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Simulation of Three-Phase Fluidized Bioreactors for Denitrification

A. V. Hamza
J. F. Dolan
E. W. Wong

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ABSTRACT

Fluidized-bed bioreactors were developed and operated at three scales (diameters of 0.1, 0.2, and 0.5 m) by the Chemical Technology Division. The performance of these reactors in denitrification was simulated using the following modified form of Monod kinetics to describe the reaction kinetics:

$$\text{rate} = V_{\max} \left(\frac{\text{NO}_3^-}{K_s + \text{NO}_3^-} \right) (\% \text{ biomass})$$

In the fluids-movement portion of the simulation the tanks-in-series approximation to backmixing was used. This approach yielded a $V_{\max}$ of 3.5 g/m³-min (% biomass) and a K_s of 163 g/m³ for the 0.5-m bioreactor. Values of $V_{\max}$ and K_s were also determined for data derived from the 0.1-m bioreactor, but inadequate RTD data reduced the confidence level in these results. A complication in denitrification is the multi-step nature of the reduction from nitrate to nitrite to hyponitrite and finally to nitrogen. An experimental study of the effect of biomass loading upon denitrification was begun. It is recommended that the experimental work be continued.

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1. SUMMARY

The Chemical Technology Division at Oak Ridge National Laboratory has developed a biodenitrification process for wastewater, using *Pseudomonas denitrificans*. In this process bacteria are immobilized on coal particles, which are fluidized by the nitrate wastewater stream. The bacteria catalyze the denitrification of nitrates in the presence of a carbonaceous energy source to N_2 and CO_2 . The direct application of this technology is in the nuclear-fuel-processing cycle where nitrates are waste products of a number of steps. The technology may be applied to a wide variety of other waste streams and to the production of certain chemicals such as methane and ethanol.

A simulation of the fluidized-bed bioreactor was required for the design of a larger-scale plant. Existing pilot-plant data and a review of the literature indicated that a modified Monod kinetics model of the form:

$$\text{rate} = V_{\max} \left(\frac{NO_3^-}{K_s + NO_3^-} \right) (\% \text{ biomass})$$

was found to describe the denitrification reaction adequately. In the operating range of pilot-plant data (pH values between 7.0 and 8.6 and $C/N > 1.7$), pH and ethanol concentration had little effect on the reaction rate. An earlier residence-time-distribution study was used to describe the backmixing in the 0.5-m reactor. Two reactor models were used to simulate the contacting pattern in the bioreactor: the tanks-in-series model and the plug-flow-in-parallel model. The simulation models were derived from material balances incorporating the rate expression and the biomass loading profile in the reactor. A non-linear regression model, based on Marquart's algorithm, was used to determine optimal values of $V_{\max}$ (maximum rate of reaction) and K_s (saturation constant) from both models.

No significant difference between the plug-flow-in-parallel model and the tanks-in-series model was observed other than the large standard error in K_s in the case of the plug-flow model. The fitted parameters were insensitive to the shape of the biomass loading profile within the bioreactor; hence a tanks-in-series model with a linear biomass loading profile was chosen to simulate the bioreactor.

Values for $V_{\max}$ and K_s were also determined for a 0.1-m-diam reactor to aid in the scaleup analysis. Values for $V_{\max}$ and K_s for the 0.1-m-diam column were $20 [g \cdot m^{-3} \cdot min^{-1} (\% \text{ biomass})^{-1}]$ and 1300 g/m^3 , respectively, as compared with $3.5 [g \cdot m^{-3} \cdot min^{-1} (\% \text{ biomass})^{-1}]$ and 160 g/m^3 for the 0.5-m-diam column. The differences are possibly attributable to the use of an inappropriate RTD and to problems associated with mixed cultures. Since differences between the two sets of parameters are large, data from other columns will be needed to determine an effective scaleup method.

The biodenitrification reaction follows a reduction path from nitrate to nitrite to hyponitrite and finally to nitrogen. Since at least nitrite appears in the product in substantial quantity, it is recommended that a better understanding of the process may be gained by studying the behavior of the intermediate reduction products.

An experimental program to study the effect of biomass loading on the denitrification rate, using a bench-scale tapered fluidized-bed bioreactor, was begun. It was recommended that this program be continued.

2. INTRODUCTION

Nitrate-containing wastewater presently generated by several steps in the nuclear fuel cycle and other commercial processes may cause stream eutrophication. Therefore they represent a health and environmental hazard. Biological reduction of nitrate to nitrogen provides an economical process for treating these wastes. The Chemical Technology Division of Oak Ridge National Laboratory has developed fluidized-bed bioreactors beginning at the bench-scale and proceeding to the pilot-plant scale for the biological destruction of nitrate (1, 2). In this process, anthracite coal particles laden with anaerobic bacteria (*Pseudomonas*) are fluidized by the nitrate wastewater stream. In the presence of a carbonaceous energy source (for the most part ethanol), the bacteria catalyze the denitrification reaction, producing relatively harmless wastes: nitrogen and carbon dioxide.

A fluidized-bed bioreactor (FBR) has three main advantages over conventional, continuous, stirred-tank reactors (CSTR). First, the CSTR operates at its outlet concentration, which therefore must be the maximum permissible effluent concentration. Since the reaction rate in the low concentration range is proportional to concentration, the destruction rate of the nitrate will of necessity be relatively low. On the other hand, a FBR can capitalize on high inlet concentrations, resulting in higher overall rates. Actual waste systems fall between the CSTR and plug-flow reactors in their reaction behavior. Therefore they tend to less efficiently utilize reactor volume. The conventional waste disposal units tend to require a great deal of space. In a confined plant, a FBR would offer very definite advantages. Secondly, by providing high surface area for biomass growth, the FBR can support higher biomass concentrations (10 to 20 fold) than conventional reactors, thus promoting still higher reaction rates (1). Because of the faster rate, FBR equipment can be much smaller and have a lower capital cost. Thirdly, since the residence time is much less (200 fold) in the FBR bacteria, toxins or inhibitors which appear after long residence times have a reduced effect on the reaction.

After preliminary testing, the pilot-plant-scale bioreactor (0.5-m diam, 0.7-m height) was continuously operated for two and one-half months. Concentrations, temperature, flow rate, pH, and biomass loading were monitored

throughout this period. As part of this investigation, Roadcap *et al.* (3) measured the residence-time distribution for both the 0.5-m-diam column and a smaller column (0.1-m diam) in which water, air, and clean coal were studied. In addition to these studies, earlier data on 0.1-m- and 0.2-m-diam columns were taken and were available to the current modeling effort. The objective of this study was to develop a simulation model of the pilot-plant reaction behavior and to determine acceptable scaleup criteria that would be useful in designing full-scale biodenitrification operations.

3. PILOT-PLANT OPERATION

The pilot plants on which this study was based consisted of fluidized-bed columns (various diameters and height) and their supporting equipment. A schematic layout of these units is given in Fig. 1. The fluidized-bed reactor consists of four sections. The conical entry section at the bottom of the column acts as a fluid distributor and prevents the backflow of bacteria and coal into the feed system. The main cylindrical section of the column is 0.5 m in diameter and 7 m high in the case of the large pilot plant and contains the fluidized bed. A second conical section above the fluidized bed slows the fluid rate, allowing for disengagement of the solid and liquid. Some of the biomass-laden coal is removed in this section. A short cylindrical section at the top of the column permits disengagement of the liquid stream and the gas produced by the reaction.

The bed consists of 30/60-mesh coal particles, to which a mixed culture of bacteria (mainly consisting of *Pseudomonas denitrificans*), attach themselves and grow. Initially an inoculum of bacteria is mixed with nutrient and clean coal. Over a short time period (1 day) biomass grows on the coal, and the bed is ready to be exposed to the waste stream. As the weight of biomass attached to the coal increases, the average density of the material decreases, and the bacteria-laden coal rises in the column. Eventually particles with a sufficiently high level of biomass will float. These particles are removed from the bed, and the pendent biomass is shaken from the coal by a vibrating screen. The cleaned coal with a remaining thin layer of biomass is then returned to the column. Therefore, in continuous operation a gradient of biomass loading can be expected from the bottom of the column to the point at which the bacteria-laden coal is removed. Four sample points are located in the fluidized section of the column, permitting the measurement of biomass loading as a function of position in the column.

A synthetic feed mixture was prepared which would be typical of nitric acid wastewater that had been neutralized with ammonium hydroxide. For storage convenience a concentrated solution (Table 1) was mixed, containing, in addition to ammonium nitrate, ethanol which served as a carbonaceous source, other nutrients, and an antifoaming agent. The concentrated solution was diluted to the desired nitrate level with water before it entered the bioreactor.

Table 1. Composition of Synthetic Nitrate Wastes (1)

<u>Concentrated Feed Solution</u>	
<u>Component</u>	<u>Concentration (g/liter)</u>
HNO ₃	300
NH ₄ OH	120
EtOH	200
MgSO ₄	1
Dow-Antifoam "A"	1
Trace metal solution	0.1
<u>Trace Metal Solution</u>	
KI	10
H ₃ BO ₃	1
Fe-chelate	200
ZnSO ₄ ·7H ₂ O	0.4
(NH ₄) ₆ Mo ₇ O ₂₄ ·4H ₂ O	0.2
MnSO ₄ ·7H ₂ O	0.25
CuSO ₄ ·5H ₂ O	0.45
FeSO ₄ ·7H ₂ O	0.25

Each day during the experimental program the nitrate, nitrite, ethanol, and other nutrient concentrations were measured as were the average biomass loading, temperature, and feed flow rate. The concentrations were measured at 8 points in the system: the concentrated feed tank, the inlet, the four sample ports, the exit, and the drain. The average biomass loading was determined by sampling the bed at the four ports, blending the samples, and then analyzing for percentage biomass.

