Numerical Methods of Solution for Continuous Countercurrent Processes in the Nonsteady State

Part I: Model Equations and Development of Numerical Methods and Algorithms

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Simple, efficient and noniterative algorithms are developed for the calculation of the dynamics of continuous countercurrent processes described by hyperbolic differential equations. The algorithms are derived using the method of characteristics and are particularly useful for either general quadratic or hyperbolic isotherms such as the Langmuir isotherm. The use of characteristic coordinates for the numerical solution avoids accumulating errors that would arise from computations based on a rectangular grid of real time and space coordinates.

The proposed methods can provide an efficient framework for extension to transport processes with general nonlinear rate expressions. The algorithms and methods initially derived for simple models can be extended to more complex systems such as countercurrent flow with accumulating stationary phases and response to distributed disturbances.

The application of the algorithm and methods to a number of countercurrent mass and heat transfer processes will be illustrated in Part II, where the accuracy and efficiency of the proposed methods will also be demonstrated by comparison to available analytic solutions. An example demonstrating the extension of the method to a system with complex coupled boundary conditions will also be discussed.

SCOPE

The purpose of this paper is to present a simple, efficient and accurate numerical method which can facilitate the determination of the dynamic behavior of countercurrent heat and mass transfer processes. Although the steady-state behavior of these processes can be usually analyzed quantitatively, the same cannot be said for the transient state. Simple general analytic solutions for the nonsteady state are not readily obtainable, partly due to the presence of split boundary conditions. The most general form of analytic solution (Jaswon and Smith, 1954) is in a complicated series form and the evaluation even for relatively simple boundary conditions is difficult and time-consuming, requiring lengthy computer calculation. The simultaneous partial differential equations for nonsteady-state countercurrent processes have thus been evaluated numerically by many authors in a variety of ways. These include application of finite difference methods and the use of cell or lumped parameter models. Both methods have been shown to implicitly involve a dispersion term which smooths and spreads the discontinuous wave behavior of the hyperbolic equations often used to model countercurrent processes. Attempts to represent the discontinuity by decreasing the size of the increments of finite difference schemes or by increasing the number of cells in lumped parameter models can lead to lengthy computation.

The method of characteristics transforms the simultaneous hyperbolic partial differential equations to a set of ordinary differential equations which can be integrated numerically by standard methods. Acrivos (1954) indicated the possibility of applying the method of characteristics to countercurrent systems. However, most of the published examples using the method of characteristics have been in the field of fixed bed operations in which the split boundary conditions of countercurrent systems do not arise because one of the two contacting phases is stationary.

In this paper, the applications of the method of characteristics for the numerical solution of countercurrent processes are given in sufficient detail that they may be readily applied to a wide variety of heat and mass transfer processes. Basic algorithms for processes with simple boundary conditions for linear systems and mass transfer processes with Langmuir type of isotherms are first derived. Methods making use of the characteristic grid which enable the direct calculation of transients are derived. The determination of profiles without the accumulating errors due to internal interpolation are discussed.

Although the basic algorithms are derived for simple physical models, it will be shown that the numerical methods and algorithms presented here can be extended to more complex systems. These extensions include efficient methods for dealing with distributed disturbances and accumulating interfaces. The basis of extension of the methods for use with general nonlinear rate expressions is also examined.

CONCLUSIONS AND SIGNIFICANCE

The algorithms derived for the numerical solution of countercurrent processes are brief and efficient since they are explicit and equivalent to those obtained by the modified Euler's method with infinite iteration. The use of the characteristic coordinates in the computation contributes to the accuracy and efficiency.

The basic simple algorithms and methods presented in this paper can be efficiently and accurately extended for application to a number of more complex models of countercurrent and noncountercurrent processes.

INTRODUCTION

Many mass and heat transfer processes between contacting phases are conducted in countercurrent flow. An understanding of process dynamics for such systems is important for efficient design, operation and control. However, practical and useful quantitative analyses for countercurrent processes are difficult to obtain. The most general analytic solution available for linear systems which could be applicable to more than the simplest boundary conditions is that of Jaswon and Smith (1954). Even for the simple linear models used, the solutions are cumbersome for practical use and require the use of a computer for evaluation of the complicated series solutions. Numerical methods which are accurate and efficient for at least these linear models are thus highly desirable. If an efficient algorithm is available, extension to relatively more complex systems will be facilitated.

The numerical methods used to solve the type of hyperbolic partial differential equations arising in countercurrent processes can be roughly grouped into three categories: (a) finite difference schemes applied directly to the flow equations (Ramirez, 1976; Privott and Ferrell, 1966); (b) cell or lumped parameter models which convert the distributed parameter system into a set of ordinary differential equations which are then integrated by standard numerical techniques (Rosenbrock, 1966); and (c) replacing the original equations by characteristic equations which can then be integrated along the characteristic lines (Acrivos, 1954).

The implementation and results of finite difference schemes vary, depending on the finite difference approximations used to replace the time and space derivatives and the average values of the dependent variables. The accuracy and stability of the methods depend not only on the relative time and space increment used, but also on the particular finite difference scheme used (Ames, 1977; Smith, 1978). It has been shown by Stone and Brian (1963) that the finite difference scheme implicitly includes a term equivalent to axial dispersion. The cell model also implicitly includes a dispersion term as shown by Rosenbrock (1966) and thus cannot accurately represent the hyperbolic equations except with a very large number of cells. The explicit inclusion of axial dispersion in system models would be desirable. If an efficient algorithm for the numerical solution of the basic hyperbolic differential equations can be developed then a framework for extension to such models would be provided.

Acrivos (1954) has shown the usefulness of the method of characteristics for solving a number of chemical engineering problems. He also indicated the possible application to countercurrent processes. Most of the publications in the chemical engineering literature illustrating the details of the numerical calculations used with the method of characteristics are applications to fixed bed processes (Dranoff and Lapidus, 1958; Gonzalez and Spencer, 1963). In these systems, the special difficulties resulting from the split boundary nature of countercurrent processes do not arise. A few papers (Bradley and Andre, 1972; Lee et al., 1973; Gawdzik, 1979) on countercurrent processes do not focus on the details of the numerical methods and are primarily studies of process dynamics or control of specific systems. These papers do not provide accuracy and efficiency checks of their numerical solutions and do not provide sufficient detail enabling the facile extension of the numerical methods to other systems.

In this work, a simple numerical method based on the method of characteristics and applicable to many simple models used in chemical engineering will be presented. The particular features of the proposed methods and the derived algorithms which will be discussed are:

(1) The use of the modified Euler's method to obtain explicit forms of algorithms which lead to accuracy and efficiency.

(2) The use of a grid of characteristic coordinates which avoids the approximations and interpolation required for methods using a rectangular grid based on real time and space coordinates.

(3) The direct conversion of the characteristic coordinates of the dependent variable output to real time and space coordinates.

(4) The facile extension of the derived basic algorithms for simple models to more complex systems dealing with transient response to distributed disturbances, accumulating interfaces, general nonlinear isotherms, nonlinear rate expressions and noncountercurrent processes.

Finally, the advantages and disadvantages of the proposed method relative to other methods will be examined.

