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

Part II: Application of Numerical Methods

The numerical methods developed in Part I are applied to a number of important countercurrent processes. Examples involving simultaneous input disturbances, distributed disturbances, Langmuir isotherms, and nonlinear coupled boundary conditions are tested. These examples, if solved by previous methods, would have required interpolation or iterative procedures, but are solved efficiently and accurately by the explicit algorithms and coding sequence developed in Part I.

The solutions for a linear system are in excellent agreement with the analytic solution. Numerical solutions obtained from explicit algorithms based on a nonlinear rate expression also shows very good agreement with the analytic solutions of Thomas (1944) for a fixed bed process. In both cases good accuracy is obtained with as few as sixteen increments.

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SCOPE

The methods and algorithms developed in Part I are expected to be efficient and accurate because of their noniterative nature and the absence of internal interpolation. Nevertheless, it is desirable to test the accuracy and efficiency of the proposed methods against an analytic solution. The only analytic solution for a countercurrent heat or mass transfer system is that of Jaswon and Smith (1954) for a linear driving force rate equation with a linear isotherm. A countercurrent heat exchanger to which a step input disturbance is applied is used to check the accuracy and efficiency of the basic numerical method. The ease of extending the algorithms for a linear system is illustrated by the use of time dependent input changes, step flow rate changes and the inclusion of a stationary accumulating phase. The flexibility of the basic method is further demonstrated by applying the method of Part I for simultaneous disturbances to a packed column absorber with a linear isotherm.

The algorithms developed for a countercurrent system with a Langmuir isotherm are tested for accuracy by comparing a numerical solution to an analytic solution (Thomas, 1944) for a second-order kinetic model for a fixed-bed sorption process.

The straightforward extension of the methods of Part I is illustrated by application to a batch distillation with packed column rectification. The application for this system involves the use of the method for a step flow rate (reflux ratio) change together with the application of algorithms derived for Langmuir isotherms. This distillation example also serves to illustrate the simple method of handling coupled boundary conditions that arise because of the reboiler and overhead conditions. The possible errors due to the often used assumption of negligible vapor holdup are examined by comparison to the more accurate model without this assumption.

CONCLUSIONS AND SIGNIFICANCE

The proposed noniterative numerical algorithm using a characteristic grid gives results that agree with the analytic solution for a countercurrent heat exchanger to less than 0.1% relative error for an increment size as large as 0.1 of the normalized total length parameter. The computation time required for obtaining this level of accuracy is about 0.2 s for 1,024 values of both cold and hot fluid temperature, less than about 2% of the time required for evaluating the analytic solution on the same computer (IBM 370/165II). Comparison between an analytic solution for a nonlinear fixed-bed process and an explicit numerical solution based on algorithms derived in Appendix

3 of Part I also shows agreement to within three to five significant figures. Examples for a heat exchanger and a packed gas absorber serve to illustrate the ease of application of the algorithms for linear systems to step flowrate changes, time-dependent input, simultaneous input disturbances and countercurrent flow with an accumulating phase. The example of batch distillation with packed column rectification demonstrates that the proposed methods can efficiently and accurately handle a nonlinear system with Langmuir form of isotherm and coupled boundary conditions.

INTRODUCTION

The numerical methods developed in Part I will be illustrated by application to a variety of heat and mass transfer processes. The accuracy and efficiency will be determined for both linear and nonlinear rate expressions. The numerical examples will not only illustrate the application of the algorithms of Part I but will also serve to demonstrate the facile adaptation of the proposed basic numerical methods for dealing with the dynamic behaviour of more complex chemical engineering transport processes.

In the first example, a countercurrent flow heat exchanger will be used to check the accuracy of the algorithms for a linear model with step input change in the dependent variable against the analytic solution of Jaswon and Smith (1954). In addition, this example will serve to demonstrate the flexibility of the numerical methods for the calculation of the transient response for other types of disturbances such as a step flowrate change and a time dependent inlet temperature change. The implementation of the algorithm derived for an accumulating stationary phase given in Appendix 2 of Part I will also be illustrated with this example.

In the second example, gas absorption of a dilute component will be used to illustrate the numerical methods for calculation of the dynamics of the start-up operation and the handling of simultaneous input changes.

The algorithm developed for a countercurrent system with a linear driving force rate equation and a Langmuir isotherm could not be tested for its accuracy directly since no analytic solution is available. However, an analytic solution is available for a nonlinear fixed-bed sorption process in which the governing rate equation could be rearranged in formal correspondence to a linear driving force rate expression with Langmuir isotherm. This analytic solution (Thomas, 1944) will be compared to the solution obtained by using the numerical methods developed in Part I.

For the last example, a nonlinear model for which an analytic solution is not available will be used to illustrate the facile adaptation of the proposed numerical method to a complex system. This example involves a packed column batch distillation with Langmuir isotherm and coupled boundary conditions arising from the mass balances on the overhead condenser and reboiler. The response of this system to changes in reflux ratio will be examined. An approximate model assuming negligible vapor holdup will be compared to a model without this assumption.