4. MODEL DEVELOPMENT

4.1 Literature Search

A literature search (3, 5, 6, 7, 8, 12) was conducted to guide the selection of a suitable kinetic model of the denitrification reaction. Biological denitrification requires a carbonaceous energy source. With ethanol as the source, the reaction may be written in unbalanced form (1) as:

The composition of the biomass is approximately $\text{C}_5\text{H}_7\text{O}_2\text{N}$ with a yield of 0.1 gram per gram of nitrate consumed. The intermediate nitrite concentration is only measured at entry and exit points of the system. Any nitrite departing the system will eventually be reoxidized to nitrate and therefore, from a design viewpoint, reaction to the nitrite state only is of no value. In modeling the behavior of the system, an accounting for the nitrite is of importance, since significant quantities of the material occur in all reactions. The stoichiometry of the reaction expressed as the mole ratio of carbon in the form of ethanol consumed to nitrate-nitrogen reduced to nitrogen was previously shown to be between 1.1 and 1.5 (2). This ratio is studied in more detail in this report.

Lee (4) studied denitrification by *Pseudomonas* and found the reaction rate to be described by Monod kinetics (5). Pitt et al (2) found the data generated in a denitrification study by *Pseudomonas* in a fluidized-bed bioreactor fit the Monod model satisfactorily. Therefore it is natural that this model be selected as the starting point for our simulation efforts.

It has been found that bacterial growth is first-order in the viable biomass which is present. This relation may be written as:

$$\frac{dX}{dt} = \mu X \quad (2)$$

where X is the microbial concentration of a given species and μ is the specific growth rate for the type of organism at the temperature, pH, and for the specific nutrient medium of interest.

The growth rate is proportional to the concentration of the limiting substrate in the low concentration range, while at high concentrations the limitation is associated with metabolic functions of the micro-organism. Monod (5) found that these facts may be expressed mathematically as:

$$\frac{dX}{dt} = \hat{\mu} \left(\frac{S}{K_S + S} \right) X \quad (3)$$

where

S = substrate concentration

$\hat{\mu}$ = maximum specific growth rate

K_s = saturation constant and represents the concentration at which the reaction rate is one half the maximum

The empirically derived Monod expression is similar to the Michaelis-Menton equation in its substrate functionality. The latter theory describes the reactions between enzymes and substrates (16). Since enzyme reactions are the basis for biological reactions, the connection between Michaelis-Menton kinetics and Monod model is expected.

In biological denitrification of nitrates and nitrites to gaseous N_2 and CO_2 it is normal to use a mixed culture of bacteria from soil. Typically the bacteria which are active are *Pseudomonas denitrificans* or *Pseudomonas stutzeri*, both of which are facultative anaerobes. The disposition of both the nitrogen and the carbon in the process is discussed by Pitt et al. (2).

As mentioned earlier, anaerobic denitrification requires two substrates: nitrate and a carbonaceous energy source. Therefore a Monod-type expression describing this reaction may be written as (12):

$$\frac{dX}{dt} = k \left[\frac{[NO_3^-]}{K_s^{NO_3} + [NO_3^-]} \right] \left[\frac{[C]}{K_s^C + [C]} \right] X \quad (4)$$

where

$[NO_3^-]$ = nitrate concentration

$K_s^{NO_3}$ = saturation constants for nitrate

$[C]$ = ethanol concentration

K_s^C = saturation constant for ethanol

An expression of similar form was used by Eckenfelder and Argaman (7) in describing aerobic denitrification with two limiting substrates.

Since the removal of nitrate from the waste stream is the objective of the process, the rate expression is most conveniently stated in terms of denitrification rate. There exists a stoichiometric relationship between substrate consumed and microorganism produced:

$$\frac{dX}{dt} = -Y \frac{d[NO_3^-]}{dt} \quad (5)$$

where Y is a stoichiometric coefficient called the yield coefficient. Equations (4) and (5) are combined to yield:

$$\frac{d[\text{NO}_3^-]}{dt} = V_{\max} \left[\frac{[\text{NO}_3^-]}{K_s^{\text{NO}_3} + [\text{NO}_3^-]} \right] \left[\frac{[\text{C}]}{K_s^{\text{C}} + [\text{C}]} \right] \quad (6)$$

where $V_{\max} = \hat{\mu}/Y$ = maximum velocity of the reaction if all substrates are present in excess.

Biological reduction of nitrate occurs in a number of known steps. Nitrate (NO_3^-) is first reduced to nitrite (NO_2^-) before reacting to form nitrogen. Any nitrite present in the bioreactor effluent will be oxidized back to nitrate upon contact with oxygen. Since the design objective is to attain a minimum nitrate concentration in the exit stream, both nitrate and nitrite concentrations must be considered in studying the process. Therefore the nutrient concentration is expressed in terms of the total unreduced nitrogen which is the sum of the nitrate (NO_3^-) and nitrite (NO_2^-) concentrations:

$$\frac{d[\text{N}]}{dt} = V_{\max}^n \left[\frac{[\text{N}]}{K_s^n + [\text{N}]} \right] \left[\frac{[\text{C}]}{K_s^{\text{C}} + [\text{C}]} \right] \quad (7)$$

The changes in the reaction constants $V_{\max}^n$ and K_s^n are necessary because the concentration basis has been modified.

This rate expression will apply if the rate of nitrite reduction is similar in functionality and rate to the nitrate removal. Concentration profiles of the two species in the reactor indicate agreement with this premise. The nitrate profile monotonically decreases with length, while the nitrite concentration, which is very low at the inlet, is usually significant at the exit.

A fundamental study of the two sequential reactions would be needed before one could justify a more sophisticated model. It is not possible to ignore the nitrite since it represents as much as 25% of the original unreduced nitrogen in some cases. As a first step in the analysis of this complication, the stoichiometry of the two-reaction sequence was studied.

4.2 Reaction Stoichiometry

As an initial inquiry into the nature of the reactions which occur in denitrification, the stoichiometric relationships between nitrate, nitrite, and ethanol were examined. On a mass basis, two balances are written:

$$\Delta \text{NO}_3^- = x''(\Delta \text{C}_2\text{H}_5\text{OH}) \quad (8)$$

and

$$\Delta \text{NO}_2^- = \beta'' (\Delta \text{C}_2\text{H}_5\text{OH}) \quad (9)$$

where Δ is the overall change in concentration in ppm. In any given experiment there will be a change in both the nitrate and nitrite levels. Therefore Eqs. (8) and (9) can be combined and rearranged to give:

$$\frac{\Delta \text{C}_2\text{H}_5\text{OH}}{\Delta \text{NO}_3^-} = \frac{1}{\alpha''} - \frac{1}{\beta''} \frac{\Delta \text{NO}_2^-}{\Delta \text{NO}_3^-} \quad (10)$$

It then remains to gather a reliable set of data and to perform a linear regression analysis on the data.

The data selected were those collected for the operation of the dual 20-cm columns. Five time periods were selected in which the columns were operated under steady feed conditions for at least four days. The results for each column were averaged. There appeared to be little anomalous behavior in any of the sets of results. The averaged data along with the linear regression line are shown in Fig. 2. Negative values of $\Delta \text{NO}_2^- / \Delta \text{NO}_3^-$ indicate that there was a net increase in NO_2^- concentration from inlet to outlet of the column in question. This is expected in most operations. One would never expect a negative $\Delta \text{C}_2\text{H}_5\text{OH} / \Delta \text{NO}_3^-$ ratio because both ethanol and nitrate are continuously depleted. On a molar basis the results are:

$$\text{mole ratio C/NO}_3^- = 1.14$$

$$\text{mole ratio C/NO}_2^- = 0.72$$

$$r^2 = 0.816$$

The coefficient of correlation (r^2) is within expectation for these data. Previously reported C/NO₃⁻ ratios in the range of 1.1 to 1.5 are in agreement with our result. It is interesting to note that nearly two-thirds of the carbon is utilized in reducing from NO₃⁻ to N₂. Since it is postulated that the sequence is a three-step reaction [Eq. (1)], this result is expected.

It would be of interest to attempt to isolate the hyponitrite species and its kinetics. The hyponitrite ion occurs as a dimer:

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FIG.
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One of the known reactions of the hyponitrite of alkali metals is with CO_2 , yielding N_2O (17). Since the medium rapidly saturates with CO_2 , it is possible that this reaction occurs. It would be of interest to determine whether nitrous oxide (N_2O) occurs in the effluents from the reactors. Usually hyponitrites behave as reducing agents; therefore it is anticipated that if it exists in the mixture being released from the column, it will probably be oxidized back to NO_3^- . Since the NO^- levels were not measured, it is impossible to assess the influence of hyponitrite ion on the reaction system.

4.3 Data Trends

An initial scrutiny of the data collected in the pilot denitrification indicates a wide variability. A significant number of variables are evidently at play in the denitrification operation. A statistical analysis by Hancher (14) showed that the important variables that might affect the outlet nitrate concentration from the bioreactor are the flow rates into the reactor, the inlet nitrate concentration, the biomass loading, the ethanol concentration, and the pH. Hence, plots of average nitrate removal rates as a function of the various variables were analyzed qualitatively. Equation (7) was then simplified according to the trends observed from these plots, before a more sophisticated modeling procedure was performed. In this initial study, effects of nitrite were not included.

A plot of average nitrate removal rate vs the arithmetic average nitrate concentration in the bioreactor for all the 0.5-m pilot-plant data is shown in Fig. 3. There is a positive correlation between these two variables although the large scatter at higher concentrations clearly indicates that other factors are at work. The functionality appears to decrease from first order in the $[\text{NO}_3^-]_{\text{avg}} < 500 \text{ g/m}^3$ range to zero order at higher concentrations. These trends support the use of a hyperbolic function in $[\text{NO}_3^-]_{\text{avg}}$ in the kinetic model and also lend support to the Monod kinetics.