MODELS FOR GENERAL CONTINUOUS COUNTER-CURRENT PROCESSES

A basic simple model will be presented first. Extensions and applications to more complex models and other flow arrangements will be discussed in a later section. The basic model will be applicable to two moving contacting phases with negligible axial dispersion and absence of chemical reaction or internal generation of heat. The rate of interphase mass or energy transport will be approximated by simple linear driving force rate equations. Holdup in both phases is assumed to be significant. The physical properties of the flowing streams are assumed to be constant. For mass transfer systems, it is assumed that the molar flow rates in both phases are constant, an assumption that is reasonable in the case of gas absorption of dilute components and in many continuous distillation processes. With the above assumptions, the model equations are:

For mass transfer:

$$G_x \frac{\partial x}{\partial z} + \phi_x \frac{\partial x}{\partial t} = K_y aS(y - y^*) \tag{1}$$

$$-G_y \frac{\partial y}{\partial z} + \phi_y \frac{\partial y}{\partial t} = K_y aS(y^* - y) \tag{2}$$

where $y^* = f(x)$

Two types of equilibrium relationship will be considered. The first is the linear isotherm:

$$y^* = mx + m_o \tag{3}$$

where m and m_o are respectively the slope and intercept of the equilibrium line.

The second equilibrium relation is the nonlinear isotherm of Langmuir form:

$$y^* = \frac{rx}{1 + r'x} \tag{4}$$

TABLE I. DIMENSIONLESS VARIABLES AND PARAMETERS FOR MASS OR HEAT TRANSFER FOR EQS. 5 AND 6

	Mass Transfer		
	Linear Isotherm	Langmuir Isotherm	Heat Transfer
X	y^*	x	$\frac{T_1 - T_2(H)^*}{T_1(0) - T_2(H)}$
Y	y	y	$\frac{T_2 - T_2(H)^*}{T_1(0) - T_2(H)}$
$f(x)$	$mx + m_o$	$\frac{rx}{1 + r'x}$	$x = X = \frac{T_1 - T_2(H)^*}{T_1(0) - T_2(H)}$
h	$K_y aSz/G_y$	$K_y aSz/G_y$	$UaSz/(C_PG)_2$
θ	$K_y aSt/\phi_y$	$K_y aSt/\phi_y$	$UaSt/(C_P\phi)_2$
A	$(G_x/G_y)/m$	G_x/G_y	$(C_PG)_1/(C_PG)_2$
B	$(\phi_x/\phi_y)/m$	ϕ_x/ϕ_y	$(C_P\phi)_1/(C_P\phi)_2$

* where $T_1(0)$ and $T_2(H)$ are the inlet temperatures. Other normalized forms may be used.

where r and r' are constants.

For liquid-vapor equilibria, the equilibrium relationship is usually expressed in terms of a constant relative volatility for binary systems and is identical in form to Eq. 4 with $r' = r - 1$. It should be noted that an equation identical to Eq. 4 can be used for homovalent ion exchange where $r' = r - 1$ and r is defined as the separation factor (Helfferich, 1962).

Equations 1 and 2, used in the development of the numerical algorithms, are written for y phase rate controlling. Analogous equations and algorithms can be formulated for x phase rate controlling.

For heat transfer:

$$(C_PG)_1 \frac{\partial T_1}{\partial z} + (C_P\phi)_1 \frac{\partial T_1}{\partial t} = UaS(T_2 - T_1) \qquad (1A)$$

$$-(C_PG)_2 \frac{\partial T_2}{\partial z} + (C_P\phi)_2 \frac{\partial T_2}{\partial t} = UaS(T_1 - T_2) \qquad (2A)$$

Equations 1, 2, 1A and 2A can then be transformed to the following identical form:

$$A \frac{\partial X}{\partial h} + B \frac{\partial X}{\partial \theta} = Y - f(x) \qquad (5)$$

$$-\frac{\partial Y}{\partial h} + \frac{\partial Y}{\partial \theta} = f(x) - Y \qquad (6)$$

The dimensionless variables and parameters, as well as $f(x)$ are defined in Table 1.

The total and partial differential relations lead to a linear transformation which further simplifies Eqs. 5 and 6 (Jaswon and Smith, 1954).

Letting:

$$\alpha = \frac{\theta + h}{A + B}, \qquad \beta = \frac{A}{A + B}\left(\theta - \frac{B}{A} h\right)$$

where α and β are the two characteristics, the following characteristic equations are obtained:

$$\frac{\partial X}{\partial \alpha} = \left.\frac{dX}{d\alpha}\right|_\beta = Y - f(x) \qquad (7)$$

$$\frac{\partial Y}{\partial \beta} = \left.\frac{dY}{d\beta}\right|_\alpha = f(x) - Y \qquad (8)$$

The characteristic grid is illustrated in Figure 1a.

The boundary conditions for Eqs. 5 and 6 correspond to X and Y inlet conditions at their respective entrance positions. For uncoupled boundary conditions, these conditions are known and can be expressed as general functions of time.

In continuous distillation processes and systems with recycle streams or systems with control loops, coupled boundary conditions arise. For example, the boundary condition at the top of a distillation column is related to a mass balance on the condenser, while the bottom condition is related to a mass balance on the reboiler. The solutions of systems with these types of coupled boundary conditions will be discussed in more detail in the application examples of Part II.

The initial conditions for Eqs. 5 and 6 as applied to the illustrated numerical examples will be limited for brevity to practical cases, i.e., start-up conditions or processes initially operating at steady state. In the former case, one of the two contacting phases is usually of uniform composition or temperature. For the latter case, the initial composition or temperature is determined from the solution to the steady-state equations. Since axial dispersion was assumed to be neglible in the basic model equations, a disturbance in inlet temperatures or composition is propagated as a discontinuity. Thus the initial condition at a particular space coordinate is applicable up to the time of arrival of the disturbance front at that particular position.

NUMERICAL METHODS OF SOLUTION

The disturbances to the initial state can be introduced in the X stream, in the Y stream or in both X and Y streams. The disturbances to be considered here for illustrative purposes are: arbitrary time-dependent changes in the inlet composition or temperature. Figures 1a, 1b and 1c are diagrams of the coordinate system used for the numerical solutions. In all three cases, the boundary conditions for X and Y inlets are known. The basic difference equation used in this paper is very simple and corresponds to integrating Eqs. 7 and 8 along characteristic lines α and β by the modified Euler's method. If a single-step integrating method is used along the characteristics, advantage can be taken of the simplicity of the linear driving force rate equation to obtain an explicit algorithm for the simultaneous equations. Any single-step method such as modified Euler or Runga Kutta is suitable for calculation along the boundaries or along the initial characteristic. However, the modified Euler's method was chosen because of its simple, unambiguous application to interior points. In addition, the use of the modified Euler's method results in simple, explicit algorithms which lead to efficiency and accuracy of the numerical solution.

Linear Isotherm

For a system in which $f(x) = X$, application of the modified Euler's method to Eq. 7 gives:

$$X(i,j) - X(i-1,j) = \frac{\Delta\alpha}{2}[Y(i,j) - X(i,j) + Y(i-1,j) - X(i-1,j)] \qquad (11)$$

Similarly, application of the modified Eulers method to Eq. 8 gives:

$$Y(i,j) - Y(i,j-1) = \frac{\Delta\beta}{2}[X(i,j) - Y(i,j) + X(i,j-1) - Y(i,j-1)] \qquad (12)$$

where the i and j indices locate the mesh point coordinates along the β and α characteristics respectively.

Note that the value of X or Y at mesh points of $(i-1)$ or $(j-1)$ are known from calculations for the preceding mesh points or from the known initial and/or boundary conditions.

