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New Algorithms for the Computation of Column Dynamics of Multicomponent Liquid Phase Adsorption

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Abstract. New and efficient numerical algorithms were developed for simulating column dynamics of multicomponent liquid phase adsorption. Simple and realistic models are used for the simulation. Langmuir form of isotherm and linear driving force rate expressions are employed in the model equations. Algorithms were formulated for three different rate control mechanisms, namely, film diffusion control, particle diffusion control and combined film and particle diffusion control. The algorithms derived are explicit with the exception of the requirement of solving a nonlinear equation in one single variable which is the concentration of a reference species. Thus the tedious iterative calculation procedure for solving simultaneous nonlinear equations in a multicomponent fixed bed system is avoided. Example calculations indicated very good numerical accuracy as verified from an independent check by means of an overall mass balance.

Keywords: column dynamics, liquid adsorption, multicomponent, algorithms

Introduction

Fixed bed liquid phase adsorption is widely used in industrial separation and environmental purification applications. The study on the performance of the column operation of multicomponent adsorption system is usually carried out with local equilibrium assumption (Helfferich and Klein, 1970; Moon and Tien, 1988). The use of equilibrium theory enables relatively simple analysis of the performance of multicomponent sorption process and provides extensive physical insight on limiting system behavior. However, in most operations it is expected that both the solution and adsorbent phase are far from equilibrium. Thus, assumptions neglecting mass transfer effects within the solid and liquid phases are not realistic for most practical operating conditions.

There have been numerous studies on the numerical solution of fixed bed multicomponent liquid phase adsorption under nonequilibrium conditions (Hsieh et al., 1977; Liapis and Rippin, 1978; Balzli et al., 1978; Wang and Tien, 1982). A comprehensive review in this area of work up to 1980 is covered by Mansour et al. (1982). In this work we utilize the simple model equations from which efficient and accurate numerical algorithms are developed to facilitate the simulation and computation of column dynamics for multicomponent liquid phase adsorption. In previous studies (Cooney and Strusi, 1972; Hsieh et al., 1977; Omatete et al., 1980; Wang and Tien, 1982), plug flow assumption and simple rate expressions were used in the analysis of multicomponent fixed bed liquid adsorption or ion exchange. The simplified rate expressions include the use of linear driving force rate equation as an approximation for particle diffusion (Glueckauf, 1955). With the plug flow model and the linear driving force rate expression, we have developed in this work numerical algorithms which are applicable for three different rate control mechanisms, namely, film diffusion, particle diffusion and combined film and particle diffusion. These algorithms can be easily extended to the case of nonuniform presaturation, variable feed condition, composition dependent mass transfer coefficients and cyclic operation which includes the regeneration step.

The important features of the algorithms developed in this work are their simplicity and the derivation of an explicit relation between the concentration of any species to that of an arbitrary reference species. This unique relation is obtained because of the application of the modified Euler's method and the use of a linear driving force rate expression with Langmuir type of isotherm. The derived algorithms enable the initial determination of the concentration of a reference species from an implicit polynomial expression. Once the concentration of this reference species is known, concentrations of all other species are calculated explicitly and directly. The avoidance of extensive iterative calculations results in high efficiency in the simulation and computation of column dynamics for multicomponent liquid phase adsorption system.

Model Equations

Assuming isothermal condition, constant physical properties for feed solution and plug flow with no axial dispersion, the continuity equations for n species of a multicomponent fixed bed liquid adsorption system are

$$V\frac{\partial C_i}{\partial Z} + \beta\frac{\partial C_i}{\partial t} + \rho\frac{\partial Q_i}{\partial t} = 0, \quad \text{for } i = 1, 2, 3, \ldots, n \tag{1}$$

where C_i is the concentration of species i in the solution, Q_i is the concentration of species i in the adsorbent, V is the superficial linear velocity, β is the void fraction of the bed, ρ is the bulk density of the adsorbent in the column, Z is axial distance of the bed and t the absolute time.

For liquid phase rate control, the rate equations are

$$\rho\frac{\partial Q_i}{\partial t} = K_{li}(C_i - C_i^*), \quad \text{for } i = 1, 2, 3, \ldots, n \tag{2A}$$

where C_i^* is the equilibrium liquid phase concentration of specie i with respect to solid phase concentration, Q_i. K_{li} is the overall liquid phase mass transfer coefficient for species i.

For solid phase rate control, the linear driving force approximation is employed and he rate equations are

$$\rho\frac{\partial Q_i}{\partial t} = K_{si}(Q_i^* - Q_i), \quad \text{for } i = 1, 2, 3, \ldots, n \tag{2B}$$

where Q_i^* is the equilibrium solid phase concentration of species i corresponding to liquid phase. K_{si} is the overall solid phase mass transfer coefficient for species i.

For the case of combined liquid and solid phase rate controlling, the rate equations are

$$\rho\frac{\partial Q_i}{\partial t} = k_{li}(C_i - C_i^{\ddagger}) = k_{si}(Q_i^{\ddagger} - Q_i) \quad \text{for } i = 1, 2, 3, \ldots, n \tag{2C}$$

where $C_i^{\ddagger}$ and $Q_i^{\ddagger}$ represent, for i species, the liquid and solid interphase concentration respectively. k_{li} is liquid phase mass transfer coefficient while k_{si} is the solid phase mass transfer coefficient.

The Langmuir type of multicomponent adsorption isotherm employed in this study is given by

$$Q_i^{\ddagger} = \frac{a_i C_i^{\ddagger}}{1 + \sum_1^n b_j C_j^{\ddagger}} \tag{3A}$$

where a and b are the constants of the Langmuir isotherm.

To facilitate the numerical solution the following dimensionless quantities are introduced for the concentration variables (Hsieh et al., 1977)

$$X_i = C_i/C_i^0 \quad \text{and} \quad Y_i = Q_i/Q_i^0,$$

where C_i^0 is the feed concentration of species i and Q_i^0 is defined by

$$Q_i^0 = \frac{a_i C_i^0}{1 + \sum_1^n b_j C_j^0} \tag{3B}$$

$$Y_i^{\ddagger} = \frac{Q_i^{\ddagger}}{Q_i^0} = \frac{(1 + \sum_1^n b_j C_j^0)X_i^{\ddagger}}{1 + \sum_1^n b_j C_j^0 X_j^{\ddagger}} \tag{4A}$$

as shown by Hsieh et al. Equation (4A) can be solved for $X_i^{\ddagger}$ in terms of $Y_i^{\ddagger}$

$$X_i^{\ddagger} = \frac{C_i^{\ddagger}}{C_i^0} = \frac{Y_i^{\ddagger}}{1 + \sum_1^n b_j C_j^0 (1 - Y_j^{\ddagger})} \tag{4B}$$

Introduce the dimensionless length and time variables, h and θ, the normalized continuity equations become

$$\frac{\partial X_i}{\partial h_i} + \frac{\partial Y_i}{\partial \theta_i} = 0, \quad \text{for } i = 1, 2, 3, \ldots, n \tag{5}$$

