A METHOD OF MASS TRANSFER CALCULATION IN A BACK-FLOW MODEL

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Received October 18th, 1979

Instead of solving a set of N nonlinear equations (as has been proposed by the author and his coworker), the problem may be solved iteratively as a linear one. The proposed method converges rapidly and the number of iterations is practically constant regardless of the number of stages in countercurrent cascade N and the degree of nonlinearity of equilibrium formula. The method proved to be suitable for computation on desk-top calculator.

The paper deals with so-called back-flow model for the description of flow of phases in a countercurrent stage equipment. Among other methods[2-5] there has been proposed a method of calculation[1] based on the solution of N nonlinear equations (the nonlinearity is introduced in the problem by nonlinear equilibrium formula), with the number of iterations fully depending on the dimensionality of the problem. This unpleasant feature may be removed by proper reformulation of material balance equations leading to the iterative solution of a (N,N) matrix equation with corrective oin of nonlinear equilibrium calculation between successive iterations. To remove further the direct role of backflow in both phases, a concept of so-called modified concentration variables is introduced. The explicit numerical influence of the driving force for mass transfer expressed in terms of the difference between the actual and equilibrium concentration of the solute, as the most sensitive and least stable factor from the view point of the numerics, is removed too. The evaluation of the course of computation of particular problems has shown, that the number of iterations is practically independent of the number of stages N, *i.e.* the dimensionality of the problem.

FORMULATION OF MATERIAL BALANCE EQUATIONS

Schematic representation of the back-flow model with constant flow of phases and back-flow is shown in Fig. 1. The solute material balance of the feed phase in k th stage of the N stage cascade is expressed by the equations

$$Fx_0 - (F + E)\,x_1 + Ex_2 = -(S + R)\,(y_2 - y_1) = KaV(x_1 - x_1^+) \qquad (1)$$

$$(F + E)\,x_{k-1} - (F + 2E)\,x_k + Ex_{k+1} =$$
$$= -(S + R)\,y_{k+1} + (S + 2R)\,y_k - Ry_{k-1} = KaV(x_k - x_k^+) \tag{2}$$
$$k = 2, \ldots, N - 1$$

$$(F + E)\,(x_{N-1} - x_N) = -Sy_{N+1} +$$
$$+ (S + R)\,y_N - Ry_{N-1} = KaV(x_N - x_N^+)\,, \tag{3}$$

where x_0 and y_{N+1} are known inlet concentrations. If we define the back-flow coefficients

$$f = E/F\,. \tag{4}$$

$$s = R/S\,, \tag{5}$$

the mass transfer number

$$t = KaV/F\,, \tag{6}$$

distribution coefficients

$$m_k = y_k/x_k^+\,; \quad k = 1, \ldots, N \tag{7}$$

and introduce the ratio of phase flows

$$Q = F/S\,, \tag{8}$$

the set of equations (1)–(3) may be reformulated in the form

$$U_{k-1} - U_k = -(1/Q)\,(Z_{k+1} - Z_k) = t(x_k - y_k/m_k)\,; \quad k = 1, \ldots, N\,, \tag{9}$$

where the variables U, Z are so-called modified concentration variables, defined as follows:

$$U_0 = x_0\,, \tag{10}$$

$$U_k = x_k + f(x_k - x_{k+1})\,; \quad k = 1, \ldots, N - 1 \tag{11}$$

$$U_N = x_N\,, \tag{12}$$

$$Z_1 = y_1\,, \tag{13}$$

$$Z_k = y_k + s(y_k - y_{k-1})\,; \quad k = 2, \ldots, N\,, \tag{14}$$

$$Z_{N+1} = y_{N+1}\,, \tag{15}$$

(it is apparent that $U_k = x_k$ and $Z_k = y_k$ for all k when no backflow exist). Now we may express the original concentration variables x, y by means of the modified ones (using the above equations) as

$$x_k = \sum_{j=k}^{N} \alpha_{k,j} U_j \tag{16}$$

$$y_k = \sum_{j=1}^{k} \beta_{k,j} Z_j \tag{17}$$

$$k = 1, \ldots, N\,,$$

where

$$\alpha_{k,j} = \begin{cases} 1/(1 + f) & \text{for} \quad j = k \\ \alpha_{k,j-1} f/(1 + f) & \text{for} \quad k < j < N\,; \quad k = 1, \ldots, N - 1 \\ \alpha_{k,N-1} f & \text{for} \quad j = N \end{cases} \tag{18}$$

$$\alpha_{N,N} = \beta_{1,1} = 1 \tag{19}$$

$$\beta_{k,j} = \begin{cases} 1/(1 + s) & \text{for} \quad j = k \\ \beta_{k,j+1} s/(1 + s) & \text{for} \quad k > j > 1\,; \quad k = 2, \ldots, N \\ \beta_{k,2} s & \text{for} \quad j = 1 \end{cases} \tag{20}$$

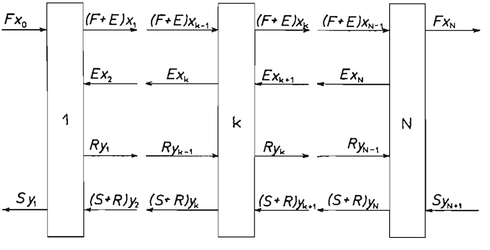

FIG. 1
Model of Countercurrent Cascade with Back-Flows

and thus remove the direct expression of the driving force. The final form of material balance equations (1)–(3) is

$$U_{k-1} - U_k = -(1/Q)(Z_{k+1} - Z_k) =$$
$$= t\left[\sum_{j=k}^{N} \alpha_{k,j} U_j - (1/m_k) \sum_{j=1}^{k} \beta_{k,j} Z_j\right]; \quad k = 1, \ldots, N, \tag{21}$$