As can be seen, the two simultaneous equations can be solved explicitly for the unknowns $X(i,j)$ and $Y(i,j)$. It will be shown later that application of the modified Euler's method to a nonlinear isotherm also leads to an explicit numerical scheme. The application of Eqs. 11 and 12 will be illustrated for the three types of disturbances previously mentioned:

Case a: Disturbance in the X Stream. Referring to Figure 1a, a complete algorithm is derived using Eqs. 11 and 12. The numerical calculation scheme is as follows:

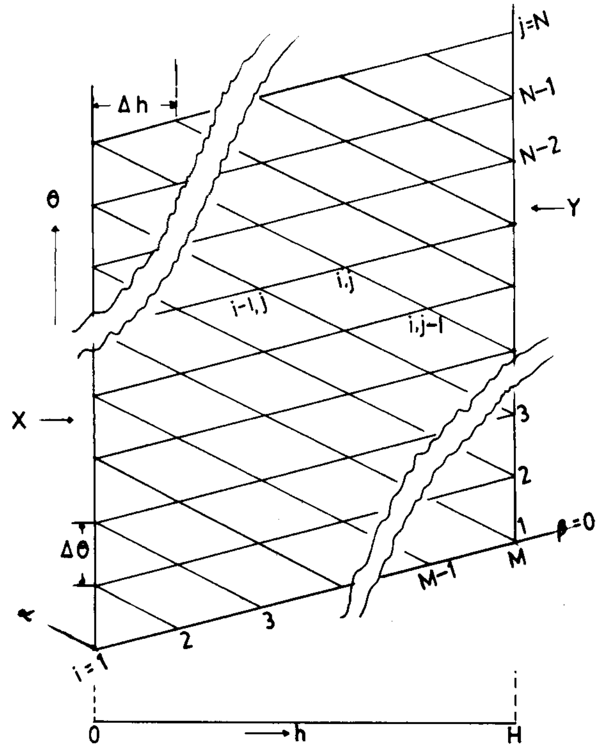

Figure 1a. Schematic diagram for calculation of response to disturbances introduced by the X stream.

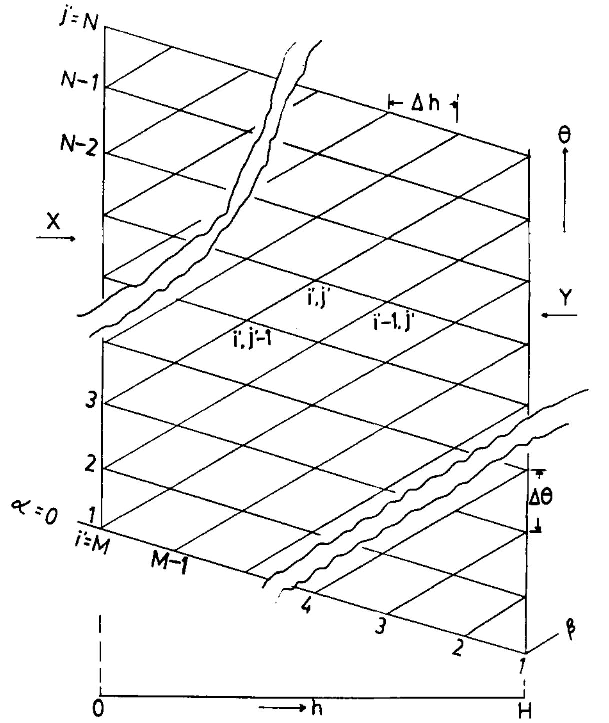

Figure 1b. Schematic diagram for calculation of response to disturbances introduced by the Y stream.

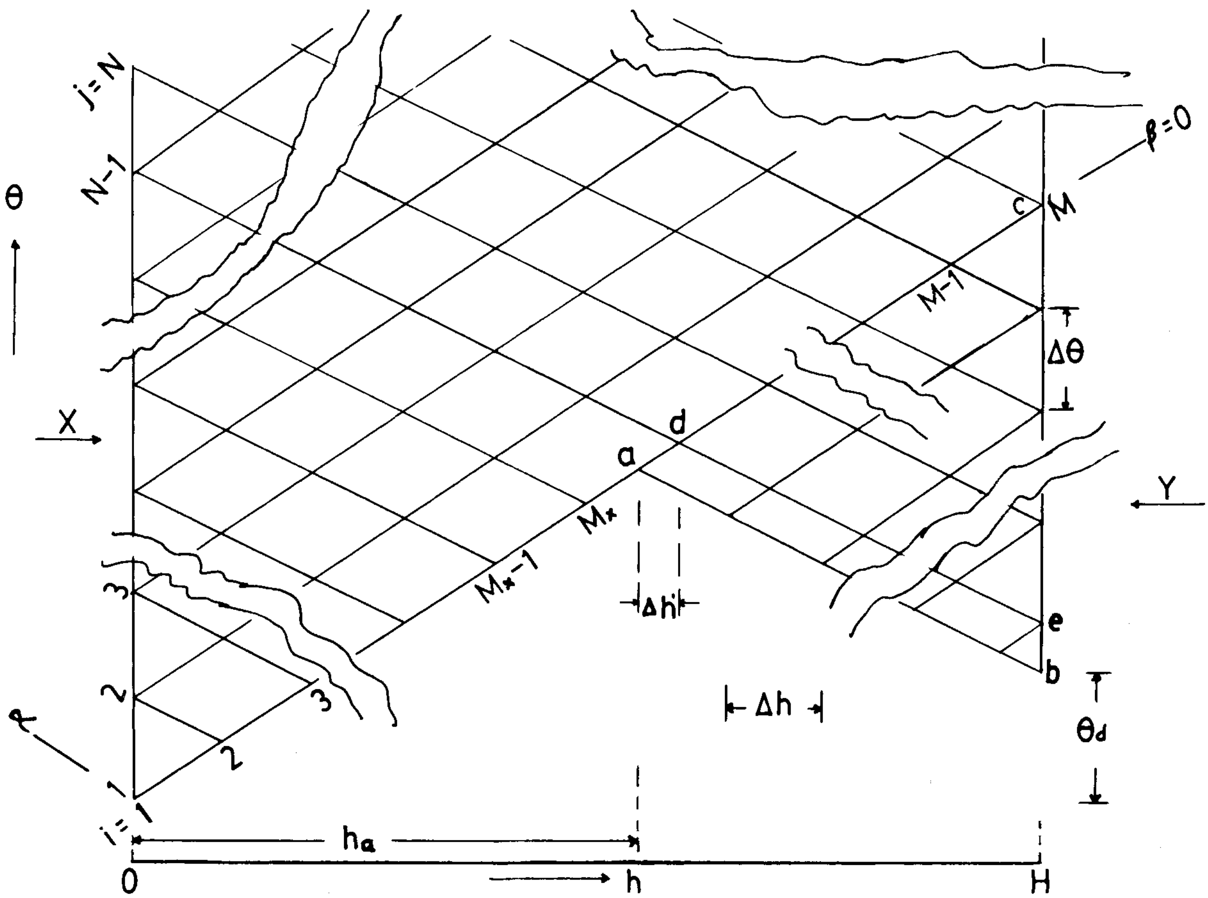

Figure 1c. Schematic diagram for calculation of response to disturbances by both X and Y streams.

(1) Calculation of the values of the front of the X stream. The initial condition of $Y = Y[h,\theta - (B/A)h \leqslant 0]$ is known, hence the values of X for $\beta = 0$ can be obtained by applying Eq. 11 for $j = 1$. Solving for $X(i,1)$:

$$X(i,1) = \frac{2-\Delta\alpha}{2+\Delta\alpha}X(i-1,1) + \frac{\Delta\alpha}{2+\Delta\alpha}[Y(i,1) + Y(i-1,1)] \tag{13}$$

for $i = 2,3,4, \ldots M$
where M is located at $h = H$ on the $\beta = 0$ characteristic.