The normalized rate equations for either liquid phase rate controlling or solid phase rate controlling ion exchange are

$$\frac{\partial Y_i}{\partial \theta_{li}} = X_i - X_i^*, \quad \text{for } i = 1, 2, 3, \dots, n \quad (6)$$

$$\frac{\partial Y_i}{\partial \theta_{si}} = Y_i^* - Y_i, \quad \text{for } i = 1, 2, 3, \dots, n \quad (7)$$

The normalized rate equations for combined liquid phase and solid phase rate controlling are

$$\frac{\partial Y_i}{\partial \theta'_{li}} = X_i - X_i^\ddagger, \quad \text{for } i = 1, 2, 3, \dots, n \quad (8)$$

$$\frac{\partial Y_i}{\partial \theta'_{si}} = Y_i^\ddagger - Y_i, \quad \text{for } i = 1, 2, 3, \dots, n \quad (9)$$

The dimensionless length and time variables are defined according to the rate controlling mechanism. For liquid phase rate controlling

$$h_{li} = \frac{K_{li} Z}{V}, \quad \theta_{li} = \frac{K_{li} G}{\rho a_i}(t - \beta Z/V)$$

where $G = 1 + \sum_1^n b_j C_j^0$.

For solid phase rate controlling

$$h_{si} = \frac{K_{si} a_i \rho Z}{VG}, \quad \theta_{si} = K_{si}(t - \beta Z/V)$$

For combined liquid and solid phase rate controlling

$$h'_{li} = \frac{k_{li} Z}{V}, \quad \theta'_{li} = \frac{k_{li} G}{\rho a_i}(t - \beta Z/V)$$

$$h'_{si} = \frac{k_{si} a_i \rho Z}{VG}, \quad \theta'_{si} = k_{si}(t - \beta Z/V)$$

To solve Eqs. (5)–(9), appropriate initial and boundary conditions should also be specified. The most general initial and boundary conditions are

$$X_i(0, \theta_i) = f(\theta_i) \quad \text{and} \quad Y_i(h_i, 0) = g(h_i)$$

They correspond to time dependent feed concentration and arbitrary initial bed composition. The common cases of zero or uniform presaturation and constant uniform feed composition are special cases of the above conditions and are defined by $Y_i(h_i, 0) = 0$ or $Y_i(h_i, 0) = Y_i^0$ and $X_i(0, \theta_i) = 1$.

Development of Numerical Algorithms

Algorithms are developed for the numerical solution of Eqs. (5)–(9). Index I and J designate the grid location for characteristic coordinates of h and θ respectively. The characteristic coordinates (I, J) refer to the current points whose X and Y values are to be calculated. $(I - 1, J)$ or $(I, J - 1)$ are grid points whose X and Y values are given or previously calculated. In particular, values of X and Y at $(I, 1)$ correspond to the initial values defined or calculated for characteristics line $\theta = 0$. Similarly, values of X and Y at $(1, J)$ correspond to boundary conditions given or to be calculated for characteristic line $h = 0$. Modified Euler's method is applied for the calculation of $X(I, 1)$, $Y(1, J)$ and the interior points of $X(I, J)$ and $Y(I, J)$. Because of the similarity of the methods used in deriving separate algorithms for liquid phase rate control, solid phase rate control and combined liquid and solid phase rate control, only the details of development of algorithms for the combined liquid and solid phase rate control are presented here. Algorithms for solid phase and liquid phase rate control are given in Appendices 1 and 2.

The following gives the derivation of algorithms for combined liquid and solid phase rate controlling.

(a) Calculation of X_i for Characteristic Line $\theta = 0$

The values of $X_i(I, 1)$ for $I = 2, 3, 4, \dots, m$, where $m - 1$ is the number of length increments, are determined by applying modified Euler's method to

$$\left.\frac{dX_i}{dh'_{li}}\right|_{\theta'_{li}=0} = X_i^\ddagger - X_i,$$

$$\frac{X_i(I,1) - X_i(I-1,1)}{\Delta h'_{li}} = \frac{X_i^\ddagger(I,1) + X_i^\ddagger(I-1,1)}{2} - \frac{X_i(I,1) + X_i(I-1.1)}{2} \quad (10)$$

solving for $X_i(I, 1)$

$$X_i(I,1) = \left(\frac{2 - \Delta h'_{li}}{2 + \Delta h'_{li}}\right) X_i(I-1,1) + \left(\frac{\Delta h'_{li}}{2 + \Delta h'_{li}}\right)[X_i^\ddagger(I,1) + X_i^\ddagger(I-1,1)]$$

$$\text{for } i = 1, 2, 3, \dots, n \quad (11)$$

From the interphase relationship of

$$X_i(I,1) - X_i^{\ddagger}(I,1) = R_i[Y_i^{\ddagger}(I,1) - Y_i(I,1)] \quad (12)$$

where R_i is the ratio of solid phase to liquid phase rate constants for species i in which

$$R_i = \frac{k_{si}\rho a_i}{k_{li}\left(1+\sum b_j C_j^0\right)} = \frac{h'_{si}}{h'_{li}}$$

Eliminating $X_i(I,1)$ from Eqs. (11) and (12) and after simplifying

$$X_i^{\ddagger}(I,1) - \frac{2+\Delta h'_{li}}{2}F_i = -\frac{2+\Delta h'_{li}}{2}R_i Y_i^{\ddagger}(I,1) \quad \text{for } i = 1,2,3,\ldots,n \quad (13)$$

where

$$F_i = \left(\frac{2-\Delta h'_{li}}{2+\Delta h'_{li}}\right)X_i(I-1,1) + \left(\frac{\Delta h'_{li}}{2+\Delta h'_{li}}\right)X_i^{\ddagger}(I-1,1) + R_i Y_i(I,1)$$

let k denote a reference species, from Eq. (13)

$$\frac{[2/(2+\Delta h'_{li})]X_i^{\ddagger}(I,1) - F_i}{[2/(2+\Delta h'_{lk})]X_k^{\ddagger}(I,1) - F_k} = \frac{R_i Y_i^{\ddagger}(I,1)}{R_k Y_k^{\ddagger}(I,1)} \quad (14)$$

Substituting equilibrium values of $X_i^{\ddagger}(I,1)$ and $X_k^{\ddagger}(I,1)$ for $Y_i^{\ddagger}(I,1)$ and $Y_k^{\ddagger}(I,1)$ and after simplification

$$X_i^{\ddagger}(I,1) = \frac{(F_i/F_k)(R_k/R_i)X_k^{\ddagger}(I,1)}{1 + \frac{2}{(2+\Delta h'_{lk})F_k}\left\{\frac{R_k(2+\Delta h'_{lk})}{R_i(2+\Delta h'_{li})} - 1\right\}X_k^{\ddagger}(I,1)} \quad \text{for } i = 1,2,3,\ldots,n, \quad i \neq k \quad (15)$$

This equation relates the equilibrium value of i species to that of a reference species k.