APPLICATION TO LINEAR SYSTEMS

Example 1: Heat Transfer in a Countercurrent Heat Exchanger

The following data were used in the calculation:

Length of exchanger (L): 7.50 m
Heat transfer coefficient (U): 700 J/m²·s·K
Heat transfer area per unit length (aS): 0.240 m²/m

Heat capacities (C_p): $(C_{P_1}) = (C_{P_2}) = 4,200$ J/kg·K
Mass flow rate (G): $G_2 = 0.80$ $G_1 = 0.300$ kg/s
Holdup (ϕ): $\phi_2 = 0.80$ $\phi_1 = 1.80$ kg/m

From these data, the calculated dimensionless parameters are: $A = 1.25$, $B = 1.25$ and $H = 1.00$. It was assumed that the system was initially at steady state with the following inlet conditions:

$$\overline{T}_1(0) = 65°C \text{ and } \overline{T}_2(H) = 10°C$$

The steady-state temperature profiles were readily obtained by solving the steady state equations.

For a step input change in X stream temperature from 65 to 90°C the numerical solution using the algorithm derived for a linear system and the analytic solution of Jaswon and Smith (1954) were compared and the results shown in Table 1.

Before discussing the results of the numerical solution it is appropriate to present and discuss Jaswon and Smith's analytic solutions.

The general solutions for equations:

$$\partial X/\partial \alpha = Y - X \tag{1}$$

$$\partial Y/\partial \beta = X - Y \tag{2}$$

were given by Jaswon and Smith as follows:

$$X = -\exp(-\alpha -\beta) \sum_0^\infty P_n \left(\frac{\alpha}{\beta}\right)^{n/2} I_n(2\sqrt{\alpha\beta})$$
$$+ \sum_1^\infty P'_n \left(\frac{\beta}{\alpha}\right)^{n/2} I_n(2\sqrt{\alpha\beta}) \tag{3}$$

$$Y = \exp(-\alpha -\beta) \sum_0^\infty Q_n \left(\frac{\alpha}{\beta}\right)^{n/2} I_n(2\sqrt{\alpha\beta})$$
$$+ \sum_1^\infty Q'_n \left(\frac{\beta}{\alpha}\right)^{n/2} I_n(2\sqrt{\alpha\beta}) \tag{4}$$

where P, Q, P', Q' are series coefficients which are determined by matching the given initial and boundary conditions, and I_n is the modified Bessel function of the first kind of order n.

For countercurrent processes with step input change in either X or Y, Jaswon and Smith discussed the matching technique and derived formulae for determining the series coefficients of Eqs. 3 and 4. For time dependent input changes and for step changes in both X and Y, the matching technique for undetermined coefficients is difficult to apply. In any case, because of the nature of the series form of solution, the analytic solutions are tedious to evaluate and cannot be used without the aid of a computer.

Numerical Results

The evaluation of the analytic series solution was carried out until the series converged to within 10^{-7} of the final correct value. Table 1 indicates that the use of 16 increments for the length parameter with $\Delta h/A = 0.05$ and $\Delta h = 0.0625$ gave values of dependent

