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The Chemical Engineering Journal 65 (1997) 77–80

CHEMICAL ENGINEERING JOURNAL

An efficient algorithm for solving hollow-fiber bioreactor design equations [1]

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Received 31 May 1996; accepted 23 July 1996

Abstract

A simple algorithm for solving the hollow-fiber bioreactor design equations has been presented. This algorithm is quite general and is applicable to any nonlinear reaction occurring in the reactor spongy matrix. This can also be applied to other reactor types having similar configurations, like the wall-coated enzyme reactors.

Keywords: Hollow-fiber membrane bioreactors; Nonlinear reaction; Algorithm; Effectiveness factor

1. Introduction

Many models are available for the theoretical description of hollow-fiber membrane bioreactors [1–3]. Waterland et al. [1] have solved both linear and nonlinear reaction cases in membrane reactors whereas Kim and Cooney [2] and Jayaraman [3] have obtained compact solutions to the first-order reaction problem in membrane reactors. Davis and Watson [4] describe special finite difference formulations to solve the annular bed catalytic reactor problems. They note that the major error lies in the discretization of the lumen side equations. Salmon and Robertson [5] have assumed the flux of the reactants into the annulus to be piecewise constant and have solved the design equations. In this communication an alternative algorithm developed by the authors to solve the annular reactor problems, is described. This algorithm is computationally simpler and is semi-analytical in nature.

2. Theoretical development

A conventional hollow-fiber bioreactor is considered in this analysis. The reactant which is fed through the inner tube (known as the lumen) passes through the membrane to the outer annular region (known as the spongy matrix) where the reaction occurs with the cells/enzymes localized therein. The membrane is permeable to the reactants and products but is impermeable to the high molecular weight enzymes/cells. The product diffuses back through the membrane to the lumen and flows with the bulk stream. The following assumptions are considered to hold good for the subsequent development of the governing equations:

1. the reactor geometry is cylindrical;
2. the reactant flow in the lumen is laminar and parabolic;
3. there is no radial convection in the membrane and the spongy matrix;
4. quasi-steady state prevails in the reactor;
5. the membrane is inert and the reaction occurs only in the spongy matrix;
6. the reaction is isothermal.

With these assumptions and taking the simple Michaelis–Menten rate expression as a test case, the governing equations for the lumen, membrane and spongy matrix can be written as:

Lumen

$$\frac{D_1}{r}\frac{\delta}{\delta r}\left(r\frac{\delta c_1}{\delta r}\right)=V_0\left(1-\frac{r^2}{a^2}\right)\frac{\delta C_1}{\delta z} \tag{1}$$

Membrane

$$\frac{D_2}{r}\frac{\delta}{\delta r}\left(r\frac{\delta c_2}{\delta r}\right)=0 \tag{2}$$

Spongy matrix

$$\frac{D_3}{r}\frac{\delta}{\delta r}\left(r\frac{\delta c_3}{\delta r}\right)=\frac{V_{\max}C_3}{Km+C_3} \tag{3}$$

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[1] NCL Communication number 6381.

PII S1385-8947(96)03155-5

The associated boundary conditions are

$$c_1 = c_0 \text{ at } z = 0 \tag{4}$$

$$\frac{\delta c_1}{\delta r} = 0 \text{ at } r = 0 \tag{5}$$

$$D_1\frac{\delta c_1}{\delta r} = D_2\frac{\delta c_2}{\delta r};\ K_a = \frac{c_2}{c_1} \text{ at } r = a \tag{6}$$

$$D_2\frac{\delta c_2}{\delta r} = D_3\frac{\delta c_3}{\delta r};\ K_b = \frac{c_2}{c_3} \text{ at } r = b \tag{7}$$

$$\frac{\delta c_3}{\delta r} = 0 \text{ at } r = d \tag{8}$$

c_1, c_2 and c_3 are the concentrations of the reactant in the lumen, membrane and spongy matrix respectively. a is the lumen radius, b is distance from the lumen center to the outer wall of the membrane and d is the distance from the lumen center to the outer wall of the spongy matrix. The other symbols are explained in the nomenclature (Appendix A).