The values of $Y(i,1)$ for $i = 1,2,3, \ldots M$ correspond to the known initial conditions and $X(1,1)$ is assumed to be the new inlet condition of X.

(2) Calculation of the values of Y outlet. The outlet condition of Y, $Y = Y(0,\theta)$ is obtained by applying Eq. 12 for $i = j$ and solving for $Y(i,j)$:

$$Y(j,j) = \frac{2-\Delta\beta}{2+\Delta\beta}Y(j,j-1) + \frac{\Delta\beta}{2+\Delta\beta}[X(j,j) + X(j,j-1)] \tag{14}$$

for $j = 2,3,4, \ldots N$
Note that $X(j,j)$ for $j = 1,2,3, \ldots N$, are known and correspond to the inlet condition of $X = X(0,\theta)$.

(3) Calculation of the values of X and Y for the interior points. For the interior points, applying both Eqs. 11 and 12 and solving the two equations simultaneously for $X(i,j)$ and $Y(i,j)$:

$$X(i,j) = \frac{\dfrac{2-\Delta\alpha}{2+\Delta\alpha}X(i-1,j) + \dfrac{\Delta\alpha}{2+\Delta\alpha}\left[Y(i-1,j) + \dfrac{\Delta\beta}{2+\Delta\beta}X(i,j-1) + \dfrac{2-\Delta\beta}{2+\Delta\beta}Y(i,j-1)\right]}{1 - \dfrac{\Delta\beta}{2+\Delta\beta}\dfrac{\Delta\alpha}{2+\Delta\alpha}} \tag{15}$$

$$Y(i,j) = \frac{2-\Delta\beta}{2+\Delta\beta}Y(i,j-1) + \frac{\Delta\beta}{2+\Delta\beta}[X(i,j) + X(i,j-1)] \tag{16}$$

for $j = 2,3,4, \ldots N$
for $i = j + 1, j + 2, j + 3, \ldots M + j - 2$

(4) Calculation of the values of X outlet. An equation similar to Eq. 13 can be obtained for the outlet conditions of X by applying Eq. 11 and solving for $X(H,\theta) = X(M + j - 1,j)$:

$$X(M+j-1,j) = \frac{2-\Delta\alpha}{2+\Delta\alpha}X(M+j-2,j) + \frac{\Delta\alpha}{2+\Delta\alpha}[Y(M+j-1,j) + Y(M+j-2,j)] \tag{17}$$

for $j = 2,3,4, \ldots N$

Note again that $Y(M + j - 1,j)$ are the known inlet conditions of $Y = Y(H,\theta)$

A logical sequence of calculation which leads to simple coding arises from following the characteristic lines. The sequence of calculations in applying Eqs. 13 to 17 is to first calculate $X(i,1)$, then the values of X and Y along the line $j = 2$, that is, applying Eq. 14 to obtain $Y(2,2)$, then Eqs. 15 and 16 to obtain values of X and Y for the interior points and finally Eq. 17 for the outlet condition of X. The process can then be repeated for $j = 3,4,5, \ldots N$, where N is a value such that the final steady state values of X and Y are closely approached.

In Eqs. 14 and 17, it is assumed that the boundary conditions of X and Y are independent. For coupled boundary conditions, modified equations may be formulated to take account of the special relations between X and Y at $h = 0$ and $h = H$. These will be illustrated with appropriate examples in Part II.

Case b: Disturbances in the Y Stream. The calculation scheme for disturbances introduced in the Y stream is identical to that of Case a as is evident from inspecting the sketches shown in Figures 1a and 1b. To make use of the equations derived for Case a, the only changes required are interchange of notation for X and Y, $\Delta\alpha$ and $\Delta\beta$ and the substitution of i' for i and j' for j.

Case c: Disturbances in both X and Y Streams. The numerical procedure for this case is somewhat more complex. To apply the complete numerical scheme written for Case a, all the values of X and Y on $\beta = 0$ must be known. For $i = 1$ to $i = M_x$ (Figure 1c), the values of Y are specified, while the values of X can be calculated from Eq. 13. The values of both X and Y along line segment ac can be determined by applying the numerical scheme of Case b to the region bounded by abc. The remaining calculations for X and Y at their respective outlets, and the interior points of X and Y proceed as given by Eqs. 14 to 17. However, some modification of the numerical scheme is necessary for general values of A and B. Referring to Figure 1c, point a gives the time and location at which the two disturbances meet for the first time. The space coordinate of a is given by:

$$h_a = \frac{H + \theta_d}{1 + B/A},$$

where B/A is the slope of the β characteristic lines and θ_d is the time delay between the two disturbances.

Only if B/A can be approximated by B'/A' where A' and B' are integers can a suitable size increment of Δh be chosen such that both h_a and H can be expressed as integer multiples of Δh, i.e., $\Delta h' = 0$. If this approximation is not adequate, then a different increment in α, $\Delta\alpha'$ must be used in the calculations for values of X and Y in region $abed$ of Figure 1c. In addition, for the calculation of $Y(i' = 2, j' = 1)$, a new increment $\Delta\beta'$ should be used in place of $\Delta\beta$. The relationship between $\Delta\alpha'$ and $\Delta\beta'$ and $\Delta\alpha$ and $\Delta\beta$ is given by:

$$\Delta\alpha'/\Delta\alpha = \Delta\beta'/\Delta\beta = \Delta h'/\Delta h$$

and as can be shown in Figure 1c, $\Delta h' = M_x\Delta h - h_a$, where $M_x - 1$ is the integer part of $h_a/\Delta h$.

Nonlinear Isotherm

The derivation of the algorithms and their application to the different types of disturbances can be extended to nonlinear isotherms such as the Langmuir form. To derive algorithms corresponding to Eqs. 13 to 17, the two equations to be solved are:

$$\frac{\partial x}{\partial\alpha} = \left.\frac{dx}{d\alpha}\right|_\beta = y - \frac{rx}{1 + r'x} \tag{7N}$$

$$\frac{\partial y}{\partial\beta} = \left.\frac{dy}{d\beta}\right|_\alpha = \frac{rx}{1 + r'x} - y \tag{8N}$$

Applying the modified Euler's method of integration to the two characteristic equations gives:

$$x(i,j) - x(i-1,j) = \frac{\Delta\alpha}{2}\left[y(i,j) - \frac{rx(i,j)}{1 + r'x(i,j)} + y(i-1,j) - \frac{rx(i-1,j)}{1 + r'x(i-1,j)}\right] \tag{11N}$$

$$y(i,j) - y(i,j-1) = \frac{\Delta\beta}{2}\left[\frac{rx(i,j)}{1 + r'x(i,j)} - y(i,j) + \frac{rx(i,j-1)}{1 + r'x(i,j-1)} - y(i,j-1)\right] \tag{12N}$$

Following a numerical procedure similar to that applied to the linear system, equations analogous to Eqs. 13 to 17 are obtained for application to Case a.