A plot of average nitrate removal rate vs biomass loading for all data is presented in Fig. 4. The trend in these data clearly indicates that one can expect biomass to have an effect on rate.

The functionality in nitrate feed concentration has not been removed from these data. Therefore, it is expected that there will be considerable scatter. Nevertheless, if we assume that there will be no reaction when the biomass loading is zero, it is possible to draw an envelope around the data and to finally draw a dotted line which indicates the effect of the biomass loading upon the overall reaction. Figure 5 shows denitrification rate as a function of biomass loading for two initial concentrations: 600 and 1500 g/m^3 . The data show average nitrate removal rates to be a positive function of biomass loading, but the points are too scattered to determine the exact functionality. Therefore, a first-order functionality between

AVERAGE NITRATE-
NITROGEN REMOVAL RATE
(kg N/m³-d)

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AVERAGE RATE AS A FUNCTION
OF BIOMASS LOADING

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average nitrate removal rate and biomass loading was drawn through the data and passed through the origin as predicted by Monod kinetics.

The ratio of average nitrate removal rate to percentage biomass loading is shown as a function of average pH at the constant average nitrate concentrations in Fig. 6. Nitrate removal rates were divided by percentage biomass loading to eliminate the effect of assumed first-order functionality in biomass. Data with average nitrate concentrations of 600 and 1500 g/m³ showed a weak functionality between (nitrate removal rate)/(% biomass) and average pH in the column for the range 7.0 to 8.6. If other data are selected, the scatter is even more pronounced and the trend is reversed in many cases. Therefore our conclusion is that there is no functionality in pH for the range studied. This conclusion agrees with a study by Dodd and Bone (8) in which it was concluded that this particular reaction runs at its maximum rate from pH 6.9 to 8.9.

Since the bacteria are a mixed culture of many different types of bacteria, it is likely that each particular strain has its highest activity at a certain pH. The overall effect of simultaneous growth masks the pH-growth-rate trend for any individual species.

The effect of the ratio of nutrients (C/N) upon reduced reaction rate is shown in Fig. 7 for average nitrate concentrations of 600 and 1500 g/m³. There was no discernible trend in the data. The average C/N in the feed solution for all runs was 2.2, while the average C/N consumed by the reaction was approximately 1.14. This suggests that the carbon source is in excess and will remain so throughout the reaction. Therefore the modified Monod kinetic expression [Eq. (7)] is likely to reduce to zero in the carbon source. As a result the functionality in carbon is neglected in this simulation of the pilot-plant operation.

The effect of flow rate on the average nitrate removal rate was incorporated into the design equation through a dispersion number which represents the flow pattern inside the bioreactor. The flow was essentially constant for all experiments.

Hence, based on theory and analysis of the pilot-plant data, a reduction of Eq. (7) was chosen as the kinetic expression to be used in the initial simulation:

$$\text{rate} = V_{\max} \left(\frac{[N]}{K_s^n + [N]} \right) X \quad (11)$$

The term [N] refers to the total unreduced nitrogen and accounts for two species: nitrate and nitrite. The latter material is in a state of partial reduction, but the means of accounting for its reaction was not studied. Therefore, nitrite was simply accounted for as being unreduced from the initial state. The entire reduction sequence in denitrification requires further study.

4.4 Design Equations

To develop a design equation, the kinetics and the contacting pattern must be incorporated into a material balance on the bioreactor. From the residence-time distribution (RTD), a model of the contacting pattern may be proposed.

Roadcap et al. (3) measured the RTD of the bioreactors used in the current study and expressed the variances of the RTD in terms of a dispersion number. Axial dispersion numbers in a continuity equation are a measure of the deviation from plug flow (9). A correlation between dispersion number and volumetric flow rate was developed for the 0.5-m column (see Appendix 10.1). Incorporating the kinetic expression in the dispersion model results in the following performance equation for the bioreactor:

$$\frac{D}{uL} \frac{d^2[N]}{dz^2} - \frac{d[N]}{dz} - \frac{V_{\max}[N]}{K_s + [N]} X = 0 \quad (12)$$

A review of the pilot-plant data made it clear that the evaluation of coefficients by the numerical solution of Eq. (12) was an expensive task and was not justified in light of our poor understanding of the scatter in the data. Hence, other reactor models having the same RTD were examined.

Since the denitrification reaction is not mathematically simple, the type of model chosen (macromixing or micromixing) might have an effect on the conversion. Thus, two single-parameter models, one describing macromixing and the other micromixing, were selected to simulate the bioreactor.

A stirred-tanks-in-series model was chosen as the micromixing model. The relationship between the dispersion number and the number of tanks in series which simulates the same dispersion characteristics is discussed by Levenspiel (9). The number of tanks (N) is given by the following equation:

$$\frac{1}{N} = 2\left(\frac{D}{uL}\right) - 2\left(\frac{D}{uL}\right)^2 \left[1 - \exp\left(-\frac{uL}{D}\right)\right] \quad (13)$$

A steady-state material balance for a single stirred tank yields the following relationship:

$$FS_1 = FS_0 + (V)(V_{\max})\left(\frac{S_0}{K_s + S_0}\right)X \quad (14)$$

Equation (14) may be rearranged to a more standard form:

$$\frac{S_i - S_o}{\tau} = V_{\max} \left[\frac{S_o}{K_s + S_o} \right] \times \quad (15)$$

where

F = volumetric flow rate

S = substrate concentration (unreduced nitrogen)

i = in

o = out

τ = residence time

V = reactor volume

By solving Eq. (15) for N tanks in series, and setting the inlet concentration for a given tank equal to the exit concentration of the previous tank, a predicted value of effluent concentration (equal to the exit concentration of the final tank) can be compared with the observed concentration. If the constants $V_{\max}$ and K_s were optimally selected, the two effluent concentrations should coincide.

A second approach is to model the reactor as a bundle of parallel plug-flow reactors of various lengths. This method was chosen as a macro-mixing model of the RTD. In this case each plug-flow reactor corresponds to a particular residence time. The flow rate into each reactor is determined by the fraction of effluent leaving the pilot-plant reactor at the corresponding residence time. The length of each tube is then calculated from the flow rate, residence time, and diameter of the tube. To use this model, an equation for the residence-time distribution must be obtained.

Both linear and nonlinear analyses were used to relate the dispersion number (Pe^{-1}) to the flow rate in the reactor (Appendix 10.1). Alternately, the RTD curve may be derived from the Peclet number using an exact relationship (15):

$$E(\theta) = e^{Pe/2} \sum_{i=1}^{\infty} \frac{(-1)^{i+1} 8\gamma_i^2}{4\gamma_i^2 + 4Pe + Pe^2} \times \exp[-\theta(Pe^2 + 4\gamma_i^2)/4Pe] \quad (16)$$

where γ_i is defined by the equation:

$$\tan \gamma_i = \frac{4Pe\gamma_i}{4\gamma_i - Pe^2} \quad (17)$$

Because of the complexity of Eq. (16), Eq. (13), relating the number of stirred tanks required to the dispersion number, was used again to model the RTD. Turning again to Levenspiel (9), the relationship between the number of tanks and the RTD may be expressed as:

$$E(\theta) = \frac{N(N\theta)^{N-1} e^{-N\theta}}{(N-1)!} \quad (18)$$

where $E(\theta)$ is the residence-time distribution, θ is the dimensionless residence time, and N is the number of stirred tanks calculated from the Peclet number.

A differential material balance for a plug flow reactor is written as:

$$FdS = V_{\max} \frac{S}{K_s + S} \times AdZ \quad (19)$$

where A is the cross-sectional area of the tubular reactor and Z is the length dimension. The material balance is rearranged and integrated:

$$\int_{S_i}^{S_o} \left(\frac{K_s + S}{S} \right) dS = \int_0^L \frac{V_{\max} XA}{F} dZ \quad (20)$$

where L is the length of the plug-flow reactor. Integration of Eq. (20) yields the outlet concentration of each plug-flow reactor. The outlet concentrations, weighted by their flow rates, are then averaged to determine predicted outlet concentrations for the whole reactor.

A modeling complication arises because the biomass loading increases with height in the column. In the tanks-in-series model, different biomass loadings must be assigned to different tanks in the train; while in the plug-flow reactor model, biomass must be described as a function of length. Only the average biomass level in the column was measured for each day. However, from measurements made early in the experimentation, it was determined that the percentage biomass varied approximately $\pm 20\%$ from the average. However, the functionality of the loading with position in the column was not determined. In the case of the 0.1-m bench-scale column for which biomass profile data were available, biomass loading varied $\pm 50\%$ from the average. The shape of the profile varied considerably; however, for simplicity in the simulation, only a linearly increasing function with height was assumed for all the 0.1-m-column data.

Fortran programs were written for both the tanks-in-series and plug-flow-reactors-in-parallel models. These along with flow charts for each program are shown in Appendix 10.2.2.

4.5 Non-Linear Regression

The two constants in the Monod rate expression [Eq. (11)] ($V_{\max}$, the maximum rate, and K_s , the saturation constant) were determined from the pilot-plant data. Marquardt's algorithm (10, 11) was used to minimize the sum of the squares of the difference or residual between the observed exit concentration and the concentration predicted by the model. This technique was used both for the case of tanks-in-series model [Eq. (15)] as well as the plug-flow-reactors-in-parallel model [Eq. (20)]. From the initial guess of $V_{\max}$ and K_s , the algorithm varies each parameter until the change in the summation of the residuals squared is less than a predetermined small value ($\sim 10^{-6}$). A routine for implementing Marquardt's algorithm is available on the PDP-10 computer in the Chemical Technology Division. Care must be taken in the selection of the initial values since the algorithm may converge on a local minimum instead of the true minimum.

