Modelling techniques for biological reaction systems 1. Mathematical description and model representation

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Abstract
This paper is the first in a series of three which deals with modelling and numeric techniques for biological reaction systems. A matrix format provides a useful method for model presentation. The matrix ensures clarity as to the compounds, processes, reaction terms and stoichiometry comprising the model. It allows ready comparison of different models and facilitates incorporating the model in a computer simulation program.

Introduction

The phenomenon of biological growth is harnessed in a wide variety of applications. These may range from, for example, a laboratory fermentation for the production of a pharmaceutical compound to the treatment of municipal waste water in a full-scale activated sludge process. The common feature in the various systems is biological growth, even though the scale of operation and the final objectives of the growth process may be very different. For example, in a fermentation process, the objective may be to maximise certain soluble products of growth whereas in sewage treatment an objective is to minimise the residual soluble material. Whatever the objective, it is useful to quantify system behaviour on the basis of a model of the process. Because biological growth is the central feature in all of these applications, it is likely that very similar considerations will be necessary in setting up and solving a mathematical model for any of the systems.

Predicting the response of a biological system on the basis of a mathematical model is usually achieved via a computer program. Such a simulation program is useful for a number of reasons. For example:

Model development: A mathematical model incorporates a number of kinetic and stoichiometric expressions which represent the biological interactions. These expressions are based on hypotheses which are proposed for the biological processes occurring within the system. In order to test these hypotheses, specific experiments are designed and data on the system response are accumulated. This experimental data can then be compared with the predictions obtained from the model. In turn, the biological model can be altered with the objective of improving the predictive capacity. A simulation program is thus an indispensable tool in facilitating the development and sophistication of a biological model.

System evaluation and optimisation: A simulation program can be a useful aid in analysing the operation of existing biological systems. If a system model can provide accurate predictions of response behaviour, then these predictions can be compared to observed responses. Any discrepancies can be useful in identifying problems in system operation. An accurate and representative computer model can also be used to optimise the performance of existing systems. Various operating strategies can be proposed and rapidly tested without having to resort to potentially difficult practical evaluation.

System design: A simulation program can be a useful tool for the design engineer. With the aid of an accurate and representative computer model, proposed system designs and configurations can be evaluated rapidly. In addition, a dynamic model can provide valuable design information which is often only available through empirical estimates. For example, a parameter such as peak oxygen utilisation rate in an activated sludge system could be obtained directly from the simulation program run under time-varying input patterns. This means that the peak aeration capacity can be quantified accurately — traditional design methods rely on empirical estimates.

Control strategy development: A simulation program allows quick and efficient evaluation of control strategies in a manner similar to evaluation of system designs. Strategies can be tested and compared in an economical way that reduces the need for field evaluation.

In this series of papers, the problem of modelling the behaviour of biological reaction systems is considered. The problem is presented in three parts:

- mathematical description and model presentation;
- analysis of steady state conditions where the inputs to the system (flow rate and concentrations) remain constant; and
- analysis of dynamic response behaviour where the inputs to the system vary with time.

Mathematical description

A comprehensive mathematical model for the simulation of biological system behaviour must account for a large number of reactions between a large number of components ("compounds"). In this presentation, the reactions will be referred to as **processes**, where processes act on certain **compounds** in the **system**, and convert these to other compounds. The set of distinct biological processes and the manner in which these act on the group of compounds constitute the biological model. The model should quantify, for each process, both the kinetics (rate-concentration dependence) and the stoichiometry (effect on the masses of compounds involved) (Henze *et al.*, 1987).

Once a model has been formulated for a biological system, simulation of the system response involves two principal steps. Firstly, the reactor configuration and the flow patterns need to be specified. Once this information is fixed, it is possible to complete mass balances over each reactor for each compound. Assuming that the system operates at constant temperature, the mass balances quantify the behaviour of each compound in the system.

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The concentrations of these compounds constitute the state variables (dependent variables). The mass balances make up the state equations which relate the dependent variables to the independent variables such as reactor volume. The mass balances form a set of simultaneous non-linear equations which, when solved, characterise the system behaviour. (The equations are usually non-linear because the kinetic expressions for biological systems generally are non-linear.) The simultaneous solution provides values of the state variables at points in space (different reactors) and time (where there is a time-varying input to the system). In this way, the change of state of the system is related to the transport (input and output) and conversion (reaction) processes occurring within the system.