From Eq. (13), solving for the reference species k and substituting $X_k^{\ddagger}(I,1)$ in terms of $Y_k^{\ddagger}(I,1)$

$$X_k^{\ddagger}(I,1) - \frac{2+\Delta h'_{lk}}{2}F_k + R_k\left(\frac{2+\Delta h'_{lk}}{2}\right)\frac{\left(1+\sum b_j C_j^0\right)X_k^{\ddagger}(I,1)}{1+\sum b_j C_j^0 X_j^{\ddagger}(I,1)} = 0 \quad (16)$$

From Eq. (15), the summation terms in Eq. (16) can be expressed as a function of $X_k^{\ddagger}(I,1)$. Thus Eq. (16) is a nonlinear equation with a single variable, namely $X_k^{\ddagger}(I,1)$. Equation (16) can then be solved by Newton-Raphson iteration method to obtain the value of $X_k^{\ddagger}(I,1)$. After $X_k^{\ddagger}(I,1)$ is determined, other values of $X_i^{\ddagger}(I,1)$ are then calculated from Eq. (15). The values of $Y_i^{\ddagger}(I,1)$ are determined from the equilibrium isotherm.

The values of $X_i(I,1)$ for $I = 2,3,4,\ldots,m$ are then calculated from Eq. (11). It should be noted that in calculating $X_i(2,1)$, we need to know $X_i(1,1)$, $Y_i(1,1)$ and $X_i^{\ddagger}(1,1)$ in order to obtain the value for F_i. The values of $X_i(1,1)$ and $Y_i(1,1)$ correspond to boundary condition and initial condition respectively and are specified. The values of $X_i^{\ddagger}(1,1)$ are calculated by using the interphase relationship of

$$X_i(1,1) - X_i^{\ddagger}(1,1) = R_i[Y_i^{\ddagger}(1,1) - Y_i(1,1)] \quad (17)$$

Using the equilibrium relationship and substituting the value of $Y_i^{\ddagger}(1,1)$ in terms $X_i^{\ddagger}(1,1)$ in Eq. (17) and after simplifying

$$X_i^{\ddagger}(1,1) - p_i = -R_i\frac{\left(1+\sum b_j C_j^0\right)X_i^{\ddagger}(1,1)}{1+\sum b_j C_j^0 X_j^{\ddagger}(1,1)} \quad \text{for } i = 1,2,3,\ldots,n \quad (18)$$

where $p_i = X_i(1,1) + R_i Y_i(1,1)$.

For a reference species k, Eq. (18) becomes

$$X_k^{\ddagger}(1,1) - p_k = -R_k\frac{\left(1+\sum b_j C_j^0\right)X_k^{\ddagger}(1,1)}{1+\sum b_j C_j^0 X_j^{\ddagger}(1,1)} \quad (19)$$

Dividing Eq. (18) by Eq. (19) and simplifying:

$$X_i^{\ddagger}(1,1) = \frac{(p_i/p_k)(R_k/R_i)X_k^{\ddagger}(1,1)}{1+\frac{1}{p_k}(R_k/R_i - 1)X_k^{\ddagger}(1,1)} \quad (20)$$

By substituting Eq. (20) to Eq. (19), a nonlinear equation with a single variable in terms of $X_k^{\ddagger}(1,1)$ can be solved by Newton-Raphson method. The values of $X_i^{\ddagger}(1,1)$ other than $X_k^{\ddagger}(1,1)$ are calculated from Eq. (20) once $X_k^{\ddagger}(1,1)$ is determined.

(b) Calculation of Y_i for Characteristics Line $h = 0$

Applying modified Euler's method to

$$\left.\frac{dY_i}{d\theta'_{si}}\right|_{h=0} = Y_i^{\ddagger} - Y_i$$

$$Y_i(1, J) = \left(\frac{2 - \Delta\theta'_{si}}{2 + \Delta\theta'_{si}}\right) Y_i(1, J-1) + \left(\frac{\Delta\theta'_{si}}{2 + \Delta\theta'_{si}}\right) \times [Y_i^{\ddagger}(1, J-1) + Y_i^{\ddagger}(1, J)] \quad \text{for } i = 1, 2, 3, \ldots, n \tag{21}$$

combining with the interphase relationship of

$$X_i(1, J) - X_i^{\ddagger}(1, J) = R_i[Y_i^{\ddagger}(1, J) - Y_i(1, J)]$$

to eliminate $Y_i(1, J)$

$$X_i^{\ddagger}(1, J) - F_i = -\frac{2R_i}{2 + \theta'_{si}} Y_i^{\ddagger}(1, J) \quad \text{for } i = 1, 2, 3, \ldots, n \tag{22}$$

where

$$F_i = R_i\left[\left(\frac{2 - \Delta\theta'_{si}}{2 + \Delta\theta'_{si}}\right) Y_i(1, J-1) + \left(\frac{\Delta\theta'_{si}}{2 + \Delta\theta'_{si}}\right) Y_i^{\ddagger}(1, J-1)\right] + X_i(1, J)$$

The relationship of $Y_i^{\ddagger}(1, J)$ to a reference species k is given by

$$X_i^{\ddagger}(1, J) = \frac{A_{ik} X_k^{\ddagger}(1, J)}{1 + B_{ik} X_k^{\ddagger}(1, J)}, \quad \text{for } i = 1, 2, 3, \ldots, n, \quad i \neq k \tag{23}$$

where

$$A_{ik} = \frac{F_i(2 + \Delta\theta'_{si}) R_k}{F_k(2 + \Delta\theta'_{sk}) R_i},$$

$$B_{ik} = \frac{1}{F_k}\left[\frac{(2 + \Delta\theta'_{si}) R_k}{(2 + \Delta\theta'_{sk}) R_i} - 1\right]$$

Substituting $X_k^{\ddagger}(1, J)$ for $Y_i^{\ddagger}(1, J)$ from the equilibrium relationship and solving for the reference species k, Eq. (22) becomes

$$X_k^{\ddagger}(1, J) - F_k + \frac{2R_k}{2 + \theta'_{sk}} \frac{\left(1 + \sum b_i C_i^0\right) X_k^{\ddagger}(1, 1)}{1 + \sum b_i C_i^0 X_i^{\ddagger}(1, J)} = 0 \tag{24}$$

After substituting the value $X_i^{\ddagger}(1, J)$ as defined by Eq. (23) to Eq. (24), a nonlinear equation with a single variable of $X_k^{\ddagger}(1, J)$ can again be solved by Newton-Raphson method. Once the value of $X_k^{\ddagger}(1, J)$ is obtained, other values of $X_i^{\ddagger}(1, J)$ are calculated from Eq. (23) directly. With the values of $Y_i^{\ddagger}(1, J)$ determined from equilibrium relationship, the values of $Y_i(1, J)$ are then calculated from Eq. (21).