5. RESULTS AND DISCUSSION OF SIMULATION

5.1 Tanks-in-Series Model

In performing the simulation of the two columns for which residence-time distributions were measured by Roadcap et al. (3) (0.1 and 0.5-m), an analytic relationship between biomass loading and column height was necessary. In the case of the 0.5-m column, a linear and a one-half power simulation were selected. A linear biomass profile was selected for the 0.1-m column. A second consideration was the type of fit one applies to the dispersion coefficient. The larger-column data were fit with both a power-law model and a linear model. Since the flow rate range was narrow, it was anticipated that the model selected would have little effect. Dispersion simulation of the 0.1-m column used only the power-law simulation. Values of $V_{\max}$, K_s , and standard error computed by the computer programs from the pilot-plant data are shown in Table 2.

Comparison of these values indicates a negligible effect of biomass profile on the accuracy of the modeling. Therefore a linear biomass profile was used for the remainder of the simulation. Flow rates in the 0.5-m-column data ranged from 95 to 150 liters/min. In this range the two models selected yielded identical results. The power-fit correlation, having a basis in theory (8), was selected for the remainder of the modeling effort (see Appendix 10.1).

5.2 Plug-Flow-in-Parallel Model

The bioreactor operation was also simulated by the plug-flow-in-parallel model. In this case the best fit $V_{\max}$ and K_s , using the 0.5-m-column data, were approximately equal to those found using the tanks-in-

Table 2. Simulation Results for Tanks-In-Series Model

	$V_{\max}$ [g-min ⁻¹ -m ⁻³ (% biomass) ⁻¹]	K_s (g/m ³)	Standard Error (g/m ³)
<u>0.5-m Column</u>			
Power fit for dispersion, Linear biomass profile	3.5 ± 10%	163 ± 25%	184.9
Power fit for dispersion, Half-order biomass profile	3.2 ± 10%	163 ± 25%	184.8
Linear fit for dispersion, Linear biomass profile	3.5 ± 10%	163 ± 25%	184.7
<u>0.1-m Column</u>			
Power fit for dispersion, Linear biomass profile	19.7 ± 10%	1285 ± 30%	415.0
$V_{\max}$ set = 3.5 Power fit for dispersion, Linear biomass profile	3.5	1.44 × 10 ⁻⁷	854.0

series model (Table 3). However, the standard error in K_s was more than twice the standard error in the tanks-in-series model. Hence the latter was used in the remainder of the modeling.

Comparison of parametric values found for the tanks-in-series model with the plug-flow-in-parallel model indicates that the calculated nitrate concentration may not be affected significantly by the flow pattern.

5.3 Mass Transfer Limitations

Mass transfer limitations may have a significant effect on the rate of denitrification. If no limitations on the diffusion of nitrate through biomass exist, the denitrification rate is proportional to the biomass loading (X), as predicted by the Monod rate equation. However, if mass transfer limitations are great, nitrates are unable to penetrate the biomass and the rate is proportional to the biomass surface area ($X^{2/3}$). In an attempt to assess the degree to which mass transfer limitations were present in the pilot-plant operation, the $\%$ biomass term X in the kinetic rate expression [Eq. (11)] was replaced by X^n . If diffusion limitations in the bacteria are present, expressions of this form may fit the data more accurately.

The simulation model was first modified so that the power dependence of the biomass loading became a third parameter to be fit by the Marquardt algorithm. Results for both the 0.5-m pilot-plant data as well as the 0.1-m column are shown in Table 4. Values calculated for the 0.5-m column indicate that a rate expression incorporating biomass to the 0.7 power provides the best fit of the data. Values calculated for the 0.1-m data indicate that a rate expression nearly independent of the biomass loading provides the best fit.

The addition of an extra parameter should lower the standard error between the observed and predicted value. Because the reduction of the standard error was small (from 184 to 174 g/m³ for the 0.5-m column), the two-parameter model was used in the remainder of the computer simulations. However, this exercise does point toward the possibility that the diffusion resistance to mass transfer might be significant. Modeling of the system in a manner similar to that used in porous-catalyst media might prove fruitful.

5.4 Effect of Biomass Loading on Parameter Values

The effect of biomass loading on the values of V_{max} and K_s were examined by grouping both the 0.1-m and 0.5-m data according to biomass loading. The resulting values of V_{max} are shown in Fig. 8.

For the 0.5-m column, V_{max} was relatively constant throughout the range of biomass loadings available and was approximately equal to the V_{max}

Table 3. Results for Plug-Flow-in-Parallel Model
(0.5-m Column)

	$V_{\max}$ [g-min ⁻¹ -m ⁻³ (% biomass) ⁻¹]	K_s (g/m ³)	Standard Error (g/m ³)
Plug-Flow-in-Parallel: Linear biomass profile, Power fit for dispersion	3.5 ± 10%	136 ± 100%	194.3
Stirred-Tank-in-Series: Linear biomass profile, Power fit for dispersion	3.5 ± 10%	163 ± 25%	184.9

24

Table 4. Determination of Mass Transfer Limitations

		$V_{\max}$ [g-min ⁻¹ -m ⁻³ (% biomass) ⁻¹]	K_s (g/m ³)	Standard Error (g/m ³)
0.5-m Column	0.7	9.0 ± 33%	146 ± 57%	174
0.1-m Column	0.0	287 ± 21%	1890 ± 21%	227

	0.1M	0.51M
V _{MAX}	19.7	3.48
BEST OVERALL FIT OF V _{MAX}		

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BEST FIT V_{MAX} AT VARIOUS
BIOMASS LOADINGS

DATE 11/21/80 DRAWN BY EW DESIGNED BY CEPSX-320G. 8

calculated using the entire range of biomass concentrations. Values of V_{max} for the 0.1-m column decreased slightly with increasing biomass. Because of the limited range of biomass values present in the 0.1-m-column data, it is difficult to assess the importance of the downward trend. Values of V_{max} were all nearly equal to the V_{max} calculated using all the data. The fact that RTD information on this column exists for the clean-coal situation only, makes any conclusion about trends somewhat tenuous.

Figure 9 shows the change in K_s as a function of the biomass loading. For the 0.1-m column, K_s increased with increasing biomass, but the values do not differ significantly from the value obtained using all the 0.1-m data. However, for the 0.5-m column, K_s varies substantially with biomass. At low biomass loadings, K_s is almost zero, indicating a zero-order reaction in substrate concentration. At higher biomass loadings, values fluctuate considerably from the value obtained using all the 0.5-m data. This indicates that the model selected here requires considerable refinement. The role of mixed-culture kinetics in the problems which were observed here is unknown.

5.5 Accuracy of Model

As a result of comparisons among the various models and model modifications as discussed in Sects. 5.1 through 5.4, a final simulation utilizing the series-of-stirred-tanks model with a linear biomass profile, a power-fit for dispersion, and a first-order dependency of the rate on biomass loading was chosen.

An assessment of the accuracy of the model was made by plotting both the average observed and average predicted rate versus the average nitrate concentration at particular ranges of biomass loadings. Figures 10, 11, and 12 show the plots for the biomass ranges >25%, between 25 and 15%, and less than 15%, respectively.

Figures 13 and 14 illustrate the ability of the stirred-tanks-in-series model to predict the profile of nitrate within the bioreactor. Two examples are presented to illustrate the range of results obtained in this study. For a number of the data points, the fit was as accurate as that shown in Fig. 13. The model frequently predicted a profile much different from the observed profile, as of Sept. 8, 1980 (Fig. 14). The poor fit may be a result of radial dispersion effects within the column. As bacteria multiply, they tend to agglomerate and to accumulate at the wall of the column. This may cause channeling within the reactor. Since the sample ports are located along the wall of the column, the measured concentrations may not be a good representation of the average concentration at that level.

In sampling the profile, no measurement was made of nitrite level. Therefore the data reported in Figs. 13 and 14 are somewhat inaccurate. Given a more complete analyses, the data might be somewhat more representative of the reaction. In spite of the deviations in the profile, the outlet concentration was predicted accurately by the model (Fig. 14).

	0.1M	0.51M
K_s	1285	163

BEST OVERALL FIT OF K_s

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OAK RIDGE NATIONAL LABORATORY

BEST-FIT K_s AT VARIOUS
BIOMASS LOADING

DATE 11/21/80	DRAWN BY EW	FILE NO. CEPS-X-324	FIG. 9
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AT			
OAK RIDGE NATIONAL LABORATORY			
COMPARISON BETWEEN PREDICTED & OBSERVED DENITRIFICATION RATE			
BIOMASS LOADING > 25%			
DATE	DRAWN BY	FILE NO.	FIG.
11/21/80	EW	X-324	10

MASSACHUSETTS INSTITUTE OF TECHNOLOGY SCHOOL OF CHEMICAL ENGINEERING PRACTICE AT OAK RIDGE NATIONAL LABORATORY			
COMPARISON BETWEEN PREDICTED AND OBSERVED DENITRIFICATION RATE 25% > BIOMASS LOADING > 15%			
DATE	DRAWN BY	FILE NO.	FIG.
11-21-80	FW	X-324	11

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COMPARISON BETWEEN PREDICTED AND
OBSERVED DENITRIFICATION RATE
BIOMASS LOADING < 15%

DATE 11-21-80	DRAWN BY EW	FILE NO. X-324	FIG. 12
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NITRATE CONCENTRATION PROFILE
ON SEPT. 29, 1980

DATE
11/21/80

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EW

FIG. NO.
CEPS-X-34 13

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NITRATE CONCENTRATION PROFILE
ON SEPT. 8, 1980

DATE 11/21/80	DRAWN BY EW	FILE NO. CEPS-X-324	FIG. 14
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5.6 Scaleup

In an attempt to assess the usefulness of the model for scaleup, the 0.1-m bioreactor was also simulated. If the 0.1-m-column data result in the same $V_{\max}$ and K_s values as for the 0.5-m column, scaleup correlations are not required. If not, the possibility of developing a correlation between the parameters and the reactor size could be investigated.