(1) Calculation of the values of the front of the X stream.

$$x(i,1) = [-(1 + r'c + r\Delta\alpha/2) + \sqrt{(1 + r'c + r\Delta\alpha/2)^2 - 4r'c}]/2r' \tag{13N}$$

for $i = 2,3,4, \ldots M$

where $c = \frac{\Delta\alpha}{2}[y^*(i-1,1) - y(i-1,1) - y(i,1)] - x(i-1,1)$

(2) Calculation of the values of Y outlet.

$$y(j,j) = \frac{\Delta\beta}{2+\Delta\beta}[y^*(j,j) + y^*(j,j-1)] + \frac{2-\Delta\beta}{2+\Delta\beta}y(j,j-1) \tag{14N}$$

for $j = 2,3,4, \ldots N$

(3) Calculation of values of X and Y for the interior points.

$$x(i,j) = \left[-\left(1 + r'c + \frac{r\Delta\alpha}{2+\Delta\beta}\right) + \sqrt{\left(1 + r'c + \frac{r\Delta\alpha}{2+\Delta\beta}\right)^2 - 4r'c}\right] / 2r' \tag{15N}$$

$$y(i,j) = y(i,j-1) - \frac{\Delta\beta}{\Delta\alpha}[x(i,j) - x(i-1,j)] + \frac{\Delta\beta}{2}[y^*(i,j-1) - y^*(i-1,j) + y(i-1,j) - y(i,j-1)] \tag{16N}$$

for $j = 2,3,4, \ldots N$

$i = j+1, j+2, j+3, \ldots M+j-2$

$$\text{where } c = \frac{\Delta\alpha}{2}\left[y^*(i-1,j) - y(i-1,j) - \frac{\Delta\beta}{2+\Delta\beta}y^*(i,j-1) - \frac{2-\Delta\beta}{2+\Delta\beta}y(i,j-1)\right] - x(i-1,j)$$

(4) Calculation of the values of X outlet.

$$x(M+j-1,j) = [-(1 + r'c + r\Delta\alpha/2) + \sqrt{(1 + r'c + r\Delta\alpha/2)^2 - 4r'c}]/2r' \tag{17N}$$

for $j = 2,3,4, \ldots N$

$$\text{where } c = \frac{\Delta\alpha}{2}[y^*(M+j-2,j) - y(M+j-2,j) - y(M+j-1,j)] - x(M+j-2,j)$$

In applying Eqs. 13 to 17 or Eqs. 13N to 17N the magnitudes of $\Delta\alpha$ and $\Delta\beta$ can be expressed in terms of Δh or $\Delta\theta$. From the functional relationship of α and β to both h and θ and applying the partial derivative relationship it can be shown that:

$$\frac{\partial X}{\partial \alpha} = A\left.\frac{dX}{dh}\right|_\beta; \qquad \frac{\partial Y}{\partial \beta} = \left.\frac{dY}{dh}\right|_\alpha$$

Hence, $\Delta\alpha$ can be replaced by $\Delta h/A$ and $\Delta\beta$ by Δh in all equations to be used for the numerical solution. The accuracy of the numerical solution is thus solely determined by the larger value of Δh or $\Delta h/A$.

Conversion of Output to Real Time and Space Coordinates

To obtain output in terms of real time (θ) and space (h) coordinates, numerical solution of the system equations by the method of characteristics have been carried out on a rectangular grid of h and θ coordinates (Lee, 1977; Gawdzik, 1979). The use of such a rectangular grid requires internal interpolation in order for the calculation to proceed along the characteristics and the approximations lead to accumulating errors. It will be shown that the α, β coordinates can be accurately converted to h and θ coordinates with minor increase in the required coding.

Transients

Figure 1a shows that the time for a disturbance in the X stream to reach a given location $h = (i-j)\Delta h$ is given by $\theta = (i-j)(B/A)\Delta h$. Thus a set of X and Y values in terms of the nonrectangular α,β coordinates can be converted to h,θ coordinates by the general expression:

$$X(i,j) = X[h = (i-j)\Delta h, \quad \theta = (i-1)(B/A)\Delta h + (j-1)\Delta h].$$

Identical expressions can be obtained for Y, or x and y.

Since the contact time for the X stream is defined as $(\theta - (B/A)h)$, an alternative conversion to a rectangular grid in terms of h and contact time of X is given by:

$$X(i,j) = X[h = (i-j)\Delta h, \quad \theta - (B/A)h = (j-1)\Delta\theta].$$

The transient at an h location given by $(i-j)\Delta h = k\Delta h$, where k is an integer, can be directly obtained without interpolation from the general expression, and is

$$X(i = j+k, j) = X[h = k\Delta h, \quad \theta = (j-1)\Delta\theta + k\Delta\theta_x]$$

for $j = 1,2,3, \ldots N$

where $\Delta\theta = (1 + B/A)\Delta h$; $\Delta\theta_x = (B/A)\Delta h$

The transient values for $h = k\Delta h$ are obtained at a time interval of $\Delta\theta$ after the elapsed time of $k\Delta\theta_x$. That is, the first value of X is

$$X(i = k+1, \quad j = 1) = X(k\Delta h, k\Delta\theta_x)$$

Profiles

For any general values of A and B, profiles at a given θ are not as readily obtained, since a line of constant absolute time of integer multiples of $\Delta\theta$ will not have many common intersections with all intersections of the characteristic lines. When B/A can be approximated by B'/A' where B' and A' are integers (Lee, 1977), then the values of X or Y at constant integer multiples of θ, i.e., $k\Delta\theta$, can be obtained directly from the numerical output at an interval of $(A' + B')\Delta h$. These values are given, for example, by:

$$X[i = k + 1 + (n-1)A', \quad j = k + 1 - (n-1)B'] = X[h = (n-1)(A'+B')\Delta h, \quad \theta = k\Delta\theta],$$

where: $n = 1,2,3, \ldots n_k + 1$; for $k \leq B'(n_m - 1)$, $\theta \leq (B'/A')h$

$n = 1,2,3,4, \ldots n_m$; for $k > B'(n_m - 1)$, $\theta > (B'/A')H$

n_k = integer part of k/B'

$n_m + 1$ = the integer part of $B'(M-1)/(A'+B')$

The profiles of X for region $\theta \leq (B'/A')h$ include a discontinuity which occurs at $\theta = (B'/A')h$. When k/B' is an integer, the value of this discontinuity is obtained directly from the α,β grid output and corresponds to the value of the data point for $n = n_k + 1$. When k/B' is not equal to an exact integer then the value of the discontinuity must be determined by some other means such as interpolation or use of an analytic solution (if available) along the characteristic $\theta - (B/A)h = 0$.

For general values of A and B, or in case B/A cannot be adequately approximated by B'/A', interpolation using output from the α, β grid can be applied to obtain profiles at any given θ. It should be emphasized that this type of external interpolation of the output data does not lead to accumulating errors.

In summary, the proposed numerical method is accurate and efficient because:

(1) The explicit algorithm is equivalent to the modified Euler's method with infinite iteration.

(2) Of the use of the method of characteristics together with numerical solution in terms of characteristic coordinates.

EXTENSION OF NUMERICAL METHODS TO OTHER MODELS AND SYSTEMS

The basic model used for derivation of the explicit algorithms was limited for clarity of presentation to important countercurrent processes represented by two first-order partial differential equations with simple linear driving force rate expressions with linear or Langmuir isotherms. In addition, the algorithms developed were limited for illustrative purposes to disturbances in inlet temperature or composition. However, the basic method can be readily extended to more complex models as well as to noncountercurrent processes.

Models for Systems with Distributed Disturbances

If the system model includes velocity changes or general space and time-dependent forcing functions $F(h,\theta)$, the transients will originate from the $\theta = 0$ line and propagate into the whole time and space domain. Thus, calculations must be carried out for a region not covered in the previous discussion. A method of calculation for this additional region is outlined in Appendix 1 and is illustrated with numerical examples in Part II. The method is applicable for any general values of A and B, whether integer or not, uses characteristic coordinates and follows a logical sequence for coding similar to that previously described. Explicit algorithms can be obtained if appropriate rate expressions are used and if the velocity changes or $F(h,\theta)$ are defined at every mesh point. The characteristic grid employed enables the direct determination of transients at any h coordinate. Profiles are readily obtained by external interpolation.