(c) Calculation of Values of X_i and Y_i at Interior Points

Applying modified Euler's method to

$$\frac{\partial X}{\partial h'_{li}} = X_i^{\ddagger}(1, J) - X_i$$

$$X_i(I, J) = \left(\frac{2 - \Delta h'_{li}}{2 + \Delta h'_{li}}\right) X_i(I-1, J) + \left(\frac{\Delta h'_{li}}{2 + \Delta h'_{li}}\right) [X_i^{\ddagger}(I, J) + X_i^{\ddagger}(I-1, J)] \quad \text{for } i = 1, 2, 3, \ldots, n \tag{25}$$

and applying modified Euler's method to

$$\frac{\partial Y_i}{\partial \theta'_{si}} = Y_i^{\ddagger} - Y_i$$

$$Y_i(I, J) = \left(\frac{2 - \Delta\theta'_{si}}{2 + \Delta\theta'_{si}}\right) Y_i(I, J-1) + \left(\frac{\Delta\theta'_{si}}{2 + \Delta\theta'_{si}}\right) [Y_i^{\ddagger}(I, J-1) + Y_i^{\ddagger}(I, J)] \quad \text{for } i = 1, 2, 3, \ldots, n. \tag{26}$$

Substituting the values of $X_i(I, J)$ of Eq. (25) and $Y_i(I, J)$ of Eq. (26) to the solid-liquid interface relation of

$$X_i(I, J) - X_i^{\ddagger}(I, J) = R_i[Y_i^{\ddagger}(I, J) - Y_i(I, J)]$$

After simplification

$$X_i^{\ddagger}(I, J) - F_i + R_i\left[\frac{(2 + \Delta h'_{li})}{(2 + \Delta\theta'_{si})}\right] Y_i^{\ddagger}(I, J) = 0 \tag{27}$$

where

$$F_i = \left[\left[\left(\frac{2-\Delta h'_{li}}{2+\Delta h'_{li}}\right)X_i(I-1,J) + \left(\frac{\Delta h'_{li}}{2+\Delta h'_{li}}\right)X_i^{\ddagger}(I-1,J)\right] + R_i\left[\left(\frac{2-\Delta\theta'_{si}}{2+\Delta\theta'_{si}}\right)Y_i(I,J-1) + \left(\frac{\Delta\theta'_{si}}{2+\Delta\theta'_{si}}\right)Y_i^{\ddagger}(I,J-1)\right]\right]\left(\frac{2+\Delta h'_{li}}{2}\right)$$

From Eq. (27), the relationship between $X_i^{\ddagger}(I,J)$ and $X_k^{\ddagger}(I,J)$ is

$$X_i^{\ddagger}(I,J) = \frac{A_{ik}X_k^{\ddagger}(I,J)}{1+X_{ik}Y_k^{\ddagger}(I,J)}, \quad \text{for } i = 1,2,3,\ldots,n, \quad i \neq k \quad (28)$$

where

$$A_{ik} = \frac{F_i(2+\Delta\theta'_{si})(2+\Delta h'_{lk})R_k}{F_k(2+\Delta\theta'_{sk})(2+\Delta h'_{li})R_i},$$

$$B_{ik} = \left(\left[\frac{(2+\Delta\theta'_{si})(2+\Delta h'_{lk})R_k}{(2+\Delta\theta'_{sk})(2+\Delta h'_{li})R_i} - 1\right]\right)\left(\frac{1}{F_k}\right)$$

Solving for $i = k$ in Eq. (27) and substituting $Y_k^{\ddagger}(I,J)$ in terms of $X_k^{\ddagger}(I,J)$

$$X_k^{\ddagger}(I,J) - F_k + R_k\left[\frac{(2+\Delta h'_{lk})}{(2+\Delta\theta'_{sk})}\right]\frac{\left[1+\sum b_j C_j^0\right]X_k^{\ddagger}}{1+\sum b_i C_i^0 X_i^{\ddagger}} = 0 \quad (29)$$

Again by combining Eqs. (28) and (29), a nonlinear equation with a variable in terms of $X_k^{\ddagger}(I,J)$ can be solved by Newton-Raphson method. After $X_k^{\ddagger}(I,J)$ is obtained, values of $X_i^{\ddagger}(I,J)$ are calculated from Eq. (28), all the $Y_i^{\ddagger}(I,J)$ values are determined from equilibrium relationship. With the known values of $X_i^{\ddagger}(I,J)$ and $Y_i^{\ddagger}(I,J)$, $X_i(I,J)$ and $Y_i(I,J)$ are then calculated from Eqs. (25) and (26).

Numerical Examples

The model equations and the algorithms developed were applied to three numerical examples studied by Hsieh et al. (1977). These examples covered liquid phase, solid phase and combined solid and liquid phase rate control. Table 1 summarizes the data used for the calculation. Since no analytic solutions are available,

Table 1. Data used for the numerical calculations of multicomponent liquid phase adsorption in fixed bed.

Example for liquid phase rate controlling, 3 component system			
$V = 0.00227164$ m/s,	$L = 0.3429$ m,	$\rho = 0.39$ g/l	
$K_{l1} = 140$/hr,	$K_{l2} = 120$/hr,	$K_{l3} = 100$/hr	
$a_1 = 40$ l/g,	$a_2 = 30$ l/g,	$a_3 = 20$ l/g	
$b_1 = 0.05$ l/μmole,	$b_2 = 0.03$ l/μmole,	$b_3 = 0.01$ l/μmole	
$C_1^0 = 20$ μmole/l,	$C_2^0 = 15$ μmole/l,	$C_3^0 = 10$ μmole/l	
Example for combined solid and liquid phase rate controlling, 2 component system			
$V = 0.00227164$ m/s,	$L = 0.0509$ m,	$\rho = 0.39$ g/l	
$k_{l1} = 2671$/hr,	$k_{l2} = 1869$/hr		
$k_{s1} = 0.246$/h	$k_{s2} = 0.405$/hr		
$b_1 = 0.14$ l/μmole,	$b_2 = 0.06$ l/μmole		
$C_1^0 = 110$ μmole/l,	$C_2^0 = 300$ μmole/l		
$a_1 = 198.8$ l/g	$a_2 = 54.3$ l/g		
Example for solid phase rate controlling, 4 component system			
$V = 0.00227164$ m/s,		$L = 0.763$ m,	$\rho = 0.39$ g/l
$K_{s1} = 0.1103$/hr	$K_{s2} = 0.1050$/hr	$K_{s3} = 0.1016$/hr	$K_{s4} = 0.0563$/hr
$a_1 = 45.1$ l/g,	$a_2 = 3.4$ l/g,	$a_3 = 3.2$ l/g	$a_4 = 2.1$ l/g
$b_1 = 0.28$ l/μmole,	$b_2 = 0.007$ l/μmole,	$b_3 = 0.003$ l/μmole	$b_4 = 0.002$ l/μmole
$C_1^0 = 4.6$ μmole/l,	$C_2^0 = 41.6$ μmole/l,	$C_3^0 = 33.3$ μmole/l	$C_4^0 = 166.5$ μmole/l

the numerical results obtained are assumed to be correct when further increased in number of increments has negligible effects on the outcome of computation. An integral mass balance for various sorption species was also incorporated into the numerical programs as an independent check on the accuracy of the numerical algorithms. The effluent i species concentration was integrated numerically by Simpson's rule and checked against the average bed composition for the given species at a given time, t. An overall mass balance for the entire column at time t gives

$$V\left[C_i^0 t - \int_0^t C_i(L,t)\,dt = \rho \int_0^L Q_i(Z,t)\,dZ\right]$$

To check the accuracy of this overall mass balance we define

$$\epsilon_i(t) = 1 - \frac{V\left[C_i^0 t - \int_0^t C_i(L,t)\,dt\right]}{\rho \int_0^L Q_i(Z,t)\,dz}$$