TABLE 1. COMPARISON OF ANALYTIC AND NUMERICAL SOLUTION FOR A LINEAR SYSTEM

H = 1.00, A = B = 1.25

| $\dfrac{\theta/H - B/A}{1 + B/A}$ | θ | \multicolumn{4}{c}{$T_1(H,\theta)$, °C} | $\dfrac{\theta/H}{1 + B/A}$ | θ | \multicolumn{4}{c}{$T_2(0,\theta)$, °C} |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | \multicolumn{3}{c}{$H/\Delta h$} | | | | \multicolumn{3}{c}{$H/\Delta h$} | |
| | | 8 | 16 | 64 | Analytic | | | 8 | 16 | 64 | Analytic |
| 0 | 1 | 53.108 | 53.114 | 53.116 | 53.116 | 0 | 0 | 38.897 | 38.897 | 38.897 | 38.897 |
| 1/4 | 3/2 | 54.792 | 54.798 | 54.800 | 54.800 | 1/4 | 1/2 | 43.963 | 43.966 | 43.967 | 43.967 |
| 1/2 | 2 | 55.685 | 55.693 | 55.695 | 55.695 | 1/2 | 1/4 | 47.351 | 47.357 | 47.358 | 47.358 |
| 3/4 | 5/2 | 56.127 | 56.131 | 56.132 | 56.132 | 3/4 | 3/2 | 49.729 | 49.735 | 49.736 | 49.736 |
| 1 | 3 | 56.295 | 56.298 | 56.299 | 56.299 | 1 | 2 | 51.470 | 51.476 | 51.478 | 51.478 |
| 5/4 | 7/2 | 56.345 | 56.346 | 56.347 | 56.347 | 5/4 | 5/2 | 51.802 | 51.805 | 51.806 | 51.806 |
| 3/2 | 4 | 56.363 | 56.365 | 56.365 | 56.365 | 3/2 | 3 | 51.947 | 51.948 | 51.949 | 51.949 |
| 7/4 | 9/2 | 56.370 | 56.371 | 56.371 | 56.371 | 7/4 | 7/2 | 52.003 | 52.004 | 52.004 | 52.004 |
| 2 | 5 | 56.373 | 56.373 | 56.374 | 56.374 | 2 | 4 | 52.022 | 52.022 | 52.022 | 52.022 |
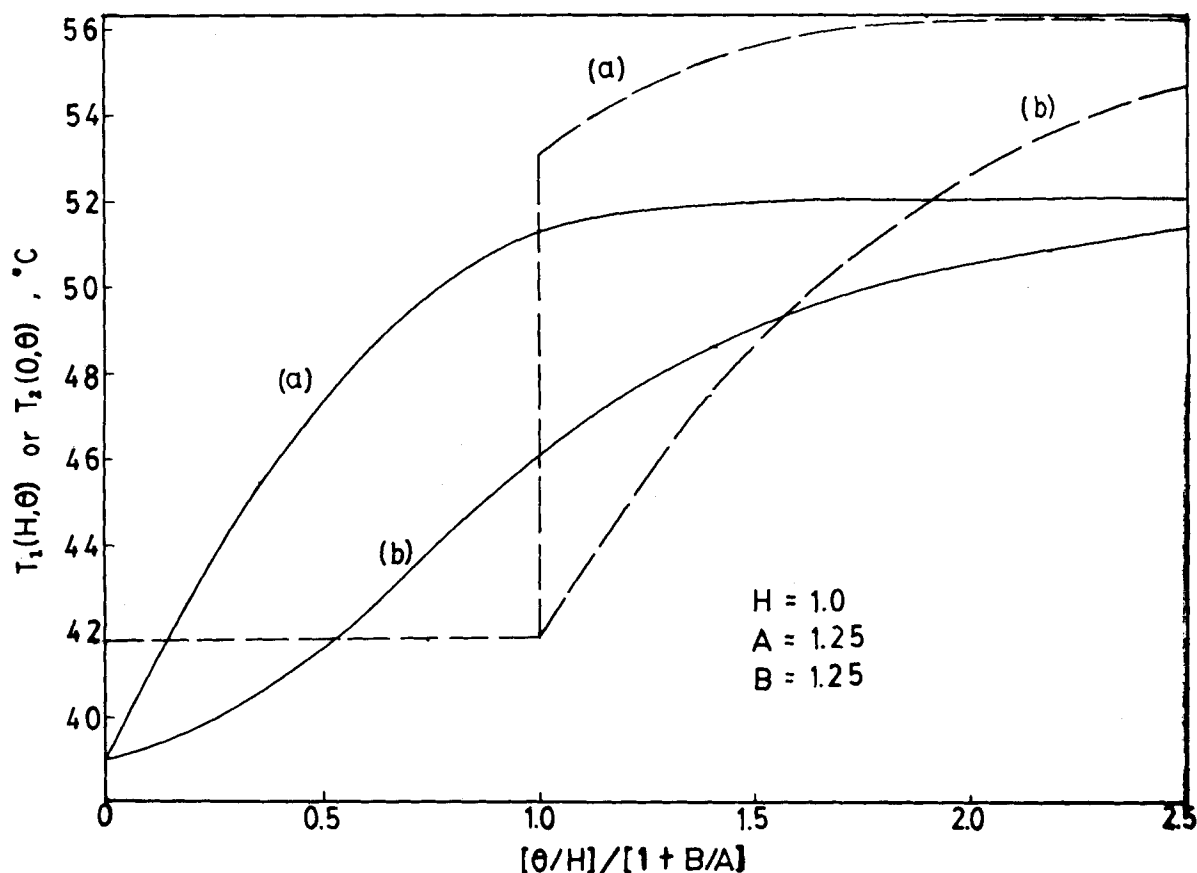
Figure 1. Response of outlet temperatures T_1 and T_2 to disturbances in the T_1 stream. (a) Step change from 65 to 90°C. (b) Time-dependent change, $T_1(0,\theta)$ $= \overline{T}_1(0) + 25[1 - \exp(-1.5\theta)]$. Dashed line, T_1; solid line, T_2.

variables which were accurate to within 99.99% of those given by the analytic solution. Using only 8 increments, the results were still accurate to about the third significant figure. Using 16 increments for Δh and a total of 64 increments for $\Delta \theta$, the total computation time required to generate 1,024 values of both X and Y was less than 0.2 of a second using the IBM 370/165II. For this same problem it required about 3 s to obtain 75 values of both X and Y using the analytic series solution.

The numerical solution along $\beta = 0$ could be initiated using either a Runge Kutta or a modified Euler's method. The fourth order Runge Kutta method showed, as expected, higher accuracy than the modified Euler's method when equal increment size was used. However, the several fold increase in computation time required would not be justified for engineering application in which accuracy up to the third or fourth significant figure is adequate. Furthermore, the Runge Kutta method cannot be applied directly to the calculation of interior points unless an iterative procedure or some other modification of the algorithm is introduced.

In addition to the response to a step input change in temperature, the transient response to several other types of disturbances was also determined using the proposed methods. Figures 1 and 2 show the response of the X and Y (T_1 and T_2) streams at their outlets with the following input changes in the X stream:

(a) A step input change of temperature from 65 to 90°C.

