(85),GP2(85),GP3(85),GP4(85),DO1(85),DO2(85),DO3(85),

2DO4(85),O2FPUR(85),O2FTON(85),QMGD(85),O2OTON(85),O2VENT(85)

DIMENSION TIME2(85),QMGD2(10),BODIN(10),BODOUT(10),RAS1(10),

1RAS2(10),CODIN(10),CODOUT(10),WAS(10)

DIMENSION TIME3(7),XM1(7),XM2(7),XM3(7),XM4(7),TIME4(85)

```

        DIMENSION AX1 (5) , AX2 (5) , AX3 (5) , AX4 (5) , AX5 (5) , AX6 (5) , AX7 (5) ,
1AX8 (5) , AX9 (5) , AX10 (5) , AX11 (5) , AX12 (5) , AX13 (5) , AX14 (5) , AX15 (5) ,
        2AX16 (5) , AX17 (5) , AX18 (5) , AX19 (5) , AX20 (5) , AX21 (5) , AX22 (5)
        DATA AX1 /5*0./ , AX2 /5*0./ , AX3 /5*0./ , AX4 /5*0./ , AX5 /5*0./ ,
1AX6 /5*0./ , AX7 /5*0./ , AX8 /5*0./ , AX9 /5*0./ , AX10 /5*0./ ,
        2AX11 /5*0./ , AX12 /5*0./ , AX13 /5*0./ , AX14 /5*0./ , AX15 /5*0./ ,
        2AX16 /5*0./ , AX17 /5*0./ , AX18 /5*0./ , AX19 /5*0./ , AX20 /5*0./ ,
        3AX21 /5*0./ , AX22 /5*0./ , JUMP /0/
        IF (JUMP.GT.0) GOTO 25
        DO 10 I=1,8
        READ (16 , * , END=15)
TIME (I) , CODIN (I) , CODOUT (I) , BODIN (I) , BODOUT (I)
10     N=I
15     CONTINUE
        DO 16 I=1,200
        READ (17 , * , END=17)
TIME2 (I) , O2FTON (I) , O2VENT (I) , O2OTON (I) , O2FPUR (I)
16     N2=I
17     CONTINUE
        N3=8
        DO 18 I=1,N3
        READ (18 , * , END=19)
TIME3 (I) , XM1 (I) , XM2 (I) , XM3 (I) , XM4 (I) , RAS1 (I) ,
        1RAS2 (I) , MLSS (I) , QMGD (I)
18     N4=I
19     CONTINUE
        DO 20 I=1,200
        READ (20 , * , END=21)
TIME4 (I) , DO1 (I) , DO2 (I) , DO3 (I) , DO4 (I) , GP1 (I) ,
        1GP2 (I) , GP3 (I) , GP4 (I)
20     N5=I
C.. CONVERT THE GAS PERCENTS TO GAS FRACTIONS
21     DO 23 I=1,N5
        GP1 (I) =GP1 (I) /100.
        GP2 (I) =GP2 (I) /100.