At this point it is worth noting certain characteristics of biological reaction systems which distinguish these from most other applications in the chemical process industry:

- A feature commonly encountered with biological systems is that the process occurs in a series of one or more completely mixed stirred tank reactors (CSTRs). (Certain reactor configurations such as oxidation ditch type systems for wastewater treatment may not appear to fit the description given here, as these are essentially plug flow reactors with recycle, and are not divided into distinct zones. However, these systems can be modelled as tanks-in-series systems by considering the plug flow zones to be made up of a number of small CSTRs in series. This is a standard approach adopted in chemical engineering process simulation.)
- An identical set of reactions often takes place in each reactor in the system. For example, in a series of aerobic activated sludge reactors, the behaviour in each reactor is governed by the same kinetic and stoichiometric expressions i.e. the same model. The only difference between the reactors would be the magnitudes of the state variables, the reactor volumes and the flow terms.
- The response of biological systems is often governed largely by the effect of recycles.

These features of biological systems are not usually encountered in operations in the chemical process industry. Those systems are generally made up of a distinct set of unit operations. Therefore, each reactor unit is governed by a different collection of reaction equations i.e. a different model. Also, the magnitude of the recycles and feedbacks is generally small. These distinguishing features of biological systems demand that specific consideration be given to their simulation.

Model representation

An important part of the simulation process is a clear and flexible representation of the model itself. Because a model may incorporate a number of different components and a large number of biological conversion processes, one convenient method of presentation is a matrix format.

The matrix method for model presentation described here is based on the approach to chemical engineering kinetic modelling of Petersen (1965). In the context of biological systems, the method has been presented and used by the IAWPRC Task Group on mathematical modelling in waste-water treatment design (Henze *et al.*, 1987). The matrix representation ensures clarity as to what compounds, processes and reaction terms are to be incorporated and allows easy comparison of different models. In addition, the method facilitates transforming the model into a computer program.

Setting up the matrix

Table 1 presents, in matrix format, the essential components of a simple Monod-Herbert model for aerobic microbial growth on a soluble substrate, accompanied by organism death.

The first step in setting up the matrix is to identify the compounds of relevance in the model. The Monod-Herbert model quantifies the growth of the biomass component (X_B) at the expense of the soluble substrate component (S_S). By keeping track of X_B and S_S, it is possible to calculate the oxygen requirement,

TABLE 1
THE MONOD-HERBERT MODEL SHOWING PROCESS KINETICS AND STOICHIOMETRY FOR HETEROTROPHIC BACTERIAL GROWTH IN AN AEROBIC ENVIRONMENT

	Component i	1	2	3	Rate expressions
j	Process	X_B	S_S	S_O	
1	Growth	1	$\frac{-1}{Y}$	$-\frac{(1-Y)}{Y}$	$\hat{\mu} X_B \frac{S_S}{(K_S + S_S)}$
2	Decay	−1		1	$b X_B$
Observed conversion rates ($ML^{-3}T^{-1}$)		$r_i = \Sigma \nu_{ij} \rho_j$			Kinetic parameters: Maximum specific growth rate: $\hat{\mu}$
Stoichiometric parameters: True growth yield: Y		BIOMASS M (COD) L^{-3}	SUBSTRATE M (COD) L^{-3}	OXYGEN (NEGATIVE COD) M (−COD) L^{-3}	Half saturation constant: K_S Specific decay rate: b

so oxygen (S_O) can be included as a third component. The compounds are presented as symbols across the top of the table, and are defined (with dimensions) at the bottom of the corresponding matrix columns. The index "i" is assigned to the range of compounds. In this case, "i" ranges from 1 to 3 for the three compounds considered in this simple model. (The recommended symbol notation of the IAWPRC has been followed: namely, X for particulate matter and S for soluble materials, Grau *et al.*, 1982).

The second step in developing the matrix is to identify the biological processes occurring in the system. These are conversions or transformations which affect the compounds considered in the model. Only two processes take place in this simple model — aerobic growth of organisms at the expense of soluble substrate, and organism decay. These are itemised one above the other at the left of the matrix. The index "j" is assigned to the range of processes: in this case "j" can only assume a value of 1 or 2.

The kinetic expressions (rate equations) for each process are recorded down the right-hand side of the matrix in the appropriate row. These are given the symbol ρ_j with j denoting the index of the biological process. The kinetic parameters incorporated in the rate expressions are defined at the lower right corner of the matrix.