The 0.1-m-diam column operation was simulated using a linear biomass profile and a power-fit for dispersion number. Results shown in Table 2 indicate an order-of-magnitude difference for both $V_{\max}$ and K_s between the 0.1-m column and the 0.5-m column. However, the effect of the high values for the 0.1-m-column parameters tend to negate each other because $V_{\max}$ is in the numerator of the rate expression, while K_s is in the denominator. This results in a rate similar to the 0.5-m column rate.

The differences in the constants do, however, have an effect on the shape of the rate-vs-substrate curve. For the 0.1-m-diam column, the rate expression does not approach zero order in nitrate as quickly as the expression determined for the 0.5-m-diam column. In theory, the kinetic curves should be the same in both cases, since presumably the reactions are the same. However, since there was a substantial time lapse between the experiments on the 0.1-m column and those on the 0.5-m column (over six months), and since mixed cultures are involved, it is entirely possible that different strains predominated in the two experiments.

To investigate the significance of the order-of-magnitude difference in $V_{\max}$ and K_s for the two columns, the simulation of the 0.1-m column was altered. $V_{\max}$ was set equal to the maximum specific rate predicted for the 0.5-m data ($3.5 \text{ g/m}^3\text{-min-\% biomass}$), and Marquardt's algorithm was used to find the new value of K_s . If the calculated K_s is close to the K_s value determined for the 0.5-m column, then the two sets of data can be approximately fit by the same set of parameters. Differences between the parameter sets originally calculated for each column could then be attributable to the effect of scattering in the data. The algorithm predicted an extremely low K_s value (10^{-7} g/m^3), yielding an apparent zero-order dependence of rate on nitrate concentration and did not converge as well as in other simulations.

One possible explanation for the difference in the apparent kinetics between the two columns is that the dispersion numbers for the 0.1-m column were measured with only clean coal in the reactor. The effect of increased particle size along the length of the column on the residence-time distribution is not known. The substitution of these dispersion numbers for those corresponding to actual column conditions might be the cause of the differences in the fitted $V_{\max}$ and K_s values. This may also account for the large standard error found in the modeling of the 0.1-m column data.

Another possible explanation for the difference in apparent kinetics is due to the data base. The average biomass loading in the 0.5-m bioreactor

was twice the level present in the 0.1-m column (~25 to ~12%). Also much higher concentrations of substrate were present in the 0.1-m-column data than in the 0.5-m-bioreactor data (see Appendix 10.2.2). Because of the significant differences between the parameters calculated for the 0.5- and 0.1-m columns, the usefulness of the model in reactor scaleup cannot be determined.

If RTD and denitrification-rate data from other columns were available, a correlation between the two kinetic parameters (V_{max} and K_s) and the size of the reactor may be found, yielding a useful scaleup tool. Denitrification data are available for a pair of 0.2-m-diam columns used by the Chemical Technology Division. RTD data should be estimated for these columns and utilized in the determination of a model scaleup method. It is recommended that these data be carefully examined for possible utility in assessing the proposed model.

6. EXPERIMENTAL

It is evident that the relationship between column performance and biomass loading is not well known. Therefore it was proposed that a transient experiment be performed to evaluate the denitrification rate as a function of biomass loading. To this end a bench-scale tapered-tube reactor was made available for experimentation.

6.1 Apparatus and Procedure

A schematic diagram of the apparatus used in the biomass-loading experiments is shown in Fig. 15. The facility consists of a 106.7-cm-long, glass, tapered fluidized bed (13) with a diameter that increases from 2.54 cm at the bottom of the reactor to 7.62 cm at the top. The bed consisted of anthracite coal particles (30 to 60 mesh) coated with a mixed culture of bacteria, mainly consisting of *Pseudomonas denitrificans*. A sharp transition between coated and uncoated coal particles was present approximately 0.5-m from the bottom of the reactor. Solids and biomass carryover are captured in a settling chamber connected to the top of the column. The water and concentrated feed streams are pumped at a ratio of approximately 100:1 and mixed before entering the column. The composition of the feed is the same as that used in the 0.5-m-diam column (see Table 1).

The fluidized bed operated continuously, and samples were taken on a daily basis. Biomass samples were prepared by mixing 25-ml samples of bed slurry taken from portals 2, 3, and 4 (Fig. 15). After drying overnight in an oven, the combined sample was weighed. The dried sample was then immersed in a caustic solution consisting of 100 g NaOH and 500 ml water to remove the bacteria from the coal. The mixture was fluidized in a funnel and the bacteria allowed to decant over the top. The remaining coal was dried in an oven and weighed to determine biomass loading. Samples were also taken at portals 1, 2, and 4 to determine the nitrate concentration

at various points along the reactor. About 10 ml of liquid was drawn from each slurry sample, using a syringe, and analyzed for nitrate ion in a Gilford spectrophotometer.

6.2 Results and Discussion

A number of problems were encountered in the experimental portion of this project. First, the concentrated-solution feed pump developed a leak, causing the inlet nitrate concentration to vary with time. Since the rate is a strong function of inlet nitrate concentration, the rate dependence on biomass loading could not be determined during that entire portion of the program.

During the second week, a fluctuation in the inlet nitrate concentration was observed. This was traced to a faulty pump. Finally a problem with the computer hardware used to analyze the nitrate concentration was discovered at the end of the week and could not be repaired in time for further experimentation. Therefore no meaningful data were obtained before the end of the project.

Although the time limited the scope of this portion of the study, its objectives are considered vital to the successful conduct of a more sophisticated simulation method. None of the pilot runs addressed biomass loading specifically, with the result that the data are bunched at specific loadings. Furthermore, a biomass profile which would be necessary for a more detailed simulation was not available.

7. CONCLUSIONS

1. The stirred-tanks-in-series reactor model simulated the performance of the fluidized-bed bionitrification pilot plant acceptably.

2. A modified Monod kinetic expression fit the data adequately. The rate expression was first-order in nitrate at low concentrations (less than 500 g/m³) and zero-order at higher concentrations. The rate generally increased with biomass loading. The effects of pH and molar carbon-to-nitrogen ratio on the rate of denitrification appeared to be negligible in the ranges encountered in pilot-plant operation.

3. Implementation of micro- and macromixing models did not significantly affect the simulation. However, the plug flows in the parallel model (macromixing) did lead to larger standard errors in the predicted kinetic constants.

8. RECOMMENDATIONS

1. Residence-time distribution for the 0.2-m-diam column should be measured or estimated. The performance data for the 0.2-m reactor could then be simulated and the kinetic constants predicted. Since six months of operating data are available on the device, these will lend significantly more weight to the constants predicted for the 0.5- and 0.1-m columns. In addition, scaleup parameters and diameter effects can be assessed. Finally, more information will be available on the effect of nitrite ion.

2. Simulation may be improved by two approaches. First, the data should be screened for anomalous points such that only actual biological and reactor phenomena are being modeled. Second, a multi-parameter reactor model may take into account such complex effects as channeling and poor mixing.

3. The Monod kinetic model should be experimentally tested on a bench-scale apparatus, as was attempted in this project. The effect of biomass loading on the rate should be investigated by allowing the bench-scale apparatus to operate without recycling the coal. In this way the biomass will increase from less than 5% to greater than 40% loading, and the effect on the rate over time can be measured. One method of reducing the pumping problems encountered is to prepare a less-concentrated feed so that the feed-to-water ratio can be increased to a more manageable range. Higher feed-to-water ratios will diminish the effects of pump variations. Also, the effect of C/N ratios on the reaction rate should be studied to verify the assumption of its negligible effect on nitrate removal rate made in Sect. 4.3. By keeping the biomass loading constant and by varying the carbon-to-nitrogen ratio in the feed between 0.5 and 1.0, the effect of carbon source could be determined.

9. ACKNOWLEDGMENTS

We thank our consultants R.K. Genung, C.W. Hancher, and J.F. Walker, for their help, ideas, and encouragement throughout the project. Special gratitude is extended to Wallace Davis, Jr., for sharing his knowledge and time with us on the use and operation of the non-linear regression routine and programming for the subroutines. Finally, we appreciate the efforts of George Dinsmore and Hal Jennings in keeping the experimental apparatus running.

10. APPENDIX

10.1 Dispersion Number as a Function of Flow Rate

Residence-time distributions and corresponding dispersion numbers for the 0.5-m-diam column were available at only two flow rates (3). Dispersion numbers at other flow rates could be obtained in a number of ways. Two were selected.

1. Linear Interpolation or Extrapolation

$$\left(\frac{D}{uL}\right) = a + bF \quad (21)$$

where a is dimensionless and b is in min/liter. a and b were determined from the two available sets of data points. $a = 0.0018$ and $b = -0.01186$ min/liter.

2. Power Correlation

Based on theoretical considerations Levenspiel (9) suggests a power law correlation:

$$\ln\left(\frac{D}{u d_T}\right) = \ln \alpha + \beta \ln\left(\frac{u d_T}{D}\right) \quad (22)$$

$$\ln\left(\frac{D}{uL}\right)\left(\frac{L}{d_T}\right) = \ln \alpha + \beta \ln\left(u d_T^2 \frac{\pi}{4}\right)\left(\frac{4}{\pi d_T D}\right) \quad (23)$$

Lumping the constants together and rearranging gives:

$$\ln\left(\frac{D}{uL}\right) = \alpha' + \beta' \ln F \quad (24)$$

α' and β' were determined from the two available set of points.

$$\alpha' = 4.85 \times 10^{-6}$$

$$\beta' = 2.07$$

Equation (24) was used in the simulation model. Similarly, the dispersion-number-vs-flow-rate data for the 0.1-m-diam column data were correlated by Eq. (24). Values of α' and β' were 0.38 and -1.48, respectively.