The calculated results for the breakthroughs of a three component liquid phase rate controlling system are tabulated in Table 2. A typical solid phase composition profile is depicted in Fig. 1. In this example the values of the rate parameters for the three individual components are very close to each other. The same is true for the values of the equilibrium parameters. The calculated total dimensionless length parameters are 4.91, 4.21 and 3.51 for components 1, 2 and 3 respectively. As can be seen from the tabulation in Table 2, with only fifty length increments, up to three significant figure of accuracy is obtained. The absolute values of $\epsilon(t)$ determined from performing an overall mass balance are found to be less than 0.005 at various values of t. In Table 3, the results of breakthroughs for a two component combined film and solid phase rate controlling system are tabulated. Figure 2 shows the bed composition and the solid particle surface composition profiles at $t = 3$ hours. As can be seen from the tabulation in Table 3, with 200 length increments and with

Table 2. Calculated results of breakthroughs for a three component liquid phase rate controlling system.

	$L/\Delta L = 50$, $\Delta t = 4$ hr			$L/\Delta L = 100$, $\Delta t = 2$ hr			$L/\Delta L = 200$, $t = 1$ hr		
hr	X_1	X_2	X_3	X_1	X_2	X_3	X_1	X_2	X_3
20	0.01527	0.03021	0.06164	0.01530	0.03024	0.06167	0.01530	0.03025	0.06168
40	0.02675	0.05171	0.10415	0.02678	0.05173	0.10417	0.02678	0.05174	0.10418
60	0.04302	0.08105	0.15939	0.04304	0.08107	0.15940	0.04305	0.08107	0.15940
80	0.06550	0.11996	0.22863	0.06552	0.11997	0.22863	0.06552	0.11997	0.22862
100	0.09586	0.17027	0.31272	0.09588	0.17026	0.31270	0.09588	0.17026	0.31270
120	0.13611	0.23385	0.41196	0.13612	0.23384	0.41193	0.13612	0.23384	0.41193
140	0.18837	0.31233	0.52548	0.18836	0.31230	0.52546	0.18836	0.31229	0.52545
160	0.25453	0.40636	0.65049	0.25451	0.40632	0.65047	0.25450	0.40632	0.65046
180	0.33556	0.51473	0.78129	0.33552	0.51469	0.78128	0.33551	0.51468	0.78128
200	0.43029	0.63302	0.90854	0.43025	0.63299	0.90857	0.43024	0.63299	0.90857
220	0.53413	0.75261	1.01955	0.53410	0.75262	1.01961	0.53409	0.75262	1.01962
240	0.63847	0.86120	1.10098	0.63846	0.86123	1.10105	0.63845	0.86124	1.10106
260	0.73253	0.94653	1.14461	0.73253	0.94657	1.14465	0.73253	0.94658	1.14465
280	0.80807	1.00246	1.15283	0.80807	1.00248	1.15282	0.80807	1.00248	1.15282
300	0.86319	1.03183	1.13748	0.86319	1.03184	1.13743	0.86319	1.03184	1.13742
320	0.90133	1.04289	1.11215	0.90132	1.04288	1.11210	0.90132	1.04287	1.11209
340	0.92751	1.04373	1.08618	0.92751	1.04372	1.08614	0.92751	1.04372	1.08613
360	0.94585	1.03987	1.06385	0.94585	1.03986	1.06382	0.94585	1.03986	1.06381
380	0.95907	1.03435	1.04626	0.95907	1.03434	1.04624	0.95907	1.03433	1.04624
400	0.96884	1.02864	1.03306	0.96884	1.02863	1.03305	0.96884	1.02863	1.03305
420	0.97619	1.02339	1.02342	0.97619	1.02339	1.02341	0.97619	1.02339	1.02341
440	0.98179	1.01884	1.01650	0.98179	1.01884	1.01650	0.98179	1.01883	1.01650
460	0.98607	1.01502	1.01159	0.98607	1.01501	1.01159	0.98607	1.01501	1.01159
480	0.98935	1.01187	1.00813	0.98935	1.01187	1.00812	0.98935	1.01187	1.00812
500	0.99187	1.00932	1.00569	0.99187	1.00932	1.00569	0.99188	1.00932	1.00569

Table 3. Calculated results of breakthroughs for a two component combined liquid phase rate controlling system.

	$L/\Delta L = 100$ $\Delta t = 0.5$ hr		$L/\Delta L = 201$ $\Delta t = 0.20$ hr		$L/\Delta L = 400$ $\Delta t = 0.1$ hr	
hr	X_1	X_2	X_1	X_2	X_1	X_2
1	0.00165	0.03149	0.00165	0.03152	0.00165	0.03152
2	0.01213	0.14365	0.01216	0.14424	0.01216	0.14432
3	0.05327	0.38929	0.05337	0.39042	0.05339	0.39058
4	0.11970	0.61445	0.11976	0.61496	0.11977	0.61503
5	0.19399	0.77258	0.19400	0.77261	0.19400	0.77261
6	0.26812	0.87781	0.26810	0.87758	0.26810	0.87754
7	0.33879	0.94598	0.33876	0.94565	0.33876	0.94560
8	0.40471	0.98902	0.40469	0.98867	0.40469	0.98862
9	0.46552	1.01523	0.46552	1.01490	0.46552	1.01486
10	0.52126	1.03032	0.52126	1.03003	0.52127	1.02999
11	0.57212	1.03813	0.57214	1.03790	0.57214	1.03787
12	0.61839	1.04128	0.61842	1.04109	0.61842	1.04106
13	0.66037	1.04149	0.66040	1.04134	0.66041	1.04132
14	0.69835	1.03993	0.69838	1.03981	0.69838	1.03979
15	0.73262	1.03736	0.73265	1.03727	0.73265	1.03726
16	0.76345	1.03429	0.76348	1.03422	0.76348	1.03421
17	0.79113	1.03104	0.79115	1.03099	0.79115	1.03098
18	0.81590	1.02780	0.81592	1.02777	0.81592	1.02776
19	0.83802	1.02471	0.83803	1.02469	0.83803	1.02468
20	0.85771	1.02184	0.85772	1.02182	0.85772	1.02181
21	0.87521	1.01920	0.87521	1.01919	0.87521	1.01919
22	0.89072	1.01682	0.89071	1.01681	0.89071	1.01681
23	0.90443	1.01468	0.90442	1.01468	0.90442	1.01468
24	0.91654	1.01279	0.91652	1.01279	0.91652	1.01279
25	0.92720	1.01111	0.92718	1.01111	0.92718	1.01111
26	0.93657	1.00964	0.93656	1.00964	0.93659	1.00964
27	0.94480	1.00835	0.94479	1.00835	0.94478	1.00835
28	0.95202	1.00722	0.95200	1.00723	0.95200	1.00723
29	0.95833	1.00624	0.95831	1.00624	0.95831	1.00625
30	0.96384	1.00539	0.96382	1.00539	0.96382	1.00539