The elements within the matrix comprise the stoichiometric coefficients, ν_{ij}, which define the mass action relationship between the components in the individual processes. For example, aerobic growth of heterotrophs (+ 1) occurs at the expense of soluble substrate (− 1/Y); oxygen is used in the metabolic process (− (1 − Y)/Y). The stoichiometric parameters are defined at the lower left of the table.

The sign convention used in the matrix is "negative for consumption" and "positive for production". Cognisance must be taken of the units used in the rate equation. For example, the rate equation for aerobic growth of biomass, ρ_1, is written as a **biomass growth rate** (not as a **substrate utilisation rate**) and has units of (mg cell COD growth)(mg substrate COD utilised)$^{-1}$ d^{-1}. The stoichiometric values are thus normalised with respect to the **biomass concentration** i.e. for growth, the stoichiometric coefficients for X_B and S_S are 1 and − 1/Y respectively, and not Y and − 1.

The stoichiometric coefficients ν_{ij} are greatly simplified by working in consistent units: in this case, all concentrations are expressed as COD equivalents. Provided consistent units have been used, continuity may be checked from the stoichiometric parameters by moving across any row of the matrix. With consistent units, the sum of the stoichiometric coefficients must be zero (noting that oxygen is equivalent to negative COD).

Use in mass balances

Within a **system** boundary, the concentration of a single compound may be affected by a number of different processes. An important benefit of the matrix representation is that it allows rapid and easy recognition of the fate of each component, which aids in the preparation of mass balance equations.

The fundamental equation for a mass balance within any defined system boundary is:

$$\begin{bmatrix}\text{Rate of accumulation}\end{bmatrix} = \begin{bmatrix}\text{Rate of input}\end{bmatrix} - \begin{bmatrix}\text{Rate of output}\end{bmatrix} + \begin{bmatrix}\text{Rate of production by reaction}\end{bmatrix} \quad (1)$$

The input and output terms are transport terms and depend upon the physical characteristics of the system being modelled. The incorporation of these is discussed later. The system reaction term [usually denoted by r_i for compound i (r_i is the production of compound i per unit time per unit volume $[M_i\ L^{-3}\ T^{-1}]$)] must often account for the combined effect of a number of processes. In the matrix format, this information is obtained by summing the products of the stoichiometric coefficients, ν_{ij}, times the process rate expression, ρ_j, for the component i being considered in the mass balance, i.e. moving down the matrix column for the specific component i and accumulating the product of ν_{ij} and ρ_j:

$$r_i = \sum_j \nu_{ij}\,\rho_j \quad (2)$$

For example, from Table 1, the rate of reaction for the compound biomass (X_B) at a point in the system would be:

$$r_{XB} = \frac{\hat{\mu}\,S_S}{(K_S + S_S)} \cdot X_B - b\,X_B \quad (3)$$

Similarly for the component soluble substrate (S_S):

$$r_{ss} = \frac{-1}{Y} \cdot \frac{\hat{\mu}\,S_S}{(K_S + S_S)}\,X_B \quad (4)$$

and for dissolved oxygen (S_O):

$$r_{so} = -\frac{(1-Y)}{Y} \cdot \frac{\hat{\mu}\,S_S}{(K_S + S_S)} \cdot X_B - b\,X_B \quad (5)$$

To create the mass balance for any component within a given system boundary (e.g. a completely mixed reactor) the conversion rate, r_i, would be combined with the reactor volume and the appropriate advective terms (input and output flow) for the particular system; this is not shown here as the system is not yet defined. (The system reaction rate or conversion rate, r_i, may be of interest on its own. For example, Eq. (5) defines the "rate of production" of S_o; therefore $-r_{so}$ defines the oxygen utilisation rate at a point within the system. This parameter is often of interest in aerobic systems.)