10.2 Least-Squares Estimation of Non-Linear Parameters and Program Listing

10.2.1 User Information

For any model f ,

$$\hat{Y}_i = f(X_{i1}, X_{i2} \dots X_{im}; p_1, p_2 \dots p_k) \quad (25)$$

which contains m independent variables (X_{il} , where $l = 1, \dots, m$) and k parameters (p_j where $j = 1, \dots, k$). Equation (25) gives the predicted value ($\hat{Y}_i$) of a dependent variable (Y_i) for (n) observations:

$$(Y_i, X_{i1}, \dots, X_{im} \text{ where } i = 1, \dots, n)$$

The computer program computes the least-squares estimates of p_j using Marquardt's algorithm.

The following must be supplied by the user:

- a) FORTRAN subroutine named "FCODE" to evaluate $\hat{Y}$ for a specific combination of X_{ij} and p_j . The subroutine evaluates the function $\hat{Y}_i$ for one data point each time it is executed.
- b) A FORTRAN subroutine named "PCODE" to evaluate the analytical derivatives of the function $\hat{Y}_i$ for the same data point just processed by FCODE. This subroutine is not required if numerical derivatives are used.
- c) A FORTRAN subroutine named "INPUT" to read in the data, the initial parameter estimates, and to compute constant or new variables required by FCODE and PCODE. This subroutine is an alternative to the following subroutine SUBZ and is optional.
- d) A FORTRAN subroutine named SUBZ, which has a similar function as INPUT. This subroutine must be included even if it is empty.
- e) A FORTRAN subroutine named "OUTPUT" to print out additional information or results of the minimization procedure which are not specified in the main program. This subroutine is optional.

Sample FCODE and INPUT program listings together with the data for each of the two simulation models are included in Appendix 10.2.2

The files are under C.W. Hancher's name and the four data files are:

CSTR.JOB tanks-in-series model with 0.51-m data

PLUG.JOB plug-flow-in-parallel model with 0.51-m data

ALEX.JOB tanks-in-series model with 0.51-m (NO_3 only) data

GRIFF.JOB tanks-in-series model with 0.1-m data

Additional questions concerning the use of the main program should be directed to W. Davis, Jr.

10.2.2 Subroutine Program

Figure 16 is a flow diagram for the calculations associated with the tanks-in-series model. Details of the routines are discussed in Appendix 10.2.1. Following are the listings of the programs which implement the tanks-in-series model. The routines are self-explanatory.

Figure 17 is a flow sheet for the calculation of parameters in the plug-flow-reactors-in-parallel model. Details of the various blocks are described in Appendix 10.2.1. Following is a listing of the program which implements the plug-flow-reactors-in-parallel model.

```

01000 C
01100 C=====
01200 C      SIMULATION MODEL FOR FLUIDIZED BIOREACTOR USING
01300 C      STIRRED-TANKS-IN-SERIES MODEL
01400 C=====
01500 C
01600 C-----THIS SUBROUTINE CALCULATES THE UNREDUCED NITROGEN CONCENTRATION,
01700 C      COMPARES WITH THE OBSERVED VALUE AND RETURNS A RESIDUAL TO THE
01800 C      MAIN PROGRAM. THE PARAMETERS AND VARIABLES REQUIRED ARE
01900 C      SUPPLIED THROUGH THE INPUT SUBROUTINE.-----
02000 C
02100 C      SUBROUTINE FCODE(B,F,PRNT,RES,X,Y,I,IB,IF,NDFM)
02200 C      IMPLICIT REAL*8 (A-H, O-Z)
02300 C      DIMENSION B(1), IB(1), PRNT(1), X(NDFM,1), Y(1)
02400 C      DIMENSION BUG(20), SIN(20), SOUT(20)
02500 C      COMMON/LBCOM1/SOUT(20),AO(10),HALF,TWO,FOUR,TWENTY,
02600 C      1      TIMEO, Z(15), N, NE, NIT, NK1, NPTS, IPR(5)
02700 C      COMMON/TAPES/NI,NO,NF,NITOC
02800 C
02900 C-----NSTATE EQUALS 0 IF ONE STEADY STATE N-CONCENTRATION RESULTS,
03000 C      1 OTHERWISE.
03100 C      NEGSO EQUALS 0 IF NO UNACCEPTABLE N-CONCENTRATION CALCULATED,
03200 C      1 OTHERWISE.-----
03300 C
03400 C      NSTATE = 0
03500 C      NEGSO = 0
03600 C
03700 C-----CALCULATE NO. OF STIRRED TANKS, N AND RESIDENCE TIME OF EACH,
03800 C      TAU FROM DISPERSION NO. (1/PECLET NO.), DIS.-----
03900 C
04000 C      DIS = AO(4) * (X(I,3) ** AO(5))
04100 C      DUMMY = 1./(TWO*DIS-(TWO*(DIS*DIS)*(1.-DEXP(-1./DIS))))
04200 C      N = DUMMY + HALF
04300 C      TAU = AO(3)/(N*X(I,3))
04400 C
04500 C-----START MATERIAL BALANCE CALCULATION IN EACH STIRRED TANK-----
04600 C
04700 C      DO 100 J = 1,N
04800 C
04900 C-----CALCULATE AVERAGE BIOMASS LOADING, BUG(J) IN TANK J,
05000 C      RELATIVE POSITION OF TANK J ALONG BIOREACTOR IS BETWEEN L1 & L2.
05100 C      BIOMASS LOADING AT INLET AND EXIT OF TANK J IS BUG1 & BUG2
05200 C      RESPECTIVELY.-----
05300 C
05400 C      L1 = (J-1)*TWENTY/N
05500 C      L2 = J*TWENTY/N
05600 C      BUG1 = X(I,5) * L1 + X(I,6)
05700 C      BUG2 = X(I,5) * L2 + X(I,6)
05800 C      BUG(J) = (BUG1+ BUG2)*HALF
05900 C
06000 C-----A QUADRATIC EQUATION IN EXIT N-CONCENTRATION, SOUT(J) RESULTS
06100 C      FROM N-CONCENTRATION BALANCE AROUND TANK J. THE COEFFICIENT &
06200 C      CONSTANT ARE FUNCTIONS OF INLET N-CONCENTRATION, SIN(J), TAU,
06300 C      VMAX AND KS.-----

```

```

06400 C
06500 SIN(1) = X(I,1)
06600 SB = B(2) - SIN(J) + B(1) * BUG(J) * TAU
06700 C = -SIN(J) * B(2)
06800 DET = (SB*SB) - FOUR*C
06900 IF (DET) 10,20,30
07000 C
07100 C-----IF ROOTS ARE IMAGINARY, REGISTER NEGS0 AND FORCE THE MAIN
07200 C PROGRAM TO SEARCH FOR A DIFFERENT SET OF VMAX, KS BY ASSIGNING A
07300 C LARGE RESIDUAL,-----
07400 C
07500 10 NEGS0 = 1. + NEGS0
07600 F = 1.D20
07700 GO TO 101
07800 C
07900 C-----IF ROOTS ARE REAL & EQUAL, CHECK FOR UNACCEPTABLE EXIT
08000 C N-CONCENTRATION BEFORE CONTINUING ON TO NEXT TANK,-----
08100 C
08200 20 SOUT(J) = -SB*HALF
08300 IF (SOUT(J).GE.SIN(J) .OR. SOUT(J).LT.0.0) GO TO 10
08400 GO TO 90
08500 C
08600 C-----IF ROOTS ARE REAL AND UNEQUAL, DISCARD THE UNACCEPTABLE ROOT;
08700 C OR IF BOTH ROOTS ARE ACCEPTABLE, REGISTER NSTATE AND SET SOUT(J)
08800 C EQUAL TO THE AVERAGE OF THE TWO ROOTS,-----
08900 C
09000 30 SOUT1 = (-SB + DSQRT(DET))*HALF
09100 SOUT2 = (-SB - DSQRT(DET))*HALF
09200 IF (SOUT1.LT.0.0) SOUT1=SOUT2
09300 IF (SOUT2.LT.0.0) SOUT2=SOUT1
09400 IF (SOUT1.LT.0.0.AND.SOUT2.LT.0.0) GO TO 10
09500 IF (SOUT1.GT.SIN(J)) SOUT1=SOUT2
09600 IF (SOUT2.GT.SIN(J)) SOUT2=SOUT1
09700 IF (SOUT1.GT.SIN(J).AND.SOUT2.GT.SIN(J)) GO TO 10
09800 SOUT(J) = (SOUT1 + SOUT2)*HALF
09900 IF (SOUT1.NE.SOUT2) NSTATE=NSTATE + 1.
10000 90 SIN(J+1)=SOUT(J)
10100 100 CONTINUE
10200 C
10300 C-----CALCULATE RESIDUAL FROM CALCULATED FINAL EXIT N-CONCENTRATION,
10400 C F AND OBSERVED VALUE, Y(I), SCALE DOWN RESIDUAL BY A CONSTANT
10500 C TO AVOID OVERFLOW DURING COMPUTATIONS,-----
10600 C
10700 F = SOUT(N)
10800 101 DIFF = Y(I)-F
10900 RES = DIFF / A0(7)
11000 C
11100 C-----PRINT INTERMEDIATE RESULTS,-----
11200 C
11300 PRNT(1) = I
11400 PRNT(2) = N
11500 PRNT(3) = TAU
11600 PRNT(4) = NSTATE
11700 PRNT(5) = NEGS0
11800 RETURN
11900 END
12000 C
12100 C