(b) A time-dependent input change in temperature of the X stream with

$$T_1(0,\theta) = \overline{T}_1(0) + 25[1 - \exp(-1.5\theta)]$$

(c) A step input change in the X stream mass flowrate from 0.300 to 0.595 kg/s with a constant U.

(d) An identical step change as for (c) except that the heat transfer coefficient varied as the 0.8 power of the mass flowrate, i.e., $U/\overline{U} = (G_x/\overline{G}_x)^{0.8}$ where the $^-$ indicates the initial value before disturbance.

The calculation for the transient response to time-dependent X input changes was straight forward. The only modification to the step input change algorithm was the expression of the continuous X input changes in sufficiently accurate discrete form. The calculations for a step mass flow rate change required the inclusion of transients for the region bounded by $\theta = 0$ and $\theta \le (B/A)h$, and therefore necessitated the use of the method outlined in Appendix 1 of Part I.

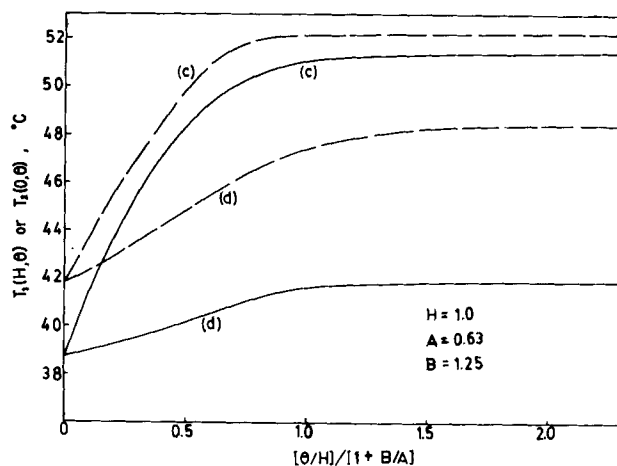The algorithm derived for an accumulating stationary phase

Figure 2. Response of outlet temperatures T_1 and T_2 to step disturbance of mass flow rate of the T_1 stream from 0.300 to 0.595 kg/s (for $A = 1.25$ to 0.63). (c) With constant heat transfer coefficient U. (d) With heat transfer coefficient change given by $U/\overline{U} = (G_x/\overline{G}_x)^{0.8}$. Dashed line, T_1; solid line, T_2.
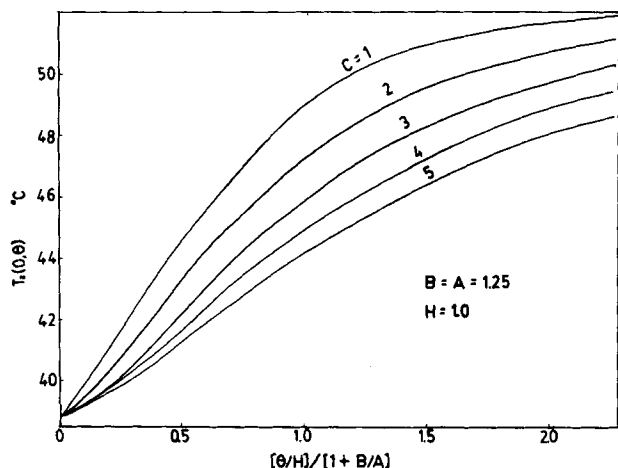
Figure 3. Response of outlet temperature of T_2 to step change in inlet temperature T_1 for different tube wall to tube fluid heat capacity ratios.

Figure 5. Response of outlet X and Y streams to simultaneous input changes in a gas absorption column.

(Appendix 2, Part I) was also used for the above heat transfer example. The only further information required in addition to the previous data given for this example was the heat transfer coefficient between the X steam and the wall and the heat transfer coefficient between the Y stream and the wall. It was assumed that:

$$1/U = U_x + 1/U_y = 1/700 \text{ and } 1/U_x = 1/U_y$$

Figure 3 shows the transient response of the outlet of the Y stream for a step input change of inlet temperature of X stream from 65 to 90°C for various heat capacity ratios of the wall to the Y stream.

Example 2: Start-Up and Transient Response to Simultaneous Feed Changes In a Gas Absorption Column

The concentration of solute being absorbed from the liquid stream was assumed to be very dilute so that the molar flowrate of liquid and gas streams remained constant and a linear isotherm was applicable. The numerical data used for calculation were as follows:

Length of the column (L): 5.00 m
Cross section area of the column (S): 0.00400 m²
Molar flow rate (G): $G_y = G_x/2.25 = 1.11 \times 10^{-4}$ kmol/s
Mass transfer coefficient ($K_y a$): 0.0278 kmol/m³·s
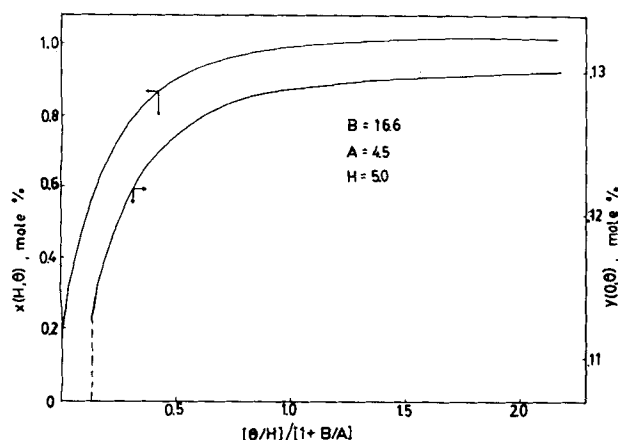Column holdup (ϕ): $\phi_x = 8.3\phi_y = 0.00400$ kmol/m
Isotherm: $y^* = 0.5x = X$