```

```

GP3 (I) =GP3 (I) /100.
23  GP4 (I) =GP4 (I) /100.
C..  CONVERT OXYGEN FLOW RATES TO GAS FLOW RATES
      DO 24 I=1,N2
      O2FPUR (I) =O2FPUR (I) /100.
      O2OTON (I) =O2OTON (I) /1004.
24  O2FTON (I) =O2FTON (I) /O2FPUR (I)
      JUMP=1
25  GOTO (70,80,90,100,110,120,130,140,150,160,170,
1180,190,200,210,220,230,240,250,260,270,280) , ITYPE
70  GDATA=MLFGEN (AX1,N5,TIM,TIME4,GP1,56)
      GOTO 950
80  GDATA=MLFGEN (AX2,N5,TIM,TIME4,GP2,56)
      GOTO 950
90  GDATA=MLFGEN (AX3,N5,TIM,TIME4,GP3,56)
      GOTO 950
100 GDATA=MLFGEN (AX4,N5,TIM,TIME4,GP4,56)
      GOTO 950
110 GDATA=MLFGEN (AX5,N5,TIM,TIME4,DO1,56)
      GOTO 950
120 GDATA=MLFGEN (AX6,N5,TIM,TIME4,DO2,56)
      GOTO 950
130 GDATA=MLFGEN (AX7,N5,TIM,TIME4,DO3,56)
      GOTO 950
140 GDATA=MLFGEN (AX8,N5,TIM,TIME4,DO4,56)
      GOTO 950
150 GDATA=MLFGEN (AX9,N2,TIM,TIME2,O2FPUR,85)
      GOTO 950
160 GDATA=MLFGEN (AX10,N2,TIM,TIME2,O2FTON,85)
      GOTO 950
170 GDATA=MLFGEN (AX11,N3,TIM,TIME3,QMGD,8)
      GOTO 950
180 GDATA=MLFGEN (AX12,N,TIM,TIME,BODIN,8)
      GOTO 950
190 GDATA=MLFGEN (AX13,N,TIM,TIME,BODOUT,8)
      GOTO 950

```

```

200  GDATA=MLFGEN (AX14 , N3 , TIM , TIME3 , RAS1 , 8)
      GOTO 950
210  GDATA=MLFGEN (AX15 , N3 , TIM , TIME3 , RAS2 , 8)
      GOTO 950
220  GDATA=MLFGEN (AX16 , N , TIM , TIME , CODIN , 8)
      GOTO 950
230  GDATA=MLFGEN (AX17 , N , TIM , TIME , CODOUT , 8)
      GOTO 950
240  GDATA=MLFGEN (AX18 , N3 , TIM , TIME3 , MLSS , 8)
      GOTO 950
250  GDATA=MLFGEN (AX19 , N3 , TIM , TIME3 , MX1 , 8)
      GOTO 950
260  GDATA=MLFGEN (AX20 , N3 , TIM , TIME3 , MX2 , 8)
      GOTO 950
270  GDATA=MLFGEN (AX21 , N3 , TIM , TIME3 , MX3 , 8)
      GOTO 950
280  GDATA=MLFGEN (AX22 , N3 , TIM , TIME3 , MX4 , 8)
950  RETURN
      END
      FUNCTION MLFGEN (AX , N , X , ARRX , ARRY , M)

```

C*****

C.. THIS FUNCTION GENERATES AN ARBITRARY FUNCTION DEFINED BY PAIRS
OF

C DATA POINTS CONTAINED IN THE ARRAYS ARRX AND ARRY, WITH THE
C NUMBER OF POINTS = N.

C NOTE THAT THE FUNCTION CHECKS FOR PROPER DATA ENTRY ON THE
FIRST

C CALL, AND CHECKS TO SEE IF X IS IN THE RANGE DEFINED IN THE
DATA

C ARRAY. QUADRATIC INTERPOLATION IS USED.

C*****

```

      REAL*4 MLFGEN

```

```

      DIMENSION ARRX (M) , AX (5) , ARRY (M)