Switching functions

At this point, it is worth introducing an aspect of the kinetic expressions used by the IAWPRC Task Group (Henze *et al.*, 1987) which is often useful — "switching functions". Consider the aerobic growth of biomass. In Table 1, the Monod growth rate equation has been used:

$$\rho_1 = \frac{\hat{\mu}\,S_S}{(K_S + S_S)} \cdot X_B \quad (6)$$

In an environment where the dissolved oxygen concentration (S_O) is zero (or perhaps close to zero), the rate of this aerobic process should also decrease to zero. Mathematically, this can be achieved by multiplying the Monod rate expression by a "switching" factor which is zero when S_O is zero, and unity when the environment is aerobic. In this case, it is convenient to write the switching function in the form:

$$\frac{S_O}{(K_O + S_O)} \quad (7)$$

where K_O = switching constant of small magnitude (say 0,1 mg0/ℓ)

The process rate equation then becomes:

$$\rho_1 = \frac{\hat{\mu} S_S}{(K_S + S_S)} \cdot \frac{S_O}{(K_O + S_O)} X_B \quad (8)$$

With this "switching function" operating on the growth rate equation, when S_O is zero the value of the function is zero, and the process rate ρ_1, will be zero. However, if S_O is say 1 mg0/ℓ then the value of the switching function is close to unity and the process rate will then be that given by the Monod equation. In this way, the process of aerobic growth is switched "on" or "off" automatically by the model depending on the dissolved oxygen concentration. The selection of a small value for K_O means that the value of the switching function decreases from near-unity to zero only at very low S_O values i.e. when the dissolved oxygen (D O) value decreases below, say 0,2 mg0/ℓ. However, the function is mathematically continuous, which helps to eliminate problems of numerical instability in simulating system behaviour; such problems can arise if the rate is switched "on" and "off" discontinuously.

In certain situations, the switching "off" of one process may be linked to the switching "on" of another. If, for example, the oxygen input to a nitrifying activated sludge system were terminated periodically, there would be a switch from aerobic to anoxic growth. The latter process is governed by kinetic and stoichiometric expressions which differ from those for the aerobic growth process. To account for this phenomenon in a single model, the rate equations for aerobic and anoxic growth can be multiplied by the appropriate switching functions as follows:

$$\text{Observed } \rho_{\text{aerobic}} = \rho_{\text{aerobic}} \cdot \frac{S_O}{(K_O + S_O)} \quad (9)$$

$$\text{Observed } \rho_{\text{anoxic}} = \rho_{\text{anoxic}} \cdot \left[1 - \frac{S_O}{(K_O + S_O)}\right]$$

$$= \rho_{\text{anoxic}} \cdot \frac{K_O}{(K_O + S_O)} \quad (10)$$

In this instance, it is apparent that the selection of K_O will influence the point at which there is a switch from aerobic to anoxic growth, and *vice versa*. That is, K_O now influences the model predictions and is not only serving a mathematical objective. Therefore, whenever switching functions are used, care should be taken in the selection of the magnitude of the switching constant (K_O here) to ensure that the model predictions are not incorrectly biased.

The consequence of using switching functions to switch between processes within a model should be highlighted. The example of anoxic and aerobic growth illustrates how switching functions enable incorporation of qualitative changes in system behaviour within a single model. Without switching functions, different models would be required to simulate the behaviour either in an aerobic or an anoxic environment.

Biological model used in this study

The matrix approach to model representation becomes particularly advantageous when presenting models incorporating many biological processes operating on a large number of compounds. An example of such a model would be that of Wentzel *et al.* (1987) for describing the behaviour of an enhanced culture of

TABLE 2
THE REDUCED IAWPRC MODEL FOR UTILISATION OF CARBONACEOUS MATERIAL IN AN AEROBIC ACTIVATED SLUDGE SYSTEM

	Component i	1	2	3	4	5	Rate expressions
j	Process	X_B	X_E	X_S	S_S	S_O	
1	Growth	1			$\frac{-1}{Y}$	$-\frac{(1-Y)}{Y}$	$\hat{\mu} X_B \frac{S_S}{(K_S + S_S)} \cdot \frac{S_O}{(K_O + S_O)}$
2	Decay	−1	f	(1 − f)			$b X_S$
3	Solubilisation			−1	1		$\frac{K_H (X_S/X_B)}{(K_X + (X_S/X_B))} X_B$
Stoichiometric parameters: True growth yield: Y Endogenous residue fraction: f		PARTICULATE BIOMASS M (COD) L^{-3}	ENDOGENOUS RESIDUE M (COD) L^{-3}	PARTICULATE SUBSTRATE M (COD) L^{-3}	SOLUBLE SUBSTRATE M (COD) L^{-3}	OXYGEN (NEGATIVE COD) M (COD) L^{-3}	Kinetic parameters: Maximum specific growth rate: $\hat{\mu}$ Maximum solubilisation rate: K_H Half saturation constants: K_S, K_O, K_X Specific decay rate: b

phosphorus removing organisms. The matrix for this model comprises 15 rows and 16 columns. Without the matrix format it would be very difficult to develop, describe or use this model. A biological model of limited complexity has been selected as the "demonstration" model in this series of papers. That is, only a limited number of compounds and processes have been incorporated. The objective of limiting model size has been to enable rapid evaluation of numerical modelling techniques. Despite its limited size, however, the model nevertheless incorporates a range of characteristics encountered in biological systems.