Figure 4. Response of outlet X and Y streams for start-up operation in a gas absorption column.
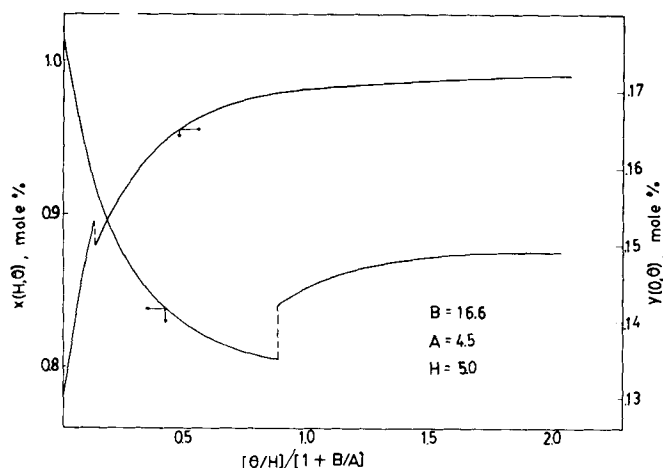
From these data, the calculated dimensionless parameters were: $A = 4.50$, $B = 16.6$, and $H = 5.00$.

For the start-up operation, it was assumed that the column was initially filled with the X stream having a composition of $x(h) = 0.002$ for $0 \le h \le H$. A y stream having a composition of $y(H) = 0.02$ was then introduced at the bottom of the column while an X stream having a composition of $x(0) = 0.002$ was fed simultaneously to the top of the column.

For demonstrating the application of the proposed method to the simulation of transient response to simultaneous inlet feed composition changes, it was assumed that after the steady state had been attained from start-up, the simultaneous changes (i.e., θ_d, the time delay between changes in the two streams was assumed to be zero) of x from 0.002 to 0.003 and of y from a value of 0.02 to 0.015 were introduced. Figures 4 and 5 show the calculated transient response (at the outlets of x and y) for the start-up operation and for simultaneous input composition changes, respectively.

As discussed in Part I, for input changes in both X and Y streams, the location at which the two simultaneous disturbance fronts meet for the first time is given by $h_a = H/(1 + B/A)$ and for this example the value of h_a/H was calculated to be 45/211. Thus, the location of h_a would not coincide with the intersection of the two characteristic lines unless the number of increments used was exactly 211 or multiples of 211. By approximation such as setting $45/211 \doteq \frac{1}{5}$ and use of a number of increments equal to multiples of 5, the location of h_a could have been made to coincide with the intersection of the two characteristic lines. However, for this example, the more exact method outlined in Part I, with 64 increments of Δh, corresponding to $\Delta h = 0.078125$ and $\Delta h' = 0.027399$, was used in the calculation.

Numerical Results

In Example 1, in which identical algorithms were used, it was shown that accurate numerical results were obtained for a single input disturbance with a normalized space increment as large as 0.125. It was, therefore, reasonable to conclude that the numerical values obtained in the present example with much smaller increment size would show little deviation from the analytic solution if such solution was available.

APPLICATION TO NONLINEAR SYSTEMS

Example 1N: Fixed-Bed Sorption Process, Second-Order Kinetic Model

Before using the numerical schemes for a countercurrent flow system with Langmuir isotherm it was desirable to have a similar algorithm checked against an analytic solution for a nonlinear

Calculated values of $x(\alpha_H,\beta)$

$\alpha_H = H/A = 4.00$, $\beta_f = \theta_f - (B/A)H = 8.00$, $\Delta\beta/\Delta\alpha = 1.00$

Throughput	r = 0.20				r = 20.0			
	$\alpha_H/\Delta\alpha$				$\alpha_H/\Delta\alpha$			
β/α_H	8	16	64	Analytic	8	16	64	Analytic
1/4	0.33581	0.34203	0.34398	0.34412	0.05122	0.05177	0.05195	0.05196
1/2	0.52617	0.52778	0.52833	0.52837	0.13019	0.12981	0.12970	0.12970
1	0.70502	0.70494	0.70491	0.70491	0.50774	0.50762	0.50756	0.50755
3/2	0.79388	0.79331	0.79312	0.79310	0.87410	0.87461	0.87475	0.87476
2	0.84868	0.84781	0.84752	0.84750	0.97962	0.97935	0.97926	0.97926

system. The only available analytic solution was that for a fixed-bed sorption process with a second-order kinetic model derived by Thomas (1944). The characteristic model equations for fixed-bed system (Appendix 3, Part I) are:

$$\frac{\partial x}{\partial \alpha} = y(1 - x)/r - x(1 - y) \tag{1}$$

$$\frac{\partial y}{\partial \beta} = x(1 - y) - y(1 - x)/r \tag{2}$$

where $\alpha = h/A$ and $\beta = \theta - (B/A)h$

The analytic solutions of Eqs. 5 and 6 corresponding to the following simple initial and boundary conditions:

$x(0,\beta) = x(0,\theta) = 1.00$ for $0 \le \theta \le \theta_f$, i.e., $0 \le \beta \le \beta_f$

$y(\alpha,0) = y(h,\theta = Bh/A) = 0$ for $0 \le h \le H$, i.e., $0 \le \alpha \le \alpha_H$

were:

$$x = \frac{J(\alpha/r,\beta)}{J(\alpha/r,\beta) + [1 - J(\alpha,\beta/r]\exp[(\alpha - \beta)(r - 1)/r]} \tag{3}$$

$$y = \frac{1 - J(\beta,\alpha/r)}{J(\alpha/r,\beta) + [1 - J(\alpha,\beta/r)]\exp[(\alpha - \beta)(r - 1)/r]} \tag{4}$$

where $J(u,v)$ is tabulated mathematical function (Helfferich, 1962; Sherwood et al., 1975).

Using the numerical algorithm derived in Appendix 3 of Part I the values of x and y were calculated for a wide range of values of α and β. The analytic solutions were calculated using either the tabulated J function or using an efficient series expansion scheme given by Chang et al. (1973). In all the calculations, double precision was used since the results of the numerical and analytic solution were compared up to the fifth significant figure.

Numerical Results

Table 2 gives the results of numerical and analytic solutions for values of x for $r = 0.2$ as well as $r = 20.0$. Even for an increment of $\Delta\alpha$ as large as 0.25, three correct significant figures were obtained. One or two more correct figures were obtained by halving the increment size. Calculations for the values of y also showed similar good agreement.

As mentioned in the introduction, the fixed-bed example was introduced to enable some accuracy check to be made of the nonlinear countercurrent algorithm of the numerical method section of Part I. Equations 1 and 2 can be rearranged (Hiester and Vermeulen, 1952) to give:

$$\frac{\partial x}{\partial \alpha} = \frac{1 + r'x}{r}\left(y - \frac{rx}{1 + r'x}\right) \tag{5}$$

$$\frac{\partial y}{\partial \beta} = \frac{1 + r'x}{r}\left(\frac{rx}{1 + r'x} - y\right) \tag{6}$$

The form of these equations corresponds almost identically to Eqs. 7N and 8N of Part I except with the additional factor of (1 +

$r'x)/r$. The presence of this term can be viewed as the inclusion of a composition dependent mass transfer coefficient in the basic Langmuir isotherm model equations. Although the same numerical method was used, the algorithms for the calculation for the fixed-bed system with a second-order kinetic rate expression were more complex than those based on a linear driving force rate equation with Langmuir isotherm. Since the numerical results for the fixed bed system were quite accurate, it was reasonable to expect that the accuracy of a numerical solution based on the algorithms derived for a countercurrent system with Langmuir isotherm, (Eqs. 13N to 17N of Part I) would be at least as good.

Example 2N: Batch Distillation with Packed Column Rectification

The following data were used in the calculation:

Length of the column (L): 1.20 m
Cross-sectional area of the column (S): 0.0250 m^2
Mass transfer coefficient $(K_y a)$: 0.01389 kmol/m^3·s
Vapor molar flow rate (G_y): 1.389×10^{-4} kmol/s
Hold up in the column (ϕ): $\phi_x = 20\phi_y = 0.00200$ kmol/m
Relative volatility (r): constant = 2.50

The calculated dimensionless parameters were $H = 3.00$ and $B = 20.0$. Although a constant relative volatility was assumed in this example, a composition dependent relative volatility could also be included in the calculation if desired (Part I).

For simplicity, constant molar flow throughout the column and reboiler was assumed. The column was equipped with a total condenser of negligible holdup so that at the top of the column, $x(0) = y(0)$. Initially, the column was operated at steady state at total reflux, i.e., $\bar{G}_x = \bar{G}_y$ and $A = \bar{A} = 1$ (initial steady-state value). The steady-state values of x and y were determined from the solution of the following equations:

$$\bar{A}\frac{d\bar{x}}{dh} = \frac{d\bar{y}}{dh} = \bar{y} - \frac{r\bar{x}}{1 + (r - 1)\bar{x}}$$

The boundary conditions were $y(H) = 0.725$ and $x(0) = y(0)$.

With an initial reboiler holdup of $W'(0) = 0.0400$ kmol and the system initially at steady state, a top product was withdrawn so that a finite reflux ratio (corresponding to a step change in flow rate in the liquid phase) was instantaneously established. The resulting new value of A was given by $A = R/(R + 1)$, where R was the external reflux ratio. The value of $K_y a$ was assumed constant although variation with G_x could have been readily included (Example 1).