Δt set equal to 0.2 hour, convergence to within four significant figure is approached. The values of $\epsilon_i(t)$ calculated for this example are less than 0.01 for most values of t and for any species i.

The last example illustrates a four component solid phase rate control system. The data listed in Table 1 indicate that species 1 is a much preferred species than the other three components. The calculated values for the separation factors are $\alpha_2^1 = 13.3, \alpha_3^1 = 14.1$ and $\alpha_4^1 = 21.5$. Thus it is expected that the breakthroughs for species 1 is to come much later than the breakthroughs for species 2, 3 and 4. Table 4 gives breakthrough data for components 1 to 4. It is seen that with 50 and 100 increments almost the same effluent concentration histories are obtained for components 2, 3 and 4. However for component 1, at least 100 or more length increments are needed for obtaining correct concentration history especially for the early breakthroughs. The overall mass balance calculation for this example gives $\epsilon_i(t)$ values less than 0.005 when 200 length increments are used. Figure 3 is a typical bed composition profile at $t = 20$ hours. The proximity of the bed composition profiles between components 2 and 3 is due to fact that the equilibrium and kinetic

Table 4. Calculated results of breakthroughs for a four component solid phase rate controlling system.

	$L/\Delta L = 50$, $\Delta t = 1$ hr			$L/\Delta L = 100$, $\Delta t = 1$ hr				$L/\Delta L = 100$ $\Delta t = 1$ hr	$L/\Delta L = 200$ $\Delta t = 1$ hr
hr	X_2	X_3	X_4	X_2	X_3	X_4	hour	X_1	X_1
5	0.00133	0.00243	0.09713	0.00134	0.00244	0.09714	300	0.00001	0.00001
10	0.00561	0.00921	0.16169	0.00564	0.00924	0.16169	320	0.00003	0.00004
15	0.01585	0.02399	0.23604	0.01588	0.02402	0.23602	340	0.00018	0.00021
20	0.03562	0.05050	0.31727	0.03566	0.05053	0.31725	360	0.00097	0.00106
25	0.06841	0.09181	0.40197	0.06845	0.09182	0.40195	380	0.00503	0.00523
30	0.11652	0.14923	0.48657	0.11652	0.14922	0.48654	400	0.02480	0.02530
35	0.18012	0.22170	0.56775	0.18010	0.22166	0.56773	420	0.10682	0.10671
40	0.25705	0.30582	0.64287	0.25700	0.30576	0.64286	440	0.32378	0.32242
45	0.34319	0.39668	0.71018	0.34312	0.39660	0.71018	460	0.60884	0.60822
50	0.43352	0.48896	0.76885	0.43344	0.48889	0.76885	480	0.81408	0.81431
55	0.52317	0.57796	0.81880	0.52309	0.57790	0.81881	500	0.91988	0.92025
60	0.60816	0.66019	0.86055	0.60810	0.66014	0.86056	520	0.96691	0.96718
65	0.68575	0.73350	0.89492	0.68571	0.73347	0.89493	540	0.98659	0.98674
70	0.75442	0.79698	0.92289	0.75439	0.79697	0.92291	560	0.99461	0.99469
75	0.81366	0.85063	0.94546	0.81365	0.85063	0.94548	580	0.99785	0.99788
80	0.86369	0.89508	0.96355	0.86369	0.89509	0.96357	600	0.99914	0.99916
100	0.98838	1.00144	1.00587	0.98841	1.00147	1.00588	620	0.99966	0.99966
200	1.06169	1.05763	1.03534	1.06169	1.05763	1.03534	640	0.99986	0.99986
300	1.06160	1.05748	1.03599	1.06160	1.05748	1.03599	660	0.99994	0.99994
400	1.0602	1.05622	1.03544	1.06010	1.05610	1.03537	680	0.99997	0.99996
500	1.00514	1.00491	1.00516	1.00505	1.00482	1.00513	700	0.99998	0.99997
600	1.00006	1.00006	1.00009	1.00005	1.00005	1.00009	800	0.99999	0.99998

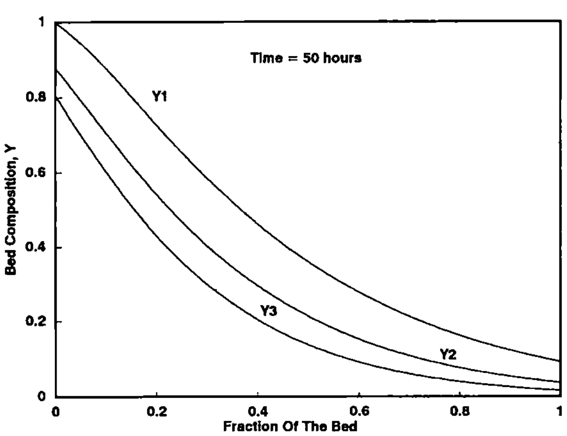

Figure 1. Bed composition profile for a three component liquid phase rate controlling system.

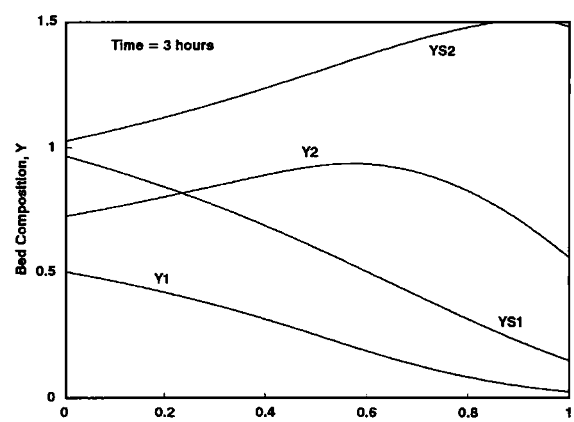

Figure 2. Bed composition and particle surface composition profile for a two component combined liquid and solid phase rate controlling system.