Table 2 presents the limited model in matrix format. This model is a reduced version of that proposed by the IAWPRC Task Group for mathematical modelling in waste-water treatment design (Dold and Marais, 1985; Henze *et al.*, 1987). The model incorporates only those features which relate to the utilisation of carbonaceous material in an aerobic activated sludge system.

Five compounds are identified in the demonstration model. These are:

- heterotrophic organism mass (X_B);
- endogenous residue (X_E);
- particulate biodegradable substrate (X_S);
- soluble biodegradable substrate (S_S); and
- dissolved oxygen (S_O).

These processes operate on the compounds in a manner defined by the stoichiometry and the process rate equations:

Aerobic growth of heterotrophs: Soluble substrate (S_S) is used for growth by the heterotrophic organisms (X_B). There is an associated use of oxygen (S_O). The process is modelled by the Monod expression together with a switching function which reduces the rate to zero in the absence of oxygen.

Death of heterotrophs: Organism decay is modelled according to the "death-regeneration" hypothesis. The heterotrophic organism mass dies at a certain rate; a portion (f) of the material from death is non-degradable and adds to the endogenous residue (X_E) while the remainder (1 – f) adds to the pool of biodegradable particulate COD (X_S).

Hydrolysis of particulate COD: Biodegradable particulate COD in the effluent is assumed to be enmeshed in the sludge mass within the system. The enmeshed material is broken down extracellularly, with the products of breakdown adding to the pool of readily biodegradable substrate (S_S) available to the organisms for synthesis purposes. This "hydrolysis/solubilisation" process is modelled on the basis of Levenspiel's surface reaction kinetics (Levenspiel, 1972).

A number of features incorporated in this model, and which may be encountered with other biological systems, should be noted. These are:

Dual substrate: The model distinguishes between soluble and particulate biodegradable influent material, and the manner in which these are removed in the system.

Non-linear expressions: The non-linear nature of certain of the process rate equations introduces non-linear terms into the mass balance equations. This aspect influences the numerical techniques for solution of the simulation problem.

Single and series reactions: Use of soluble substrate directly by the organism is modelled as a single reaction. However, use of particulate material is modelled as a series reaction occurring in two steps: hydrolysis to soluble substrate followed by use of the soluble substrate.

Bulk versus surface concentration terms: Process rate expressions are usually formulated in terms of the bulk concentration of certain species in the system (i.e. the mass per unit system volume). For example, the concentration of soluble substrate (S_S) as used in the Monod growth rate expression is given by the mass of S_S in the system divided by the volume of the system. However, in certain cases, the basis for quoting concentration is some parameter other than the system volume. For example, hydrolysis of particulate substrate is hypothesised as being dependent on the concentration of particulate material adsorbed onto the organism mass, i.e. the surface concentration. The ratio of two bulk concentrations (X_S/X_B) is used to approximate the surface concentration, and this term appears in the rate expression for hydrolysis.

Setting up the mass balance equations

In a system consisting of a series of completely mixed reactors, the set of equations defining the state of the system is obtained by performing a separate mass balance over each reactor for each compound. Where a solids/liquid separator, such as a gravity settling tank, is included in the configuration, an additional set of mass balance equations is required.

The reactor

Consider a single component in the i^{th} reactor in a series of n completely mixed reactors (Fig. 1). Let C_i denote the concentration of this component in the i_{th} reactor.

The inputs to the reactor could comprise some or all of the following:

- an influent feed stream at a flow rate Q_{feed} and a concentration C_{feed};
- flow from the previous reactor [$(i-1)^{th}$] in the series, at a flow rate Q_{i-1} and a concentration C_{i-1};
- a mixed liquor recycle (a) from the k^{th} reactor in the series, at a flow rate Q_a and a concentration C_k; and
- underflow from the settling tank at a flow rate Q_r and a concentration C_r.