```

```

12200 C
12300 C
12400 C-----THIS SUBROUTINE READS IN THE DATA CONTAINING OBSERVED
12500 C      EXIT N-CONCENTRATION, INLET N-CONCENTRATION, BIOMASS LOADING
12600 C      AND VOLUMETRIC FLOWRATE.-----
12700 C
12800      SUBROUTINE INPUT(B,PRNT,X,Y,FMT,TITLE,IREAD,NDP,NDPM)
12900      IMPLICIT REAL*8(A-H, O-Z)
13000      DIMENSION B(1), FMT(1), PRNT(1), TITLE(18,3)
13100      DIMENSION X/NDPM,1), Y(1)
13200      COMMON/LBCOM1/52(10), A(10), AO(10), HALF, TWO, FOUR, TWENTY,
13300      1      TIMEO, Z(15), IMAX, NE, NIT, NK1, NPTS, IPR(5)
13400      COMMON/TAPES/NI,NO,NTTOD,NP
13500      INTEGER FMT
13600 C
13700 C-----DEFINE NUMERICAL VALUES USED IN SUBROUTINE FCODE AS VARIABLES
13800 C      TO FACILITATE COMPUTATIONS.-----
13900 C
14000      REAL*4 TITLE
14100      HALF = 5.0D-01
14200      TWO = 2.0D0
14300      FOUR = 4.0D0
14400      TWENTY = 2.0D01
14500      AO(1) = 1.8D-03
14600      AO(2) = 1.186D-01
14700      AO(3) = 1.212D03
14800      AO(4) = 4.858D-06
14900      AO(5) = 2.07D00
15000      AO(7) = 1.0D03
15100 C
15200 C-----Y(I) = EXIT CONCENTRATION OF UNREACTED NITRATE AND NITRITE
15300 C      X(I,1) = INLET CONCENTRATION OF NITRATE AND NITRATE, G/M3
15400 C      X(I,2) = BIOMASS LOADING IN BIOREACTOR (PER CENT)
15500 C      X(I,3) = VOLUMETRIC FLOWRATE, LITRES/MIN
15600 C
15700      READ (NI,9001) (TITLE(I,1), I=1,18)
15800      READ (NI,9001) (TITLE(I,2), I=1,18)
15900      READ (NI,9001) (TITLE(I,3), I=1,18)
16000      I = 0
16100      101 I = I + 1
16200      READ (NI,FMT) Y(I), X(I,1), X(I,2), X(I,3)
16300      IF (X(I,2) .LE. 0.0) GO TO 121
16400 C
16500 C-----CALCULATE CONSTANTS USED IN THE BIOMASS LOADING PROFILE
16600 C      EXPRESSION.-----
16700 C
16800      X(I,5) = X(I,2) * 4.0D-01 / TWENTY
16900      X(I,6) = X(I,2) * 8.0D-01
17000      GO TO 101
17100      121 NDP = I - 1
17200      321 IREAD = 0
17300      9001 FORMAT (18A4)
17400      RETURN
17500      END
17600 C
17700 C
17800 C
17900 C
*
```

```

01000 C
01100 C
01200 C      SIMULATION MODEL FOR FLUIDIZED BIOREACTOR USING
01300 C      PLUG-FLOW REACTORS-IN-PARALLEL MODEL
01400 C
01500 SUBROUTINE FCODE(B,F,PRNT,RES,X,Y,I,IB,IF,NDPM)
01600 IMPLICIT REAL*8 (A-H, O-Z)
01700 DIMENSION B(1), IB(1), PRNT(1), X(NDPM,1), Y(1)
01800 DIMENSION THETA(100),E(100),L(100),SOUT(100),V(100)
01900 COMMON/LBCOM1/BB(10),A0(10),HALF,TWO,FOUR,TWENTY,
02000 1      TIME0, Z(15), N, NE, NIT, NK1, NPTS, IPR(5)
02100 COMMON/TAPES/NI,NO,NP,NTT0C
02200 C
02300 C      DIS = DISPERSION NUMBER, OR 1/PECLET NO.
02400 C      N = NO. OF STIRRED-TANK REACTORS
02500 C
02600 DIS = A0(4) * (X(I,3) ** A0(5))
02700 DUMMY = 1./(TWO*DIS-(TWO*(DIS*DIS)*(1.-DEXP(-1./DIS))))
02800 N = DUMMY + HALF
02900 SUMSO = 0.
03000 DO 90 J= 1, 100
03100 THETA(J)= J / TWENTY
03200 C      CALCULATE (N-1) FACTORIAL
03300 NEND = N - 1.
03400 NF = 1.
03500 DO 80 K = 1, NEND
03600 80 NF = NF*K
03700 C      CALCULATE E-THETA CURVE FROM TANKS-IN-SERIES MODEL
03800 DTHETA = A0(1)
03900 E(J) = (N**N/NF)*(THETA(J)**(N-1.))*DEXP(-N*THETA(J))
04000 C      CALCULATE L(J) PER UNIT X-S AREA FOR EACH PFR
04100 V(J) = E(J)*DTHETA*X(I,3)
04200 L(J) = A0(3)*THETA(J)*(E(J)*DTHETA)
04300 C
04400 C      CALCULATE EXIT CONC. FOR EACH PFR BY NEWTON RAPHSON
04500 C
04600 A = 1./B(2)
04700 SB = DLOG(X(I,1))+X(I,1)/B(2)-B(1)*X(I,4)*L(J)/B(2)/V(J)
04800 SOUT(J)= A0(4)
04900 1 FSOUT = DLOG(SOUT(J))+A*SB
05000 DFSOUT = 1./SOUT(J)+A
05100 SOUT(J)= SOUT(J)-(FSOUT/DFSOUT)
05200 IF (SOUT(J) .LT. 0.0 ) GO TO 2
05300 DELF = DABS(FSOUT/DFSOUT)
05400 IF (DELF .GT. A0(2)) GO TO 1
05500 SUMSO = SOUT(J)*V(J)+SUMSO
05600 90 CONTINUE
05700 F = SUMSO/X(I,3)
05800 GO TO 3
05900 2 PRNT(2)= THETA(J)
06000 PRNT(3)= FSOUT
06100 PRNT(4)= DFSOUT
06200 PRNT(5)= SB
06300 F = 1.0D20
06400 3 RES = (F-Y(I))*A0(6)
06500 PRNT(1)= I
06600 RETURN
06700 END
06800 C
06900 C
*
```

10.2.3 Data Listing

This section presents a collection of the entire data set used in the simulation activities. Listed are the inlet and outlet unreduced nitrogen concentration, the % biomass loading, and the flow rate of nutrient.

```

23600      20  2  0  3  0  0  1
23700              1 02100
23800                                  1.0 D-06
23900      3.48000D00  1.63000D02
24000      (8F10.0)
24100      SIMULATION OF 20 INCH COLUMN
24200      OUTLET NO3      INLET NO3      BIOMASS      FLOW
24300      G/M3            G/M3            %            L/MIN
24400      58.             1050.           27.7          115.
24500      4.              1080.           17.9          103.
24600      35.             1170.           17.1          107.
24700      93.             1140.           12.2          105.
24800      280.            980.             14.6          115.
24900      95.             1050.           15.5          107.
25000      160.            1020.           12.5          110.
25100      1000.           1990.            9.9          112.5
25200      1660.           2100.           13.9          105.
25300      1740.           2250.           10.8          110.
25400      1600.           1900.           23.5          115.
25500      1200.           2000.           22.1          115.
25600      1030.           1980.           20.           115.
25700      420.            1220.           21.1          105.
25800      1340.           2650.           20.6          105.
25900      816.            2100.           20.8          120.
26000      880.            2000.           29.4          115.
26100      360.            1700.           36.4          130.
26200      750.            2100.           22.6          120.
26300      49.             678.            40.2          115.
26400      20.             640.            32.4          115.
26500      13.             610.            30.1          130.
26600      6.              620.            27.7          115.
26700      14.             660.            27.5          140.
26800      5.              500.            25.1          128.
26900      36.             500.            36.5          125.
27000      23.             510.            29.2          120.
27100      21.             460.            28.7          115.
27200      11.             410.            28.1          115.
27300      2.              233.            27.0          110.
27400      8.              410.            33.2          110.
27500      5.              530.            28.3          130.
27600      20.             500.            32.6          140.
27700      24.             1400.           36.4          120.
27800      17.             520.            33.1          140.
27900      17.             450.            36.0          150.
28000      8.              500.            27.6          150.

```

28100	2.	520.	33.3	140.
28200	22.	710.	35.6	145.
28300	25.	1050.	36.8	115.
28400	35.	1170.	17.5	115.
28500	49.	860.	17.2	105.
28600	22.	960.	14.8	117.
28700	110.	900.	13.5	115.
28800	150.	1160.	18.7	95.
28900	930.	2200.	47.4	120.
29000	1070.	2030.	14.9	110.
29100	1640.	2710.	12.7	95.
29200	1490.	2410.	15.4	105.
29300	35.	870.	35.0	145.
29400	2470.	2910.	10.8	105.
29500	1100.	1600.	22.0	115.
29600	660.	1800.	22.4	115.
29700	810.	1660.	23.3	115.
29800	1220.	2130.	18.7	105.
29900	1040.	1800.	20.2	115.
30000	720.	1630.	27.5	120.
30100	560.	1800.	30.3	130.
30200				
30300	\$END DATA			
30400	/*			
30500	//			
*				

16900	20	2	0	3	0	0	1
17000	1	02100					
17100						1.0	D-06
17200	3.00000D00	1.60000D02					
17300	(8F10.0)						
17400	SIMULATION OF 20 COLUMN						
17500	OUTLET URN	INLET URN	BIOMASS	FLOW RATE			
17600	G/M3	G/M3	%	L/MIN			
17700	301.	1069.	27.7	115.			
17800	217.	1091.	17.9	105.			
17900	314.	1188.	17.1	107.			
18000	406.	1188.	12.2	105.			
18100	655.	1011.	14.6	115.			
18200	429.	1070.	15.5	107.			
18300	543.	1053.	12.5	110.			
18400	1410.	2009.	9.9	112.5			
18500	1801.	2194.	13.9	105.			
18600	1874.	2254.	10.8	110.			
18700	1765.	1912.	23.5	115.			
18800	1433.	2022.	22.1	115.			
18900	1304.	2045.	20.	115.			
19000	669.	1294.	21.1	105.			
19100	1668.	2691.	20.6	105.			
19200	1196.	2156.	20.8	120.			