Stationary Accumulating Phases

If a linear driving force rate expression can be assumed for the interface(s), explicit algorithms can be derived for a system with accumulation of mass or energy in stationary phases. The derivation of such an algorithm for an accumulating tube wall in a double-pipe countercurrent heat exchanger is given in Appendix 2 and its application illustrated in Part II. It is interesting to note that the simplicity of the derived algorithm arises not only from the simple rate equations used, but also from the ability to use a third characteristic line on the same mesh used for the system without a stationary phase. Thus, the addition of an accumulating shell wall with a linear driving force rate expression will also lead to explicit algorithms. These examples illustrate the possibility of extending the basic model to other systems with more than two dependent variables and more than two characteristics.

Nonlinear Isotherms in Linear Driving Force Expressions

Explicit algorithms to Eqs. 13N to 17N can be obtained for isotherms somewhat more complex than the Langmuir isotherm. For example, the general hyperbolic isotherm, $f(x) = (a + bx)/(1 + cx)$ and the general quadratic isotherm, $f(x) = a + bx + cx^2$ also lead to explicit algorithms.

The methods described can provide an efficient and accurate framework for handling general nonlinear isotherms. For example, using different hyperbolic or quadratic isotherm parameters for specified composition ranges will result in explicit algorithms of the form of Eqs. 13N to 17N. Piecewise fitting with Langmuir isotherms has been used previously (Tan and Spinner, 1971).

The above methods may not provide an adequate representation of a complex nonlinear isotherm. In such case, the isotherm can be fitted by using composition dependent parameters in the quadratic or hyperbolic forms of isotherm (Tan and Spinner, 1971). Explicit algorithms are still obtainable by approximating the parameters at a given mesh point with the parameters of previously calculated mesh points. Calculation has shown that using a small mesh size leads to more efficient algorithms than iterative algorithms of equivalent accuracy.

General Rate Expressions

If the rate expression is a general quadratic form in terms of X and Y, explicit algorithms similar to those given by Eqs. 13N to 17N can be derived. A special case of the general quadratic is the second-order kinetic rate expression for adsorption or ion exchange which is illustrated in another context in the following section and Appendix 3. Further examples arise from second-order chemical reaction or mass transfer accompanied by second-order chemical reaction.

The rate expressions are complex and usually highly nonlinear for systems involving internal heat generation and temperature dependent chemical reaction. However, explicit algorithms can still be obtained by approximation of the rate parameters, making use of the previously calculated values of the dependent variables. Sketris (1981) found that the proposed algorithms used with small mesh size was about two times more efficient than an iterative method with equivalent accuracy. However, investigation would be required to check the accuracy, stability and efficiency of the above proposed method with other rate expressions and as compared to other numerical methods which employ different iterative or internal interpolation procedures.

An alternative method for complex rate expressions which leads to explicit quadratic algorithms can be obtained by a second order Taylor series expansion around the previously calculated mesh point. If a small mesh size is used with these approximations, efficiency and accuracy can be maintained without the use of iterative methods.

Noncountercurrent Processes

The numerical methods discussed in this paper are directly applicable to cross-flow (Evans and Smith, 1962; Wnek and Snow, 1972) and fixed-bed processes with proper modification of the characteristic lines and boundary conditions. The dynamics of a nonisothermal tubular packed bed reactor with infinite heat transfer between the packing and the flowing reactant streams (Crider and Foss, 1966) can be considered as a cocurrent process. Since the temperature and composition changes are propagated in the same direction with different velocities, the proposed methods are applicable.

In fixed-bed processes, the second-order kinetic model (a quadratic form) for adsorption or ion exchange can also be solved numerically by the explicit algorithm derived in Appendix 3. This algorithm will be used in Part II to check the numerical results against the analytic solution (Thomas, 1944), since no analytic solution exists for a nonlinear system involving countercurrent flow.

In studies of transients and the periodic steady state of cyclic fixed bed processes with countercurrent regeneration where short beds with low loading are used, an efficient numerical scheme is essential. The basic algorithms and numerical methods developed in this paper have been applied successfully to nonlinear binary and ternary systems in such fixed bed ion exchange processes (Tan and Spinner, 1971).

SUMMARY AND CONCLUSIONS

The proposed methods using the characteristic coordinates can be shown to be more accurate than other applications of the method of characteristics which perform the calculations on a rectangular grid of real time and space coordinates of equivalent increment size. For equivalent accuracy the proposed methods are more efficient. Finite difference methods based on the original model equations when applied to systems with linear isotherms can be very efficient and like the proposed methods lead to simple coding. However, this simplicity is obtained at a sacrifice of accuracy in solving the relevant hyperbolic differential equations.

Systems involving complex rate expressions when solved iteratively by finite difference methods or by use of cell models can lead to shorter main program coding than the proposed methods. However, greater overall efficiency (at equivalent accuracy) is obtained using the proposed methods with small mesh size.

In common with other methods of solving hyperbolic differential equations, the coding using the proposed algorithms can be generalized to handle a variety of problems. This generalization involves for example, merging of the algorithms for distributed disturbances, accumulating interfaces, coupled boundary conditions (Part II) and general nonlinear rate expressions. Such generalization leads to somewhat lengthier coding than finite difference solutions or cell model application using iterative techniques. However, at equivalent accuracy, the proposed methods can be expected to provide more efficient numerical calculation.

The model equations used in this paper were hyperbolic and therefore explicitly excluded the axial dispersion often present in practical systems. Calculations using cell models or finite difference methods implicitly result in contributions equivalent to axial dispersion. The numerical solution of models explicitly including axial dispersion using the proposed characteristic grid as a framework for numerical calculation are currently under investigation.

NOTATION

- a = interfacial area per unit volume of contactor
- A = ratio of mass or molar flow rates
- B = ratio of holdup in the two contacting phases
- C_p = heat capacity of the flowing streams
- f = fractional heat transfer resistance on the cold fluid-side
- G = mass flow rate
- h = dimensionless space parameter
- H = dimensionless total length parameter
- K_y = overall mass transfer coefficient in the light phase, mass per unit contact area per unit time)
- K_x = overall mass transfer coefficient in the heavy phase, mass per unit contact area per unit time
- L = total length of contacting equipment
- m = slope of the linear isotherm
- m_o = intercept of the linear isotherm
- M_W = mass of wall per unit length
- r = parameter in Langmuir form of isotherm
- r' = parameter in Langmuir form of isotherm
- S = cross-sectional area of the contacting equipment
- t = real time
- T = temperature
- U = overall heat transfer coefficient, energy per unit contact area per unit temperature difference per unit time
- W = dimensionless wall temperature
- x = heavy phase composition
- X = normalized heavy phase composition, or normalized hot fluid temperature
- y = light phase composition
- Y = normalized light-phase composition or normalized cold fluid temperature
- z = axial distance along the contacting equipment

Greek Letters

- α = characteristic line or characteristic coordinate
- β = characteristic line or characteristic coordinate
- Δ = increment
- ϕ = holdup, mass/unit length of contactor
- θ = dimensionless time parameter

APPENDIX 1: METHOD FOR NUMERICAL CALCULATION FOR DISTRIBUTED DISTURBANCES

The method will be outlined for a step change in velocity of the X stream, but is readily modified to handle velocity changes in the Y stream or in both streams. General forcing functions of the form $F(h,\theta)$ can be treated in an identical manner with appropriate modification to the basic algorithms previously presented.