Following Kim and Cooney [2] and Jayaraman [3] the membrane equation can be integrated with the boundary conditions represented by Eqs. (6) and (7) to reduce the equations from three to two. The membrane function would now appear in the form of the modified boundary conditions. Defining

$$C = \frac{c}{c_0};\ K = \frac{K_b}{K_a};\ \beta = \frac{d}{b};\ \overline{Km} = \frac{Km}{c_0} \tag{9}$$

$$h = -K_a\frac{D_2}{D_1}\ln(a/b) \tag{10}$$

$$\alpha = \frac{D_3 b}{D_1 a} \tag{11}$$

$$X = \frac{r}{a} \text{ for the lumen side} \tag{12}$$

$$X = \frac{r}{b} \text{ for the matrix side} \tag{13}$$

$$Z = \frac{z}{aPe};\ Pe = V_0\frac{a}{D_1};\ \phi^2 = b^2\frac{V_{\max}}{D_3 Km} \tag{14}$$

The lumen and spongy matrix equations can be written in dimensionless form as:

Lumen

$$\frac{1}{X}\frac{\delta}{\delta X}\left(X\frac{\delta C_1}{\delta X}\right) = (1 - X^2)\frac{\delta C_1}{\delta Z} \tag{15}$$

Spongy matrix

$$\frac{1}{X}\frac{\delta}{\delta X}\left(X\frac{\delta C_3}{\delta X}\right) = \phi^2 C_3\frac{\overline{Km}}{\overline{Km} + C_3} \tag{16}$$

The relevant boundary conditions are

$$C_1 = 1 \text{ at } Z = 0 \tag{17}$$

$$\frac{\delta C_1}{\delta X} = 0 \text{ at } X = 0 \tag{18}$$

$$\frac{\delta C_1}{\delta X} = \alpha\left(\frac{\delta C_3}{\delta X}\right) \text{ at } X = 1 \tag{19}$$

$$\frac{\delta C_1}{\delta X} = h(KC_3 - C_1) \text{ at } X = 1 \tag{20}$$

$$\frac{\delta C_3}{\delta X} = 0 \text{ at } X = \beta \tag{21}$$

We can deduce from Eqs. (19) and (20) the following:

$$h(KC_3 - C_1) = \alpha\left(\frac{\delta C_3}{\delta X}\right) \text{ at } X = 1 \tag{22}$$

Kim and Cooney [2] applied the Laplace Transformation approach and obtained the solution of Eqs. (15) and (16) in terms of hypergeometric series. Jayaraman [3] simplified the approach by solving the linear matrix equation and decoupling the matrix equations from the set of equations. For nonlinear equations it is difficult to obtain closed form solutions. Thus a different strategy is needed to decouple the spongy matrix equations. This can be done by obtaining the flux to the spongy matrix or the effectiveness factor at every axial location numerically. Defining effectiveness factor as the ratio of the observed rate to the hypothetical rate at the lumen wall conditions, we can obtain an expression for it as

$$\eta(z) = \frac{2\pi b\Delta z D_3\left.\dfrac{\delta c_3}{\delta r}\right|_{r=b}}{\pi(d^2 - b^2)\left(\dfrac{V_{\max}c_1}{(Km + c_1)}\right)\Delta z|_{r=a}} \tag{23}$$

This can be written in dimensionless form as

$$\eta(Z) = \left.\frac{2(\delta C_3)/(\delta X)(\overline{Km} + C_1)}{\phi^2(\beta^2 - 1)C_1\overline{Km}}\right|_{X=1} \tag{24}$$

This can be combined with Eq. (19) to obtain

$$\left.\frac{\delta C_1}{\delta X}\right|_{X=1} = \left.\frac{\eta(Z)\alpha\phi^2(\beta^2 - 1)C_1\overline{Km}}{2(\overline{Km} + C_1)}\right|_{X=1} = f(C_w) \tag{25}$$

where $C_w = C_1(1)$ is the lumen wall concentration

It can be seen from the above equation that if the effectiveness factor is known, the solution of the problem is reduced to the solution of the lumen equation (Eq. (15)) subject to the boundary conditions represented by Eqs. (17), (18) and (25) which is nonlinear. The solution of such problems, in an analogous situation of mass transfer in reactive fibers, has been discussed by Rudisill and LeVan [6]. Following Rudisill and LeVan [6], the solution of the lumen equation can be written as:

$$C_1(X,Z) = C_w(Z) - \int_0^Z \frac{\delta C_w(Z')}{\delta Z'} C_\infty(X, Z - Z')\,dZ' \tag{26}$$

