Modelling techniques for biological reaction systems 3. Modelling of the dynamic case

A E Billing and P L Dold*
Department of Chemical Engineering, University of Cape Town. Private Bag, Rondebosch 7700, South Africa.

Abstract
This paper is the last in a series of three which deals with numeric techniques for biological reaction systems. The dynamic problem involves solving a set of coupled ordinary differential equations. A multirate technique based on Gear's approach is developed. The method incorporates a variable steplength facility.

Introduction

In practice the inputs to a biological system are unlikely to remain constant. Because the influent to the system varies with time, the mass balance equations describing the response of the system will take the form of a set of differential equations incorporating time-dependent terms [see Eqs. (14) to (21) of Part 1 in the series, for example.] This set of equations will define how the values of the concentrations of each compound in each reactor (the state variables) vary with time.

Solving the set of simultaneous differential equations is an initial value problem. The magnitudes of the concentrations of each compound in each reactor are specified as the initial condition, and thereafter the equations are solved by integrating forward in time. In this way, the changes in concentration in each reactor can be tracked, subject to the variations in the influent flow rate and concentrations. In certain circumstances, such as an activated sludge system, the influent pattern of flow rate and concentration is repeated closely from day to day i.e. a daily cyclic basis. A useful facility, therefore, is to predict the steady state cyclic response when it is assumed that the influent pattern is repeated identically from day to day. Because the initial values are only approximations, finding this solution will require integrating forward through perhaps many cycles until convergence to the solution is attained. Convergence in this case requires that the cyclic concentration response of each compound in each reactor is identical from cycle to cycle, and the values at the start and end of each cycle are the same.

The set of differential equations describing the response of a biological system under dynamic conditions will contain non-linear terms, as did the mass balance for the steady state case. The task of finding the solution to such a set of non-linear ordinary differential equations is certainly not unique to biological systems. Many systems of interest to engineers and scientists are described by non-linear differential equations. A multitude of numerical integration techniques exists for the solution of these sets of equations. Consequently, when faced with such a set of equations, the problem in finding a numerical method is the selection of an appropriate one from the many diverse methods available.

This paper outlines the selection of an integration scheme appropriate for the dynamics of biological reaction systems. In the selection, the approach taken was to first establish a rudimentary integration module which was then refined and improved. In the process of refining the module, a greater understanding of the actual dynamics of the system was generated. Thus, through an interactive process, the integration routine was gradually tailored to better meet the demands of the biological system under consideration. The chronological development of the integration module is presented here. Information concerning general aspects of integration and the earlier versions of the module are included as the detail facilitates developing a broader understanding of the dynamic problem.

General comments on using numerical integration techniques

Because the exact solution to the set of differential equations is not, in general, known and cannot be calculated analytically, a numerical integration technique will be required to provide an approximation to the solution. A common approach, which will be the focus of this presentation, is to use a time-stepping or difference method which approximates the solution by its value at a sequence of discrete points called the mesh points. Given a differential equation $y'(x) = 0$, a difference method provides some rule for approximating y at a point x_n ($y(x_n)$) in terms of the value of y at x_{n-}, and possibly at preceding points. Ideally, the solution should be represented by its actual value at each mesh point so that it can be approximated to high accuracy by interpolation between the mesh points. However, the exact solution to the differential equation is not known, so it is always an approximation that is sought. Many techniques assume that the mesh points are equally spaced. However, since the stepsize seems to have an effect on the error introduced, it is usually possible to vary the mesh spacing to account for this. For the moment, it will be assumed that the mesh spacing remains constant during the stepping procedure.

The simple Euler method

The simplest stepping technique available is Euler's rule. The value of the dependent variable at one point is calculated by straight line extrapolation from the previous point. Consider the function y with

$$y1(x) = \frac{dy}{dx} = f_{(x,y)} \qquad (1)$$

The value of y at $x_{n+1} = (x_n + h)$ may be approximated by a Taylor's expansion. Truncating after the first two terms in the series yields:

$$y(x_n + h) = y(x_n) + h \quad f(x_n, y(xn) \qquad (2)$$

where h = steplength

The error in this approximation is described by the remaining terms in the Taylor's expansion:

* To whom all correspondence should be addressed.
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