Figure 1A, which is an extension of Figure 1a, is obtained by extending α characteristic lines, $\theta = -h + (i-1)(1 + B/A)\Delta h$, to intersect with vertical line $h = H$ and horizontal line $\theta = 0$. From the intersections at line $h = H$, β characteristic lines, $\theta = (B/A)h - (j'-1)(1 + B/A)\Delta h$, are constructed to intersect with line $\theta = 0$. The method of calculation is outlined for the region bounded by $\theta = 0$ and $\theta \leq (B/A)h$. The calculations above this region then follow Case a of the numerical methods previously outlined.

Referring to Figure 1A, the sequence of calculations follows $j' = j'_N, j'_N - 1$, to 1, where $j'_N - 1$ is the integer part of $(M-1)(B/A)(1 + B/A)$. For each j' line the sequence of calculation is for $i = i_s$ to $M - j' + 1$, where i_s locates the first mesh point for $\theta \geq 0$ and where $i_s - 2$ is given by the integer part of $(A/B)(j'-1)$. For the calculation from $i = i_s$ to $M - j'$, solution of the two simultaneous characteristic equations as given by Eqs. 15 and 16, or Eqs. 15N and 16N, for the interior points are required. For $i = i_s$ to i_e, where $i_e - 1$ is given by the integer part of $(A/B)j'$, initial state values and the associated irregular increments $\Delta\alpha'$ and $\Delta\beta'$ will be required. The initial state values are defined by h_j and h_i which are determined by solving the characteristic equations at $\theta = 0$. Thus, $h_j = (j'-1)(1 + A/B)\Delta h$ and $h_i = (i-1)(1 + B/A)\Delta h$. The required increments to be used with the defined initial state values can be shown to be given by:

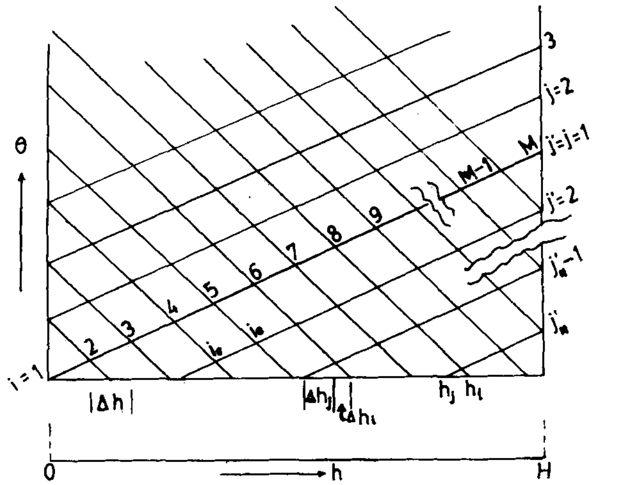

Figure 1A. Schematic diagram for calculation of response to distributed disturbances.

$$\Delta h_j/\Delta h = \Delta\alpha'/\Delta\alpha = (i_s - 1) - (j'-1)(A/B) \leq 1$$
$$\Delta h_i/\Delta h = \Delta\beta'/\Delta\beta = (i_s - 1)(B/A) - (j'-1) \leq 1$$

As can be seen in Figure 1A, for $i = i_s$ initial state values at h_j and h_i replace both "previously calculated" values and $\Delta\alpha'$ and $\Delta\beta'$ replace $\Delta\alpha$ and $\Delta\beta$ in the equations for calculating the interior points. For $i = i_s + 1$ to i_e, initial state values at h_i replace only the values from the previously determined j' line and the increment $\Delta\beta'$ replaces $\Delta\beta$. For $i = i_e + 1$ to $M - j'$, previously calculated values, together with regular sized increments are used. The calculation for a given j' line terminates with the boundary point at $i = M - j' + 1$ using Eq. 17 or 17N.

The calculation along the $j' = j'_N$ line requires some attention. If $i_s > M - j'_N + 1$, no calculation is required since the only point on the j'_N line is given by the initial state at $h = H$. If $i_s = M - j'_N + 1$, the only point to be calculated falls on the line $h = H$ and Eq. 17 or 17N is used with the initial state values defined at h_j together with the associated $\Delta\alpha'$. For $i_s < M - j'_N + 1$, the calculation proceeds as previously outlined for the general j' lines.

The method outlined above made use of a mesh obtained by extension of Figure 1a. A similar method can be obtained making use of Figure 1b. In any case, the method is general for any values of A and B, whether integer or not. In addition, the transients at any given h are directly obtainable without interpolation from the output calculated on the characteristic grid. The values for given α and β coordinates for the region $\theta \leq (B/A)h$ can be converted to h and θ coordinates by, for example:

$$X(i,j') = X[h = k'\Delta h, \theta = (i-1)(B/A)\Delta h - (j'-1)\Delta h]; \qquad k' = i + j' - 2$$

APPENDIX 2: NUMERICAL ALGORITHM FOR COUNTERCURRENT HEAT TRANSFER WITH ACCUMULATING TUBE WALL

Model equations:

$$(C_P G)_1 \frac{\partial T_1}{\partial z} + (C_P \phi)_1 \frac{\partial T_1}{\partial t} = (UaS)_1(T_w - T_1)$$

$$(MC_P)_w \frac{\partial T_w}{\partial t} = (UaS)_1(T_1 - T_w) + (UaS)_2(T_2 - T_w)$$

$$-(C_PG)_2 \frac{\partial T_2}{\partial z} + (C_P\phi)_2 \frac{\partial T_2}{\partial t} = (UaS)_2(T_w - T_2)$$

Normalized equations:

$$A\frac{\partial X}{\partial h} + B\frac{\partial X}{\partial \theta} = \frac{1}{1-f}(W - X)$$

$$C\frac{\partial W}{\partial \theta} = \frac{X}{1-f} + \frac{Y}{f} - \frac{W}{f(1-f)}$$

$$-\frac{\partial Y}{\partial h} + \frac{\partial Y}{\partial \theta} = \frac{1}{f}(W - Y)$$

where $h = \frac{(UaS)z}{(C_PG)_y}$, $\theta = \frac{(UaS)t}{(C_P\phi)_y}$, $C = \frac{(MC_P)_w}{(C_P\phi)_y}$

$A = \frac{(C_PG)_x}{(C_PG)_y}$, $B = \frac{(C_P\phi)_x}{(C_P\phi)_y}$,

$$\frac{1}{(UaS)} = \frac{1}{(UaS)_x} + \frac{1}{(UaS)_y}, \quad f = \frac{(UaS)}{(UaS)_y},$$

$$X = \frac{T_1 - T_2(H)}{T_1(0) - T_2(H)}, \quad Y = \frac{T_2 - T_2(H)}{T_1(0) - T_2(H)},$$

$$W = \frac{T_w - T_2(H)}{T_1(0) - T_2(H)}$$

Characteristic Equations

$$\frac{\partial X}{\partial \alpha} = A\left.\frac{dX}{dh}\right|_\beta = \frac{1}{1-f}(W - X)$$

$$\frac{\partial W}{\partial \theta} = \left.\frac{dW}{d\theta}\right|_h = \frac{X}{C(1-f)} + \frac{Y}{Cf} - \frac{W}{Cf(1-f)}$$

$$\frac{\partial Y}{\partial \beta} = \left.\frac{dY}{dh}\right|_\alpha = \frac{1}{f}(W - Y)$$

In the following algorithms for a disturbance introduced in the X stream, X, Y and W denote values at i and j, subscript ij denotes values at $i-1$ and $j-1$, subscript i denotes values at $i-1$ and j, subscript j denotes values at i and $j-1$.