```

C.. CHECK FOR INITIAL ENTRY

```

      NW=6

```

```

      IF (AX (1)) 10,10,90

```

```

10    AX(1)=1
      IF(N-2) 20,20,30
20    WRITE(NW,1000) N
1000  FORMAT(//,' LESS THAN THREE DATA POINTS (' ,I6,
      1' WERE SUPPLIED FOR AN MLFGEN FUNCTION' ,//,
      2' EXECUTION TERMINATING')
      STOP 20
30    AX(4)=0
C.. CHECK TO SEE IF THE DATA WAS ENTERED CORRECTLY IN ASCENDING
ORDER
      DO 40 I=2,N
      IF(ARRX(I-1).GT.ARRX(I)) GOTO 50
40    CONTINUE
      GOTO 60
50    K=I-1
      WRITE(NW,1010) I,ARRX(I),K,ARRX(K)
1010  FORMAT(//,' THE INDEPENDENT VARIABLE FOR A MLFGEN FUNCTION
HAS ',
      1'NOT BEEN' ,/, ' ENTERED IN ASCENDING ORDER' ,/, ' THE' ,I3, 'TH
POINT='
      2,2X,E17.6,2X,'WHILE THE' ,I3, 'TH POINT=' ,2X,E17.6,/, '
EXECUTION TER
      3MINATING')
      STOP 30
60    AX(3)=0.
      IF(X.LT.ARRX(1)) AX(3)=-1.
      IF(X.GT.ARRX(N)) AX(3)=1.
      IF(AX(3)) 70,80,70
70    WRITE(NW,1020) X,ARRX(1),ARRX(N)
1020  FORMAT(' THE INITIAL ENTRY TO A MLFGEN FUNCTION IS OUT OF
RANGE', 1/,
      1/, ' THE VALUE OF THE INDEPENDENT VARIABLE IS',E17.6, ' WHILE
THE',
      2/, ' MINIMUM VALUE OF THE FUNCTION IS',E17.6, ' AND THE
MAXIMUM',
      3/, ' VALUE OF THE FUNCTION IS',E17.6)

```

```

      IF (AX(3)) 240,80,210
80    AX(2)=1
C.. NORMAL ENTRY FOR MLFGEN
90    IF (X-ARRX(1)) 220,100,110
100   AX(2)=1
      AX(4)=0
      MLFGEN=ARRY(1)
      GOTO 300
110   IF (X-ARRX(N)) 120,115,190
115   AX(2)=N
      AX(4)=0
      MLFGEN=ARRY(N)
      GOTO 300
120   I=IFIX(AX(2)+0.5)
130   IF (X.LT.ARRX(I)) GOTO 140
      I=I+1
      IF (I.GT.N) GOTO 190
      GOTO 130
140   I=I-1
      IF (I.LT.1) GOTO 220
150   IF (X.GE.ARRX(I)) GOTO 160
      GOTO 140
160   I=I+1
      IF (I.GT.N) GOTO 190
      AX(2)=I
      IF (I-2) 170,170,180
170   MLFGEN=ARRY(I-1) + (X-ARRX(I-1)) * (ARRY(I) - ARRY(I-1)) /
      1 (ARRX(I) - ARRX(I-1))
      AX(4)=0.
      GOTO 300
180   A1=ARRX(I-1) - ARRX(I-2)
      A2=ARRX(I) - ARRX(I-1)
      A3=ARRX(I) - ARRX(I-2)
      A4=X-ARRX(I-1)
      A5=X-ARRX(I)
      A6=X-ARRX(I-2)

```

```

      MLFGEN=ARRY(I-2)*A4*A5/(A1*A3)-ARRY(I-1)*A6*A5/(A1*A2)+
1ARRY(I)*A6*A4/(A3*A2)
      AX(4)=0.
      GOTO 300
190  IF(AX(4)) 210,200,200
200  WRITE(NW,1030) X,ARRX(N)
1030  FORMAT(' INDEPENDENT VARIABLE FOR MLFGEN FUNCTION ABOVE
RANGE',/,
      1' INDEPENDENT VARIABLE=',E12.6,' MAXIMUM FOR THIS MLFGEN
FUNCTION'
      2,',' ,E12.6)
210  MLFGEN=ARRY(N)
      AX(4)=-1
      AX(2)=N
      GOTO 300
220  IF(AX(4)) 230,230,240
230  WRITE(NW,1040) X,ARRX(1)
1040  FORMAT(' INDEPENDENT VARIABLE FOR MLFGEN FUNCTION BELOW
RANGE',/,
      1' INDEPENDENT VARIABLE=',E12.6,' MINIMUM FOR THIS MLFGEN
FUNCTION'
      2,',' ,E12.6)
240  AX(2)=1
      AX(4)=+1
      MLFGEN=ARRY(1)
300  RETURN
      END

```