Coupled boundary condition at $h = H$.

Since the reboiler holdup was finite the value of $y(H,0)$ was not independently defined and Eq. 17N in Part I for determining the boundary condition had to be solved using a mass balance around the reboiler. The component mass balance gave:

$$\frac{dWx_w}{d\theta} = Ax(H,\theta) - y(H,\theta) \tag{1}$$

where x_w was the reboiler composition and W was the normalized

reboiler holdup at any time, $W = K_y a S W'/(G\phi)_y$. An overall mass balance with $W'(0) = 0.0400$ or $W(0) = 1,000$, gave:

$$W(\theta) = 1,000 - (1 - A)\theta \qquad (2)$$

It was further assumed that the reboiler vapour was in equilibrium with the reboiler liquid, i.e.,

$$y(H,\theta) = \frac{r x_w}{1 + (r - 1)x_w} \qquad (3)$$

The determination of the unknowns $y(H,\theta)$, $x(H,\theta)$ and $x_w(\theta)$ required the solution of Eqs. 1, 2 and 3 together with Eq. 17N of Part I. Integrating Eq. 1 with the modified Euler's method gave:

$$W(\theta)x_w - W(\theta - \Delta\theta)x_{wj} = (\Delta\theta/2)[A(x + x_j) - (y + y_j)] \qquad (4)$$

Equation 17N (shown here in implicit form for brevity) was required to relate $x(H,\theta)$ and $y(H,\theta)$:

$$\frac{x - x_i}{\Delta h/A} = \frac{y + y_i}{2} - \frac{r}{2}\left[\frac{x}{1 + (r - 1)x} + \frac{x_i}{1 + (r - 1)x_i}\right] \qquad (5)$$

where

x,y,x_w = values at H and θ

x_j,y_j,x_{wj} = values at H and $\theta - \Delta\theta$

x_i,y_i = values at $H - \Delta h$ and $\theta - \Delta\theta/(1 + A/B)$

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

The determination of the composition unknowns, $x(H,\theta)$, $y(H,\theta)$ and $X_w(\theta)$ would normally have required an iterative solution since two simultaneous quadratic relations were involved. It was of interest to examine whether an explicit solution could give adequate accuracy.

The three unknowns could be determined explicitly without iteration by using the value of x_{wj} as an approximation for x_w in Eq. 4 and $y(H,\theta)$ could then be calculated from Eq. 3. With the calculated value of $y(H,\theta)$, the value of $x(H,\theta)$ was then determined from the explicit quadratic form of Eq. 5. Finally the value of x_w was calculated from Eq. 4. It was found that the initial estimate and the final calculated value of x_w were identical to at least three significant figures when 16 increments were used in the calculation. Preliminary iterative calculation showed that convergence to five significant figures could be obtained with about four iterations. It was therefore decided to employ the explicit method of solution with 16, 24, or 32 increments in all subsequent calculations. This avoidance of iteration will lead to simpler coding and greater efficiency for the numerical calculation and as will be seen, good accuracy can be obtained.

Calculation for the Region $0 \leqslant \theta \leqslant (B/A)h$. Since the transient due to the step change in flow rate originates on the $\theta = 0$ line, the sequence of calculation must start with the deter-mination of values of x and y for the region bounded by $\theta \geqslant 0$ and $\theta \leqslant (B/A)h$ using the method outlined in Appendix 1 of Part I. Special attention was given to the calculation of the first value of x and y at $h = H$ since an irregular increment and an initial state value were required. The calculation for this region terminated on the characteristic $\theta = (B/A)h$.

Calculation for $\theta \geqslant (B/A)h$ and the Coupled Boundary Condition at $h = 0$. The remaining calculations for $\theta \geqslant (B/A)h$ followed the method of Case a of the numerical method section of Part I, starting with the calculation for the $j = 2$ line. The sequence of calculation for each β characteristic line in region $\theta \geqslant (B/A)h$ started with the calculation of x and y at $h = 0$. Because of the coupled boundary condition at the top of the column, Eq. 14N of Part I had to be modified to make use of the relation $x(0,\theta) = y(0,\theta)$. The application of this relationship led to:

$$x(0,\theta) = y(0,\theta) = [-b + \sqrt{b^2 + 4r'c}]/2r' \qquad (6)$$
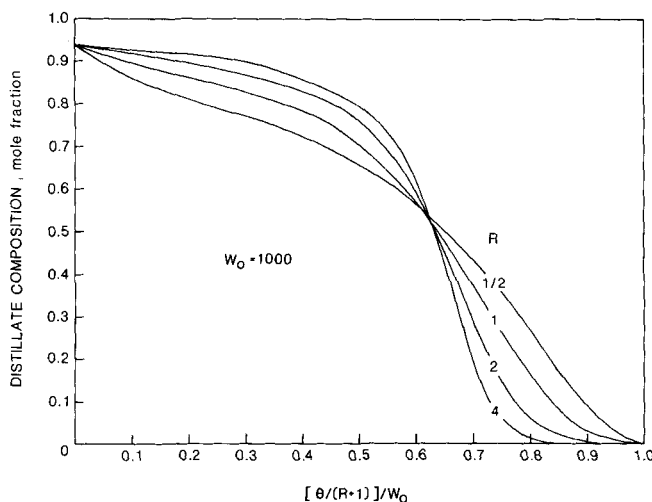
where