parameters of these two species are very close to each other. For engineering and other practical application, usually only three of four significant figures in the calculated results are required. In all these three examples of calculation, about 50 to 200 increments are sufficient to obtain this kind of accuracy. The numerical algorithms developed in this work are easy to implement using a 386 or 486 PC. All these sample calculations are

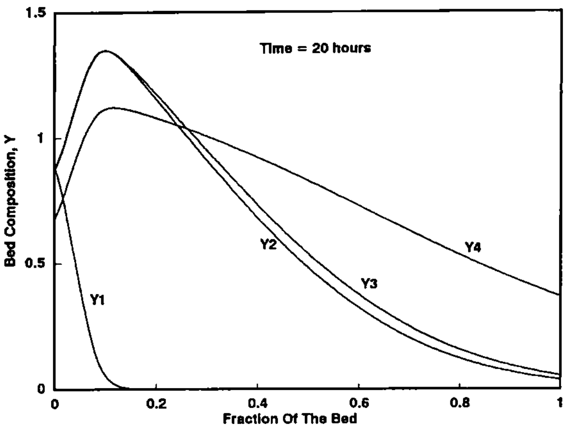

Figure 3. Bed composition profile for a four component solid phase rate controlling system.

carried out with a 486 DX2–66 PC and with programs written in Fortran. The computation time for each run is about a few seconds to less than half a minute.

Conclusions

In this paper, new and efficient algorithms are developed for the calculation of fixed bed multicomponent liquid phase adsorption. Langmuir form of isotherm is assumed for the multicomponent system. Linear driving force rate equations are employed in the model equations and algorithms are developed for the three rate controlling mechanisms. The numerical algorithms developed in this work are explicit with the exception of the requirement for solving an implicit polynomial equation for one of the species in the multicomponent system. This polynomial equation arises because of the interaction of multicomponent equilibrium relationship. Once the concentration of this arbitrarily chosen species is determined, concentrations of other species are obtained explicitly and directly. In this way the algorithms are more efficient than solving simultaneous multiple nonlinear equations by iterative procedure or by the use of predictor-corrector methods. The usefulness of equilibrium theory for analyzing multicomponent liquid adsorption processes is well recognized. However, since most fixed bed sorption processes are conducted with finite mass transfer resistance, the rate effect should always be included for practical applications. We have shown by means of numerical examples how the developed algorithms can be utilized for such studies. We have demonstrated the accuracy and efficiency of the proposed algorithms with the calculated results check by an independent mass balance and with all the calculations carried out with a personal computer.

Nomenclature

- C Concentration of species i in the solution, mol/l
- h_i Dimensionless length variable for species i.
- H_i Dimensionless total length parameter for species i.
- k_{li} Liquid phase mass transfer coefficient for species i, 1/sec
- K_{li} Overall liquid phase mass transfer coefficient for species i, 1/sec
- k_{si} Solid phase mass transfer coefficient for species i, 1/sec
- K_{si} Overall solid phase mass transfer coefficient for species i, 1/sec
- L Total bed height, m
- Q_i Concentration of species i in the adsorbent, mol/g solid
- t Absolute time, second
- V Linear superficial flow rate, m/sec
- X_i Normalized liquid phase i species concentration
- Y_i Normalized liquid phase i species concentration
- Z Axial distance of the bed, m

Greek Letters

- β Void fraction of the bed, dimensionless
- θ Normalized time variable, dimensionless
- ρ_b Bulk density of adsorbent in the column, g solid/l

Superscripts

- 0 Feed or initial
- ‡ Interface equilibrium composition
- $*$ Equilibrium with respect to bulk solution or average solid composition

Appendices

Appendix 1: Algorithms for Film Diffusion Rate Controlling

1. Calculation of X_i for Characteristic Line $\theta = 0$

$$\left.\frac{dX_i}{dh_{li}}\right|_{\theta_{li}=0} = X_i^* - X_i$$

Since the initial conditions of $Y_i(h_i, 0)$ are known, the values of X_i^* can be determined readily from the equilibrium relation. Thus by the modified Euler's method, values of X_i are calculated explicitly by

$$X_i(I,1) = \frac{2-\Delta h_{li}}{2+\Delta h_{li}} X_i(I-1,1) + \frac{\Delta h_{li}}{2+\Delta h_{li}} [X_i^*(I,1) + X_i^*(I-1,1)] \tag{A1}$$

2. Calculation of Y_i for Characteristic Line $h = 0$

Applying modified Euler's method to

$$\left.\frac{dY_i}{d\theta_{li}}\right|_{h_{li}=0} = X_i - X_i^*$$

$$Y_i(1,J) = F_i - (\Delta\theta_{li}/2) X_i^*(1,J), \quad \text{for } i = 1,2,3,\ldots,n \tag{A2}$$

where

$$F_i = Y_i(1,J-1) + [X_i(1,J) + X_i(1,J-1) - X_i^*(1,J-1)](\Delta\theta_{li}/2)$$

From Eq. (A2), it can be shown that

$$Y_i(1,J) = \frac{A_{ik} Y_k(1,J)}{1 + B_{ik} Y_k(1,J)}, \quad \text{for } i = 1,2,3,\ldots,n, \quad i \neq k \tag{A3}$$

where

$$A_{ik} = \frac{F_i \Delta\theta_{lk}}{F_k \Delta\theta_{li}}, \quad B_{ik} = \left[\frac{\Delta\theta_{lk}}{\Delta\theta_{li}} - 1\right]\left(\frac{1}{F_k}\right)$$

Substituting the equilibrium relation of Eq. (A2) and solving for $i = k$

$$Y_k(1,J) - F_k + (\Delta\theta_{lk}/2) \frac{Y_k(1,J)}{1 + \sum_1^n b_i C_i^0 [1 - Y_i(1,J)]} = 0 \tag{A4}$$

Substituting Y_i in terms of Y_k as given by Eq. (A3)

$$Y_k(1,J) - F_k + (\theta_{lk}/2) \frac{Y_k(1,J)}{1 + \sum_1^n b_i C_i^0 \left[1 - \frac{A_{ik} Y_k(1,J)}{1 + B_{ik} Y_k(1,j)}\right]} = 0 \tag{A5}$$

This is a polynomial equation with a single variable $Y_k(1, J)$. An iteration procedure by Newton Raphson method is applied for its solution. Once the value of Y_k is obtained, the values of Y for species $i = 1, 2, 3, \ldots, n$, $i \neq k$, can be readily calculated from Eq. (A3).