$C_\infty(X,Z)$ is the solution of the lumen equation with the lumen wall boundary condition replaced by

$$C_1 = 0 \text{ at } X = 1,\ Z > 0 \tag{27}$$

This can be recognized as the celebrated Graetz problem with an infinite wall Sherwood number [7,8]. The solution for the Graetz problem can be obtained in terms of hypergeometric series by separation of variables and is

$$C_\infty(X,Z-Z') = \sum_{n=1}^{\infty} A_n Y_n(X) \exp(-\lambda_n^2(Z-Z')) \tag{28}$$

where A_n, Y_n and λ_n are the Eigenconstants, Eigenfunctions and the corresponding Eigenvalues. The solution procedure is described by Brown [7] and Cooney et al. [8]. The Eigenvalues and Eigenconstants are tabulated by Brown [7]. Differentiating Eq. (26), the wall flux, $\delta C_1/\delta X|_{X=1}$, represented by Eq. (25) can be written as

$$-\int_0^Z \frac{dC_w(Z')}{dZ'} \frac{\delta C_\infty}{\delta Z'}(X,Z-Z')|_{X=1} dZ' = f(C_w, \eta(Z)) \tag{29}$$

Eq. (29) is a Volterra integral equation with the lumen wall concentration as the dependent variable and the axial length as the independent variable. The above equation can be evaluated by approximating the derivative by a difference formula. Thus Eq. (29) becomes

$$-\sum_{j=1}^{m} \frac{C_{wj} - C_{wj-1}}{\Delta Z} \int_0^{Z'} \frac{\delta C_\infty}{\delta Z'}(X,Z-Z')|_{X=1} dZ' = f(C_w(m), Z_m, \eta(Z_m)) \tag{30}$$

The integral of $\delta C_\infty/\delta Z'$ can be evaluated analytically. Thus the above equation becomes

$$\sum_{j=1}^{m} \frac{(C_{wj} - C_{wj-1})}{\Delta Z} \left(\sum_{n=1}^{\infty} B_n \exp(-\lambda_n^2 Z_m)(\exp(-\lambda_n^2 Z_j) - \exp(\lambda_n^2 Z_{j-1})) \right) = f(C_w(m), \eta(m)) \tag{31}$$

where

$$B_n = \frac{-A_n (dY_n/dX)|_{X=1}}{\lambda_n^2} \tag{32}$$

Defining mixing cup concentration as

$$\bar{C} = \frac{\int_0^1 C(X,Z)(1-X^2)X dX}{\int_0^1 (1-X^2)X dX} \tag{33}$$

This can be evaluated at the required axial position using the properties of the Graetz function as:

$$\bar{C}(m) = C_w(m) - \sum_{j=1}^{m} \left(\frac{C_{wj} - C_{wj-1}}{\Delta Z} \right) \times \left(\sum_{n=1}^{\infty} \frac{B_n}{\lambda_n^2} \exp(-\lambda_n^2 Z_m) \right) (\exp(\lambda_n^2 Z_j) - \exp(\lambda_n^2 Z_{j-1})) \tag{34}$$

3. Results and discussion

In order to obtain the solution, we have defined an effectiveness factor based on the actual rate relative to the hypothetical rate at the lumen wall conditions. This enables us to decouple the spongy matrix equation from the set of equations. The membrane and the spongy matrix functions now appear in the form of the modified boundary condition to the lumen equation at its wall. Eq. (25) represents this boundary condition and it can be seen that the spongy matrix function now appears in the form of the effectiveness factor. The algorithm to solve the decoupled problem can now be described as follows.