19300	1408.	2093.	29.4	115.
19400	1068.	1936.	36.4	130.
19500	1313.	2168.	22.6	120.
19600	171.	678.	40.2	115.
19700	148.	652.	32.4	115.
19800	138.	617.	30.1	130.
19900	163.	626.	27.7	115.
20000	191.	666.	27.5	140.
20100	187.	514.	25.1	128.
20200	131.	510.	36.5	125.
20300	162.	525.	29.2	120.
20400	103.	469.	28.7	115.
20500	72.	435.	28.1	115.
20600	4.	233.	27.0	110.
20700	61.	420.	33.2	110.
20800	44.	536.	28.3	130.
20900	97.	507.	32.6	140.
21000	101.	1408.	36.4	120.
21100	55.	522.	33.1	140.
21200	49.	452.	36.0	150.
21300	47.	502.	27.6	150.
21400	13.	522.	33.3	140.
21500	160.	719.	35.6	145.
21600	265.	1070.	36.8	115.
21700	303.	1188.	17.5	115.
21800	227.	872.	17.2	105.
21900	417.	1000.	14.8	117.
22000	399.	925.	13.5	115.
22100	580.	1182.	18.7	95.
22200	1579.	2264.	47.4	120.
22300	1517.	2088.	14.9	110.
22400	1966.	2716.	12.7	95.
22500	1733.	2418.	15.4	105.
22600	83.	875.	35.0	145.
22700	2614.	2923.	10.8	105.
22800	1290.	1624.	22.0	115.
22900	861.	1817.	22.4	115.
23000	1014.	1697.	23.3	115.
23100	1558.	2206.	18.7	105.
23200	1360.	1895.	20.2	115.
23300	1070.	1696.	27.5	120.
23400	1237.	1857.	30.3	130.
23500				
23600	\$END DATA			
23700	/*			
23800	//			
*				

16200	20	2	0	3	0	0	1
16300	1 02100						
16400	1.0 D-06						
16500	3.00000D03		3.00000D01				
16600	(8F10.0)						
16700	SIMULATION OF 4 INCH COLUMN						
16800	OUTLET URN	INLET URN	BIDMASS	FLOW RATE			
16900	G/M3	G/M3	%	L/MIN			
17000	3615.	5771.	7.0	4.			
17100	4050.	5500.	10.0	4.6			
17200	2793.	4250.	8.0	5.			
17300	3680.	5220.	16.0	4.2			
17400	5230.	7900.	11.0	4.			
17500	2545.	4400.	10.0	3.6			
17600	2368.	3989.	10.0	3.6			
17700	2187.	3900.	12.0	3.8			
17800	888.	2333.	10.0	3.6			
17900	503.	2261.	12.0	3.6			
18000	610.	2672.	12.0	3.4			
18100	533.	2198.	15.0	3.4			
18200	995.	2099.	16.0	3.6			
18300	937.	2420.	7.0	3.4			
18400	885.	2251.	7.0	3.6			
18500	810.	2057.	17.0	3.8			
18600	755.	1898.	16.0	4.0			
18700	1048.	2413.	19.0	3.6			
18800	525.	1650.	36.0	3.6			
18900	555.	1550.	23.0	4.0			
19000	415.	1323.	10.0	4.0			
19100	555.	2400.	11.0	3.6			
19200	558.	1400.	12.0	3.4			
19300	322.	1250.	8.0	4.0			
19400	900.	2438.	2.0	3.2			
19500	880.	1640.	15.0	4.2			
19600	858.	2118.	10.0	3.8			
19700	1435.	2400.	7.0	5.0			
19800	1400.	2000.	10.0	6.0			
19900	439.	1000.	8.0	4.0			
20000	855.	1700.	9.0	4.0			
20100	750.	1628.	7.0	4.0			
20200	535.	1238.	7.0	4.0			
20300	625.	966.	3.0	3.8			
20400	390.	1520.	15.0	3.6			
20500	1010.	1800.	15.0	3.4			
20600	550.	1800.	19.0	4.0			
20700	715.	1848.	21.0	4.1			
20800	300.	1300.	8.0	3.5			
20900	420.	1230.	4.0	3.6			
21000	430.	1078.	7.0	4.6			
21100	335.	1185.	8.0	3.8			

21200	300.	2050.	7.0	4.6
21300	300.	960.	7.0	4.0
21400	300.	1109.	7.0	3.8
21500	700.	1065.	9.0	4.0
21600	300.	1100.	10.0	4.0
21700	450.	1435.	11.0	4.0
21800	770.	1521.	9.0	3.8
21900	270.	1039.	6.0	3.6
22000	540.	1075.	6.0	4.0
22100	400.	1155.	5.0	4.0
22200	300.	914.	6.0	4.0
22300	400.	992.	7.0	3.9
22400	225.	1075.	10.0	3.6
22500	300.	1157.	7.0	3.6
22600	260.	1020.	7.0	4.0
22700	770.	1611.	7.0	3.8
22800	270.	1057.	9.0	4.2
22900	420.	1254.	9.0	3.6
23000	240.	1022.	8.0	4.0
23100	550.	997.	6.0	4.4
23200	660.	1508.	10.0	3.0
23300	650.	1278.	10.0	3.6
23400	730.	1136.	13.0	4.0
23500	220.	1110.	10.	4.
23600	180.	953.	9.	4.2
23700	250.	1080.	10.	4.
23800	250.	898.	6.0	4.2
23900	250.	1450.	8.0	4.2
24000	470.	1152.	8.0	4.0
24100	660.	1340.	7.0	3.5
24200	650.	1290.	7.0	4.0
24300	90.	926.	9.0	3.6
24400	110.	782.	14.0	4.0
24500	150.	891.	7.0	4.4
24600	520.	1368.	8.	4.0
24700	350.	1265.	9.0	4.2
24800	430.	1177.	9.0	4.4
24900	360.	1178.	10.0	4.0
25000	520.	1400.	9.0	4.0
25100	75.	962.	9.0	4.0
25200	170.	1022.	11.0	4.0
25300	170.	885.	10.0	3.6
25400	290.	1247.	12.0	3.6
25500	140.	917.	10.0	3.9
25600	150.	875.	9.0	4.4
25700	130.	990.	13.0	4.4
25800	1660.	3760.	20.	4.2
25900	2100.	3276.	12.0	4.0
26000	1910.	3230.	15.0	3.0
26100	1400.	2604.	9.0	3.8
26200	1920.	3573.	10.0	4.2

26300	3210.	4785.	7.	4.0
26400	1240.	3360.	8.0	4.0
26500	1340.	2790.	11.0	4.2
26600	1680.	3036.	9.	4.0
26700	2780.	4745.	12.	4.4
26800	2765.	4311.	12.	3.8
26900	2980.	4690.	13.	3.8
27000	3100.	4472.	32.	4.
27100	2600.	4931.	20.0	4.2
27200	4065.	5472.	14.0	3.8
27300	2330.	3553.	10.0	4.2
27400	2813.	4148.	10.0	4.6
27500	3130.	4100.	10.0	4.6
27600	3770.	5259.	10.0	4.4
27700				
27800	\$END DATA			
27900	/*			
28000	//			
*				

10.3 Nomenclature

- A cross-sectional area of bioreactor, m^2
- a constant defined in Eq. (21)
- b constant defined in Eq. (21), min/liter
- D dispersion coefficient in bioreactor, m^2/min
- D molecular diffusivity, m^2/min
- d_T diameter of bioreactor, m
- E dimensionless residence-time distribution function
- F volumetric flow rate, liter/min
- k rate constant defined in Eq. (4), $(g/m^3)^{-2}min^{-1}$
- K_s saturation constant, g/m^3
- L length of bioreactor, m
- N number of stirred tanks
- Pe Peclet number (D/uL)
- p_j parameter j in Marquardt's algorithm

- S substrate concentration, g/m^3
 t time, min
 u superficial velocity in bioreactor, m/s
 V volume of bioreactor, liter
 $V_{\max}$ maximum specific rate of reaction per % biomass, $\text{g/m}^3\text{-min/\% biomass}$
 v_j volumetric flow rate of PFR, liter/min
 X biomass loading, %
 X_{i2} independent variable x at data point i in Marquardt's algorithm
 Y yield coefficient of bacteria, % biomass/ g/m^3
 Y_i dependent variable at data point i in Marquardt's algorithm
 $\hat{Y}_i$ model predicted value of Y_i at data point i in Marquardt's algorithm
 Z axial position along bioreactor, m
 α constant defined in Eq. (22)
 α' constant defined in Eq. (24)
 α'' stoichiometric constant in Eq. (9)
 β constant defined in Eq. (22)
 β' constant defined in Eq. (24)
 β'' stoichiometric constant in Eq. (9)
 γ variable defined in Eq. (16)
 θ dimensionless residence time
 μ specific growth rate of bacteria, min^{-1}
 $\hat{\mu}$ maximum specific growth rate of bacteria, min^{-1}
 τ residence time, min

Subscripts

- i inlet
 o outlet

Superscripts

c carbonaceous substrate

N unreduced nitrogen

NO_3^- nitrate

10.4 Literature References

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