Figure 6. Distillate composition as a function of fraction of original charge distilled. Response to step changes in reflux ratio for a batch distillation with packed column rectification initially operating at total reflux.

$$b = 1 - \frac{r\Delta\beta}{2 + \Delta\beta} - r'c$$

$$c = \frac{\Delta\beta}{2 + \Delta\beta} y^*(\Delta h,\theta - \Delta h) + \frac{2 - \Delta\beta}{2 + \Delta\beta} y(\Delta h,\theta - \Delta h)$$

Equations 15N and 16N of Part I were then used for calculating the interior points and the determination of values x and y for all mesh points for each j line terminated with the use of the bottom boundary condition as given by Eqs. 3, 4 and 5. The calculations were extended to any value of j depending on the desired distillate composition or fraction of original charge distilled. In this example, in order to test the algorithm over the full range of composition changes, the calculation was terminated when the reboiler holdup was approximately equal to zero.

Numerical Results

In applying the numerical solution to this example, the increment of Δh used varied from $3/16$ to $3/32$. Output with 24 and 32 increments of Δh agreed to four or five significant figures, while those obtained from using 16 increments agreed to at least three significant figures with the solution using 32 increments.

As a separate check of the numerical solution, an integral component balance around the reboiler over the time interval $\theta = 0$ to any value of θ was performed using Simpson's rule for evaluating the integral values of $x(H,\theta)$ and $y(H,\theta)$. This balance was found to be satisfied to about 2% when 16 increments of Δh were used and to about 0.5% when 32 increments were used. The calculated results for this example are shown in Figure 6, where the distillate product composition for various values of step change in reflux ratio were plotted against the fraction of original charged distilled.

Effect of Neglecting Vapor Holdup

The vapor holdup in this example was relatively small compared to the liquid holdup. It was of interest to study the validity of the common assumption of negligible holdup in the vapor phase. Under such assumption, the residence time for the vapor phase was negligible. Thus, no calculation was required for the distributed disturbance region, as the transient changes for this region was negligible. It could be further assumed that the initial steady state values of x applied on characteristic line $\alpha = 0$ in Figure 1b of Part I. Thus, the numerical method section of Part I with reference to Case b could be directly applied.

A further simplification was possible because the contact time was approximately equal to the absolute time. New α characteristic lines defined in terms of the coordinates θ/B and h/A would be

horizontal (approximately) and the intersection of these characteristics with the new β characteristics would form a rectangular grid in absolute time and space coordinates. Although output was obtained directly from this grid, the time and space increments could not be independently chosen because of their unique relationship as defined by the β characteristic. Calculations showed that the no vapor holdup model was accurate to three significant figures.

Since neglecting the vapor holdup led to neglecting transients for the time period prior to the arrival of a new vapor composition from the reboiler, it was expected that larger values of A/B as well as larger initial composition gradients in the column would result in larger error. Further calculations showed that for either an H increase from 3 to 6 or an A/B increase from $\frac{1}{20}$ to $\frac{1}{4}$, the no vapor holdup assumption led to as much as 15% error.

SUMMARY AND CONCLUSIONS

The numerical results of the examples used can be seen to be efficient since iterative or interpolation techniques were not required. High accuracy was obtained with increments, as large as $\Delta h \doteq 0.1$, as indicated by the rapid convergence of the numerical

solutions as the size of the increments was decreased and by comparison to analytical solutions.

The coding sequence described in Part I was found to be applicable without change for the specific examples used. For more generalized problems the coding would be somewhat lengthier than that used with conventional methods. However, the proposed methods are expected to be more efficient and accurate.

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Bilayer Film Model for the Interaction between Adsorption and Bacterial Activity in Granular Activated Carbon Columns

Part I: Formulation of Equations and Their Numerical Solutions

The diffusion-reaction film model proposed by Andrews and Tien (1981) for the interaction between adsorption and bacterial activities in carbon columns was generalized. The microbial film was assumed to be composed of two regions of distinctively different microbial activity, depending on the presence or absence of dissolved oxygen. Governing equations were derived to describe the dynamics of the carbon columns in which the interaction between adsorption and bacterial growth and methods for solving these equations were developed.

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SCOPE

The application of granular activated carbon columns for treating water and waste water has become a standard treatment technology. When the dissolved organics present in the waste are both adsorbable and biodegradable, bacterial growth in the column becomes almost unavoidable. When the growth may create operating difficulties, its presence has been viewed more recently as beneficial because of the synergistic and complementary nature of adsorption and bacterial activity in

the treatment process. The present study is concerned with the formulation of a model which can predict the essential features of the interaction.

The model for the interaction is a generalization of an earlier study by Andrews and Tien (1981) and allows the bacterial activity to be either aerobic or anoxic depending on the film thickness. Equations describing column operations incorporating this interaction model were derived and algorithms for their solution were developed. Sample calculations which demonstrate the effect of various process variables were made as part of this study.

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