4. Algorithm

1. Start at the reactor entrance. At this position the lumen wall concentration is unity. Use this value in the equation for the spongy matrix boundary condition (Eq. (22)).
2. Solve the spongy matrix equation (Eq. (16)) subject to the above boundary condition along with zero flux boundary condition (Eq. (21)). This can be carried out by using a standard shooting routine.
3. Evaluate the effectiveness factor at this position using Eq. (24).
4. Use this value of the effectiveness factor for the lumen wall boundary condition (Eq. (25)) to solve the lumen equation; i.e. solve the Volterra integral equation (Eq. (30)) (by virtue of the finite difference approximation employed this reduces to solving a nonlinear algebraic equation) and obtain the value of the lumen wall concentration at the next incremental step in the axial direction.
5. Repeat steps 2 to 4 until the reactor exit is reached.

A simple Michaelis–Menten rate expression is considered as a test case. This expression was chosen because the results for this reaction occurring in a hollow-fiber membrane reactor using a complete finite difference formulation of the uncoupled equations are available [1]. Results obtained by the present method are compared with the results from the finite difference formulation in Fig. 1. It can be seen from the figure that there is excellent agreement between the methods. It was observed that a step size of 0.005 in the axial direction is sufficient to give results with an accuracy to three digits.

5. Conclusions

A simple method of solving the membrane bioreactor problem has been outlined. The first key to solving the problem

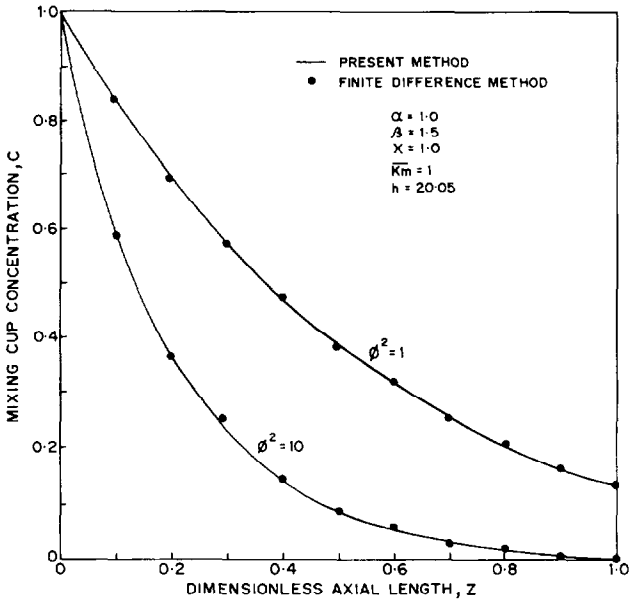

Fig. 1. Mixing cup profiles in the reactor.

is to define an effectiveness factor based on lumen wall conditions. The second key is to develop a Volterra integral equation in terms of the lumen wall concentration. This can be further simplified to a single nonlinear algebraic equation. By continuously switching between the spongy matrix problem (to evaluate the effectiveness factor) and the lumen problem (to evaluate the lumen wall concentration), the entire concentration profile can be obtained. This method is quite straightforward and can be applied to any arbitrary nonlinear rate form. This method is computationally simple but rigorous, and has an attractive semi-analytical format. It can also be applied to similar reactor configurations such as the wall-coated enzyme reactor.

Appendix A. Nomenclature

α	Lumen radius
A_n	Eigenconstants
b	Distance from lumen center to membrane outer wall
c	Concentration of the reactant
c_0	Concentration at lumen inlet
C	Dimensionless concentration of the reactant
d	Lumen side mixing cup concentration
d	Distance from the lumen center to the spongy matrix wall
D	Diffusion coefficient of the reactant
h	Parameter defined by Eq. (10)
K	Partition coefficient
K_a	Value of K at $r=a$
K_b	Value of K at $r=b$
Km	Michaelis–Menten constant
N_{Sh}	Wall Sherwood number
Pe	Peclet number defined by Eq. (14)
r	Radial coordinate
V_0	Centerline laminar flow velocity for lumen side
V_{max}	Maximum reaction rate
X	Dimensionless radial coordinate defined by Eqs. (12) and (13)
Y_n	Eigenfunctions
z	Axial distance variable
Z	Dimensionless axial distance
ΔZ	Step size in the axial direction

A.1. Greek symbols

α	Parameter defined by Eq. (11)
β	d/b
η	Effectiveness factor
ϕ	Thiele modulus
λ_n	Eigenvalues

A.2. Subscripts

1,2,3	Lumen, membrane and spongy matrix respectively
w	Wall

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