Output streams from the i^{th} reactor could comprise some or all of the following;

- flow from this reactor to the next reactor [$(i+1)^{th}$] in the series at a flow rate Q_i and a concentration C_i;
- a mixed liquor recycle (b) out of this reactor at a flow rate Q_b and a concentration C_i; and
- a sludge wastage stream may be withdrawn from the reactor at a rate q_w and a concentration C_i. (Biological sludge is withdrawn to prevent a build-up of solids in systems incorporating a solids/liquid separator. In this presentation, waste liquor will be withdrawn only from the last reactor in the series.)

The reaction terms are obtained as described previously, by summing the products of the stoichiometric coefficients and the process rate expressions for the particular component being considered. These conversion terms are combined with the flow terms to create the mass balance equations.

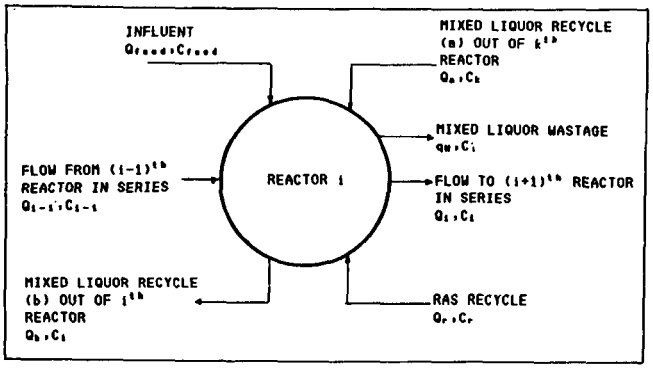

Figure 1
Schematic representation of the i^{th} reactor in a series of n completely mixed reactors.

Substituting in Eq. (1), the mass balance for a single compound in the i^{th} reactor in a series is:

$$V_i \frac{dC_i}{dt} = Q_{feed}C_{feed} + Q_{i-1}C_{i-1} + Q_a C_k + Q_r C_r - Q_i C_i - Q_b C_i - q_w C_i + rV_i \quad (11)$$

where V_i = volume of the i^{th} reactor (L^3)
C = concentration (ML^{-3})
Q = flow rate (L^3T^{-1})
q_w = wastage rate (L^3T^{-1})
r = rate of reaction or conversion rate of the compound (positive for production) ($ML^{-3}T^{-1}$)
$= \sum_j \nu\rho$

The solids/liquid separator

In certain circumstances, the output from the last reactor in the biological system passes to a solids/liquid separation device (often a gravity settler). This is usually with the intention of being able to maintain an organism retention time in excess of the hydraulic retention time and for maintaining a solids-free effluent. In this presentation it has been assumed that the process which occurs in the settling tank is merely one of physical concentration i.e. no reaction takes place. In this way, the settling tank is treated as a separation point with no hold-up. Also, the settling tank is considered to operate at 100 per cent efficiency. This means that the overflow from the settling tank comprises only soluble material and all particulate compounds entering the vessel are recycled back to the chain of reactors. Mass balances over the settler must therefore distinguish between particulate and soluble compounds.

Fig. 2 illustrates the flow terms associated with a settling tank situated at the end of a series of n reactors. These are:

- flow from the last (n^{th}) reactor at a flow rate ($Q_{feed} + Q_r - q_w$) and a concentration of C_n;
- overflow from the settling tank at a rate of ($Q_{feed} - q_w$) and a concentration of C_n for soluble material and C = O for particulate material; and
- underflow from the settling tank, at a flow rate of Q_r and a concentration C_r.

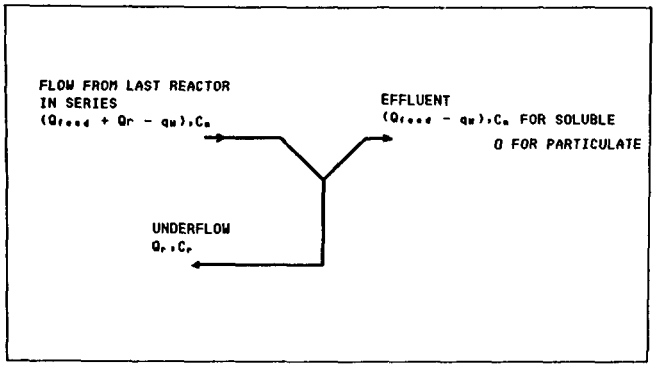

Figure 2
Schematic representation of a solids/liquid separator at the end of a series of reactors.