3. Calculation of X_i and Y_i at Interior Points

Applying modified Euler's method to

$$\left.\frac{dX_i}{dh_{li}}\right|_{\theta_{li}} = X_i^* - X - i$$

and after simplifying

$$X_i(I,J) = \frac{\Delta h_{li}}{2+\Delta h_{li}} X_i^*(I,J) + \frac{2-\Delta h_{li}}{2+\Delta h_{li}} X_i(I-1,J) + \frac{\Delta h_{li}}{2+\Delta h_{li}} X_i^*(I-1,J) \quad \text{for } i = 1,2,3,\ldots,n \tag{A6}$$

Applying modified Euler's method to

$$\left.\frac{dY_i}{d\theta_{li}}\right|_{h_{li}} = X_i - X_i^*$$

and after simplifying

$$Y_i(I,J) - F_i + \frac{\Delta\theta_{li}}{2+\Delta h_{li}} X_i^*(I,J) = 0, \quad \text{for } i = 1,2,3,\ldots,n, \tag{A7}$$

where

$$F_i = Y_i(I,J-1) + \left(\frac{\Delta\theta_{li}}{2}\right) \times \left[\frac{2-\Delta h_{li}}{2+\Delta h_{li}} X_i(I-1,J) + \frac{\Delta h_{li}}{2+\Delta h_{li}} X_i^*(I-1,J) + X_i(I,J-1) - X_i^*(I,J-1)\right]$$

From Eq. (A7), it can be shown that

$$Y_i(I,J) = \frac{A_{ik} Y_k(I,J)}{1 + B_{ik} Y_k(I,J)}, \quad \text{for } i = 1,2,3,\ldots,n, \quad i \neq k \tag{A8}$$

where

$$A_{ik} = \frac{F_i (2+\Delta h_{li}) \Delta\theta_{lk}}{F_k (2+\Delta h_{lk}) \Delta\theta_{li}},$$

$$B_{ik} = \left[\frac{(2+\Delta h_{li})\Delta\theta_{lk}}{(2+\Delta h_{lk})\Delta\theta_{li}} - 1\right]\left(\frac{1}{F_k}\right)$$

Substituting the equilibrium relation as well as Eq. (A8) to Eq. (7) and solving for species k

$$Y_k(I,J) - F_k + \left(\frac{\Delta\theta_{lk}}{2+\Delta h_{lk}}\right) \times \frac{Y_k(I,J)}{1+\sum_1^n b_i C_i^0\left[1 - \frac{A_{ik}Y_k(I,J)}{1+B_{ik}Y_k(I,J)}\right]} = 0 \quad \text{(A9)}$$

This nonlinear equation with a single variable of $Y_k(I,J)$ can again be solved by Newton-Raphson method. After the value of $Y_k(I,J)$ is obtained, values of $Y_i(I,J)$ for $i = 1,2,3,\ldots,n$, $i \neq k$, are calculated from Eq. (A8). The values of $X_i^*(I,J)$ are obtained from equilibrium relationship. Finally the values of $X_i(I,J)$ are calculated from Eq. (A6).

Appendix 2: Algorithms for Solid Phase Rate Controlling

1. Calculation of X_i for Characteristic Line $\theta = 0$

Applying modified Euler's method to

$$\left.\frac{dX}{dh_{si}}\right|_{\theta=0} = Y_i - Y_i^*$$

Using the same procedure for deriving the combined liquid and solid phase rate control algorithm, the following equation is obtained

$$X_k(I,1) - F_k + (\Delta h_{sk}/2)\frac{\left(1+\sum_1^n b_i C_i^0\right)X_k(I,1)}{1+\sum_1^n b_i C_i^0\left[\frac{A_{ik}X_k(I,1)}{1+B_{ik}X_k(I,1)}\right]} = 0 \quad \text{(B1)}$$

$$X_i(I,1) = \frac{A_{ik}X_k(I,1)}{1+B_{ik}X_k(I,1)}, \quad \text{for } i = 1,2,3,\ldots,n, \quad i \neq k \quad \text{(B2)}$$

where

$$A_{ik} = \frac{F_i \Delta h_{sk}}{F_k \Delta h_{si}},$$

$$B_{ik} = \left(\frac{\Delta h_{sk}}{\Delta h_{si}} - 1\right)\left(\frac{1}{F_k}\right)$$

$$F_i = X_i(I-1,1) + \left(\frac{\Delta h_{si}}{2}\right)[Y_i(I,1) + Y_i(I-1,1)] - \left(\frac{\Delta h_{si}}{2}\right)Y_i^*(I-1,1)$$

2. Calculation of Y_i for Characteristics Line $h = 0$

Applying modified Euler's method to

$$\left.\frac{dY_i}{d\theta_{si}}\right|_{h=0} = Y_i^* - Y_i,$$

to obtain

$$Y_i(1,J) = \left(\frac{2-\Delta\theta_{si}}{2+\Delta\theta_{si}}\right)Y_i(1,J-1) + \left(\frac{\Delta\theta_{si}}{2+\Delta\theta_{si}}\right)[Y_i^*(1,J-1) + Y_i^*(1,J)] \quad \text{for } i = 1,2,3,\ldots,n \quad \text{(B3)}$$

3. Calculation of X_i and Y_i at Interior Points

Following the procedure for deriving the liquid phase rate controlling algorithm we obtain

$$X_k(I,J) - F_k + \left(\frac{\Delta h_{sk}}{2+\Delta\theta_{sk}}\right)\frac{\left(1+\sum_1^n b_i C_i^0\right)X_k(I,J)}{1+\sum_1^n b_i C_i^0\frac{A_{ik}X_i(I,J)}{1+B_{ik}X_1(I,J)}} = 0 \quad \text{(B4)}$$

$$X_i(I,J) = \frac{A_{ik}X_k(I,J)}{1+B_{ik}X_k(I,J)}, \quad \text{for } i = 1,2,3,\ldots,n, \quad i \neq k \quad \text{(B5)}$$

where

$$A_{ik} = \frac{F_i(2+\Delta\theta_{si})\Delta h_{sk}}{F_k(2+\Delta\theta_{sk})\Delta h_{si}},$$

$$B_{ik} = \left[\frac{(2+\Delta\theta_{si})\Delta h_{sk}}{(2+\Delta\theta_{sk})\Delta h_{si}} - 1\right]\left(\frac{1}{F_k}\right)$$

$$F_i = X_i(I-1,J) + \left(\frac{\Delta h_{si}}{2}\right)[Y_i(I-1,J) - Y_i^*(I-1,J)] + \left(\frac{\Delta h_{si}}{2}\right)\left[\left(\frac{2-\Delta\theta_{si}}{2+\Delta\theta_{si}}\right)Y_i(I,J) + \left(\frac{\Delta\theta_{si}}{2+\Delta\theta_{si}}\right)Y_i^*(I,J-1)\right]$$

With the values of $X_i(I,J)$ known, $Y_i^*(I,J)$ are determined from the equilibrium relation. Finally the values of $Y_i(I, J)$ are calculated by

$$Y_i(I, J) = \left[\left(\frac{2 - \Delta\theta_{si}}{2 + \Delta\theta_{si}}\right) Y_i(I, J - 1) + \left(\frac{\Delta\theta_{si}}{2 + \Delta\theta_{si}}\right)[Y_i^*(I, J - 1)] + Y_i^*(I, J)\right] \quad \text{for } i = 1, 2, 3, \ldots, n \qquad \text{(B6)}$$

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