(1) Calculation of values of X on $\beta = 0$.

$$X = g_1(\alpha)X_1 + g_0(\alpha)(W + W_i)$$

for $i = 2,3,4,\ldots M$ and $j = 1$

where $g_1(\alpha) = \frac{2(1-f) - \Delta\alpha}{2(1-f) + \Delta\alpha}$,

$$g_o(\alpha) = \frac{\Delta\alpha}{2(1-f) + \Delta\alpha}$$

(2) Calculations of values of Y and W at the outlet of the Y stream.

$$W = \frac{g_1(\theta)W_{ij} + g_o(\theta)\left[\frac{f}{1-f}(X + X_{ij}) + Y_{ij} + g_o(\beta)W_j + g_1(\beta)Y_j\right]}{1 - g_o(\theta)g_o(\beta)}$$

$$Y = g_1(\beta)Y_j + g_o(\beta)(W + W_j)$$

for $j = 2,3,4,\ldots M$ and $i = j$

where $g_o(\beta) = \frac{\Delta\beta}{2f + \Delta\beta}$, $g_1(\beta) = \frac{2f - \Delta\beta}{2f + \Delta\beta}$

$g_o(\theta) = \frac{(1-f)\Delta\theta}{2Cf(1-f) + \Delta\theta}$, $g_1(\theta) = \frac{2Cf(1-f) - \Delta\theta}{2Cf(1-f) + \Delta\theta}$

$\Delta\theta = (1 + B/A)\Delta h$

(3) Calculation of interior points

$$X = \frac{g_1(\alpha)X_i + g_o(\alpha)W_i + D\left\{g_1(\theta)W_{ij} + g_o(\theta)\left[\frac{f}{1-f}X_{ij} + g_1(\beta)Y_j + g_o(\beta)W_j + Y_{ij}\right]\right\}}{E}$$

$$W = \frac{X - g_1(\alpha)X_i}{g_o(\alpha)} - W_i$$

$$Y = g_1(\beta)Y_j + g_o(\beta)(W + W_j)$$

for $j = 2,3,4,\ldots N$
and $i = j+1, j+2, j+3, \ldots j + M - 2$

where $D = \frac{g_o(\alpha)}{1 - g_o(\beta)g_o(\theta)}$, $E = 1 - \frac{Dfg_o(\theta)}{1-f}$

(4) Calculation of values of X and W at the outlet of the X stream:

$$W = \frac{g_1(\theta)W_{ij} + g_o(\theta)\left\{Y + Y_{ij} + \frac{f}{1-f}\left[X_{ij} + g_1(\alpha)X_i + g_o(\alpha)W_i\right]\right\}}{1 - \frac{f}{1-f}g_o(\theta)g_o(\alpha)}$$

$$X = g_1(\alpha)X_i + g_o(\alpha)(W + W_i)$$

for $j = 2,3,4,\ldots N$ and $i = M + j - 1$

APPENDIX 3: NUMERICAL ALGORITHM FOR SECOND ORDER-KINETIC MODEL FOR FIXED BED ADSORPTION OR ION EXCHANGE

Model Equations (Thomas, 1944; Vermuelen et al., 1973):

$$V\frac{\partial c}{\partial z} + \epsilon\frac{\partial c}{\partial t} + \frac{\partial q}{\partial t} = 0$$

$$\frac{\partial q}{\partial t} = k_1q(C_o - c) - k_2c(q_c - q)$$

where:
c = concentration of the fluid phase
q = concentration of the solid phase
V = linear superficial velocity
ϵ = void fraction of the bed
z = axial distance
t = time
k_1 = forward rate constant
k_2 = reverse rate constant
C_o = feed fluid concentration
q_c = ultimate exchanger capacity

Normalized Equations:

$$\frac{\partial x}{\partial h'} + \epsilon\frac{\partial x}{\partial \theta'} = y(1-x)/r - x(1-y)$$

$$\frac{\partial y}{\partial \theta'} = x(1-y) - y(1-x)/r$$

where $x = c/C_o$, $y = q/q_c$, $r = k_1/k_2$

$$h' = \frac{k'z}{V}, \qquad \theta' = \frac{k'C_o t}{q_c}, \qquad k' = k_1 q_c$$

Considering a fixed-bed process as a special case of a countercurrent process and comparing the above two normalized equations with Eqs. 5 and 6, $h' \equiv h/A$, $\theta' \equiv \theta$ and $\epsilon \equiv B$. The presence of a stationary phase in the fixed-bed process accounts for the absence of the term $\partial y/\partial h'$.

Characteristic Equations:

$$\frac{\partial x}{\partial \alpha} = A \frac{dx}{dh}\bigg|_\beta = y(1-x)/r - x(1-y)$$

$$\frac{\partial y}{\partial \beta} = \frac{dy}{d\theta}\bigg|_\alpha = x(1-y) - y(1-x)/r$$

where $\alpha = h/A, \quad \beta = \theta - Bh/A,$

Initial condition:

$$y(\alpha,0) = y(h,\theta - Bh/A) = f(h) \qquad \text{for } 0 \leq h \leq H \quad \text{or } 0 \leq \alpha \leq \alpha_H$$

Boundary condition:

$$x(0,\beta) = x(h,\theta) = g(\theta) \qquad \text{for } 0 \leq \theta \leq \theta_f \qquad \text{or } 0 \leq \beta \leq \beta_f$$

In the algorithms given below, x and y refer to values at i and j, subscript i denotes values at j and $i-1$ and subscript j denotes values at i and $j-1$.

(1) Calculation for the values of $x(h,0)$.

$$x = \frac{2 - (R'y-1)\Delta\alpha}{2 + (R'y-1)\Delta\alpha} x_i + \frac{\Delta\alpha}{2 + (R'y-1)\Delta\alpha}(y - y_i)$$

for $i = 2,3,4, \ldots M$ and $j = 1$
where $R' = R - 1$ and $R = 1/r$

(2) Calculation for the values of $y(0,\theta)$.

$$y = \frac{2 - (R - R'x)\Delta\beta}{2 + (R - R'x)\Delta\beta} y_j + \frac{\Delta\beta}{2 + (R - R'x)\Delta\beta}(x - x_j)$$

for $j = 2,3,4, \ldots N$ and $i = 1$

(3) Calculation for the values of x and y for the interior points.

$$x = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$$

$$y = d - (\Delta\beta/\Delta\alpha)x$$

for $i = 2,3,4, \ldots M$
and $j = 2,3,4, \ldots N$
where $a = R'\Delta\beta/(2 + \Delta\alpha)$

$$b = 1 + dR'\Delta\alpha/(2 + \Delta\alpha) + R\Delta\beta/(2 + \Delta\alpha)$$

$$c = \frac{2 - \Delta\alpha}{2 + \Delta\alpha} x_i + \frac{R\Delta\alpha}{2 + \Delta\alpha} y_i - \frac{R'\Delta\alpha}{2 + \Delta\alpha} x_i y_i + \frac{\Delta\alpha}{2 + \Delta\alpha} Rd$$

$$d = (\Delta\beta/2)[R'(x_j y_j - x_i y_i) + R(y_i - y_j) + (x_j - x_i)] + y_j + (\Delta\beta/\Delta\alpha)x_i$$

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