Mass balances for the particulate and soluble compounds are as follows:

Particulate:

$$(Q_{feed} + Q_r - q_w)C_n = Q_r C_r \quad (12)$$

Soluble:

$$(Q_{feed} + Q_r - q_w)C_n = Q_r C_r + (Q_{feed} - q_w)C_n$$

With $C_n = C_r$ for soluble compounds, this yields the trivial mass balance:

$$C_n - C_r = O \quad (13)$$

Dissolved oxygen mass balance

Although dissolved oxygen (S_O) is included in the matrix, a mass balance for S_O will usually not be required. This is because in aerated reactors the oxygen input to a reactor is generally regulated externally to maintain the dissolved oxygen concentration at some constant value. The reason for including S_O is that it allows computation of the oxygen utilisation rate ($-r_{SO}$), an important parameter in modelling aerobic behaviour.

A case study

Consider the system of Fig. 3 comprising a single aerobic reactor and a settling tank. Underflow from the settling tank is returned to the reactor. The system is described by eight mass balance equations, one for each of the compounds, X_B, X_E, X_S, and S_S in the reactor and in the settling tank underflow, respectively. (Additional subscripts i and r denote the concentrations in the influent and underflow recycle respectively). The eight simultaneous equations comprise a set of four non-linear ordinary differential equations for the reactor and four algebraic equations for the solids/liquid separator.

Reactor:

$$V\frac{dX_B}{dt} = Q_i X_{B,i} + Q_r X_{B,r} - (Q_i + Q_r)X_B - b X_B V + \frac{\hat{\mu} S_S X_B}{(K_S + S_S)} V \quad (14)$$

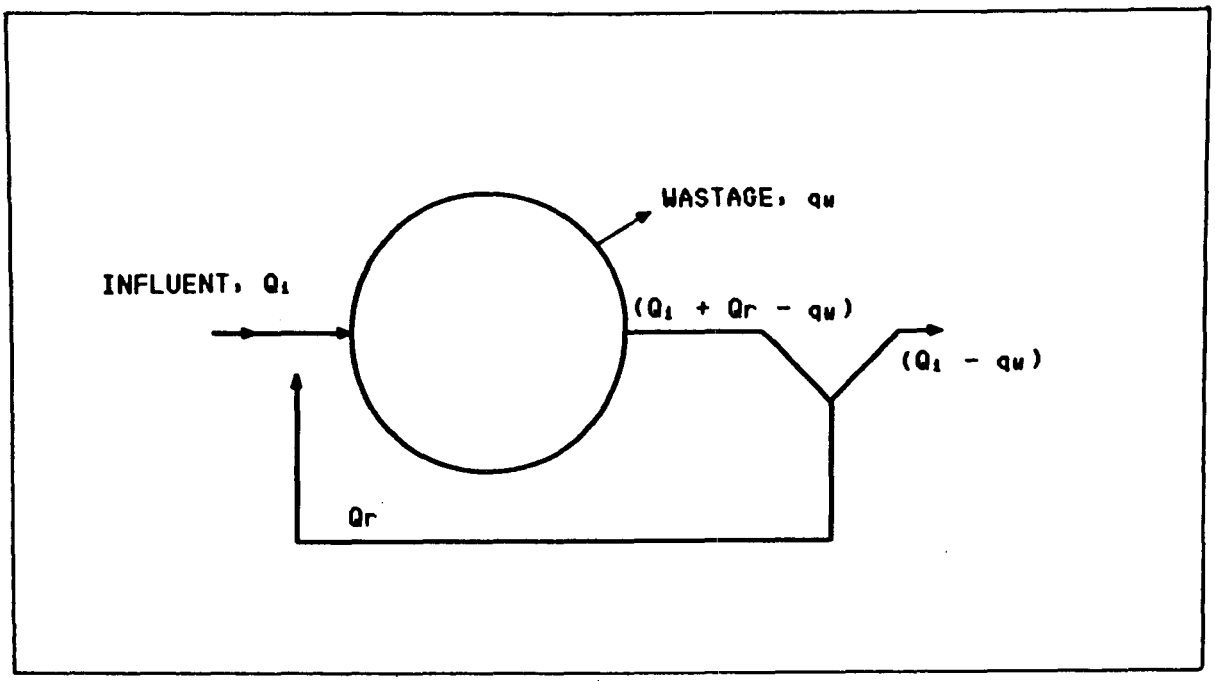

Figure 3
A case study: a single aerobic reactor with settling tank

$$V\frac{dX_E}{dt} = Q_i X_{E,i} + Q_r X_{E,r} - (Q_i + Q_r)X_E + f\,b\,X_B\,V \quad (15)$$

$$V\frac{dX_S}{dt} = Q_i X_{S,i} + Q_r X_{S,r} - (Q_i + Q_r)X_S + (1-f)\,b\,X_B\,V - \frac{K_H X_S}{(K_X + X_S/X_B)}\,V \quad (16)$$

$$V\frac{dS_S}{dt} = Q_i S_{S,i} + Q_r S_{S,r} - (Q_i + Q_r)S_S - \frac{\hat{\mu}}{Y}\cdot\frac{X_B S_S}{(K_S + S_S)}V + \frac{K_H X_S}{(K_X + X_S/X_B)}\,V \quad (17)$$

Solids/liquid separator:

$$(Q_i + Q_r - q_w)X_B = Q_r X_{B,r} \quad (18)$$

$$(Q_i + Q_r - q_w)X_E = Q_r X_{E,r} \quad (19)$$

$$(Q_i + Q_r - q_w)X_S = Q_r X_{S,r} \quad (20)$$

$$S_S = S_{S,r} \quad (21)$$

Conclusions

For the steady state situation, where the system operates under conditions of constant influent flow and load, the derivative terms in the reactor mass balance equations fall away. This reduces the single-reactor-plus-settler example problem to a set of eight simultaneous non-linear algebraic equations. In the dynamic situation, the problem remains one of solving the system of four non-linear ordinary differential equations and four algebraic equations. Solution procedures for solving the sets of simultaneous equations resulting from the steady state and dynamic situations necessitate specific considerations in each case.

The steady state problem involves finding a single value for the concentration of each compound in each reactor and in the underflow recycle stream which satisfies the set of algebraic equations. Because the biological reaction expressions introduce non-linear terms into the equations, the solution cannot be found directly and iterative techniques must be employed. These techniques range in complexity from simple successive substitution (with or without acceleration) to the various Newton-type methods. The success and efficiency of the different techniques is determined principally by the degree of non-linearity in the equations.

Under dynamic conditions, a set of coupled ordinary differential and algebraic equations describe the change in concentration of each compound in each reactor with time subject to variations in the input pattern. Because the biological system incorporates reactions involving both soluble and particulate compounds at a range of concentrations, the system will exhibit dynamics varying from fast to slow for different compounds. Therefore, use of an integration technique that exploits the differing dynamics exhibited by the compounds in a biological system is indicated.

In the second and third parts of this series of papers attention is directed at the steady state case and the dynamic situation, respectively. The objective has been to identify numerical techniques which take advantage of the particular characteristics of the equations describing the system in each case. Through exploring the nature of the non-linearities, and exploiting the specific dynamics of the biological reaction behaviour, it has been possible to identify techniques appropriate for either the steady state or the dynamic situation.

References

DOLD, P.L. and MARAIS, G.v.R. (1985) Evaluation of the general activated sludge model proposed by the IAWPRC task group. *Wat. Sci. Tech.* **18**(6) 63 - 89.

GRAU, P., SUTTON, P.M., HENZE, M., ELMALEH, S., GRADY, C.P.L., GUJER, W. and KOLLER, J. (1982) Recommended notation for use in the description of biological waste-water treatment processes. *Water Research* **16** 1501 – 1505.

HENZE, M., GRADY, C.P., GUJER, W., MARAIS, G.v.R. and MATSUO, T. (1987) Abbreviated report: A general model for single-sludge waste-water treatment systems. *Water Research* **21**(5) 505 – 515.

LEVENSPIEL, O. (1972) *Chemical reaction engineering* (2nd Edition) John Wiley and Sons, New York.

WENTZEL, M.C., DOLD, P.L., LOEWENTHAL, R.E., EKAMA, G.A. and MARAIS, G.v.R. (1987) Experiments towards establishing the kinetics of biological excess phosphorus removal. Paper presented at the International Specialised Conference on Biological Phosphate Removal from Wastewaters, Rome, September 1987.