In addition to this set we may take the material balance so that its envelope encloses the y-phase inlet and cuts between stage k and $k - 1$ to get

$$U_{k-1} - U_N = -(1/Q)(y_{N+1} - Z_k) \tag{22}$$

or (in another form)

$$Z_k = Q(U_{k-1} - U_N) + y_{N+1}; \quad k = 1, \ldots, N. \tag{23}$$

TABLE I

Example of Iterative Solution of Countercurrent Cascade

k	Iteration number 0		1		2		3		4	
	x	y	x	y	x	y	x	y	x	y
0	4·0000	—	4·0000	—	4·0000	—	4·0000	—	4·0000	—
1	3·6000	1·6000	2·2915	1·5600	2·2831	1·5653	2·2848	1·5655	2·2848	1·5655
2	3·2000	1·4400	1·7443	1·2503	1·7134	1·2594	1·7158	1·2598	1·7159	1·2598
3	2·8000	1·2800	1·3194	0·9685	1·2691	0·9721	1·2710	0·9731	1·2712	0·9731
4	2·4000	1·1200	0·9842	0·7374	0·9245	0·7312	0·9252	0·7325	0·9254	0·7325
5	2·0000	0·9600	0·7218	0·5516	0·6620	0·5371	0·6618	0·5381	0·6620	0·5382
6	1·6000	0·8000	0·5186	0·4038	0·4655	0·3849	0·4648	0·3854	0·4649	0·3855
7	1·2000	0·6400	0·3632	0·2877	0·3203	0·2680	0·3195	0·2681	0·3195	0·2682
8	0·8000	0·4800	0·2459	0·1974	0·2142	0·1799	0·2134	0·1798	0·2135	0·1799
9	0·4000	0·3200	0·1590	0·1278	0·1377	0·1144	0·1371	0·1142	0·1372	0·1142
10	0·0000	0·1600	0·1000	0·0741	0·0867	0·0653	0·0863	0·0652	0·0864	0·0652
11	—	0·0000	—	0·0000	—	0·0000	—	0·0000	—	0·0000

CALCULATION PROCEDURE

Using the expression (*23*) for Z to eliminate this variables from Eqs (*21*) and taking into account that

$$\sum_{j=1}^{k} \beta_{k,j} = 1 \quad \text{for all} \quad k\,, \tag{24}$$

we obtain the matrix equation

$$\mathbf{CU} = \mathbf{A}\,, \tag{25}$$

where $\mathbf{A}$ is a $(N, 1)$ vector with elements A_k defined as

$$A_1 = x_0 + (t/m_1)(Qx_0 + y_{N+1}) \tag{26}$$

$$A_k = (t/m_k)(Q\beta_{k,1}x_0 + y_{N+1})\,; \quad k = 2, \ldots, N \tag{27}$$

$\mathbf{C}$ is a square (N, N) matrix with elements C_{kj} defined as

$$C_{kj} = \begin{cases} -Q(t/m_k)\,\beta_{k,j+1} & \text{for} \quad k = 3, \ldots, N \\ & \qquad\; j = 1, \ldots, k-2 \\ -[1 + Q(t/m_k)\,\beta_{k,k}] & \text{for} \quad k = 2, \ldots, N \\ & \qquad\; j = k-1 \\ 1 + t\alpha_{k,k} & \text{for} \quad k = 1, \ldots, N-1 \\ & \qquad\; j = k \\ t\alpha_{k,j} & \text{for} \quad k = 1, \ldots, N-2 \\ & \qquad\; j = k+1, \ldots, N-1 \\ t(\alpha_{k,N} + Q/m_k) & \text{for} \quad k = 1, \ldots, N-1 \\ & \qquad\; j = N \\ 1 + t(1 + Q/m_N) & \text{for} \quad k = N \\ & \qquad\; j = N \end{cases} \tag{28}$$

and $\mathbf{U}$ is the $(N, 1)$ vector of the modified variables U_k $(k = 1, \ldots, N)$. By the assumption that particular formula for calculation of the distribution coefficients m_k is known, the whole problem is thus reduced to the repetitive solution of the linear equation

$$\mathbf{U} = \mathbf{C}^{-1}\mathbf{A} \tag{29}$$

together with corrective calculation of m_k (usually as a nonlinear function of phase composition $-m_k = m(x_k, y_k)$ in general case). To start the computation, the formulas

$$x_k^{(0)} = x_0(1 - k/N) \tag{30}$$

and

$$y_k^{(0)} = x_0[Q - (Q - y_{N+1})(k - 1)/N] \tag{31}$$

$$k = 1, \ldots, N$$

can be used for starting approximation of the original concentration variables. To correct the previous values of distribution coefficients, direct substitution of x, y, according to the formula

$$m_k^{(n)} = m(x_k^{(n-1)}, y_k^{(n-1)}) \tag{32}$$

(where n designates the iteration step), has proved quite satisfactory in case of mild nonlinearity of m, whilst the application of relaxation is recomended in case of strong nonlinearity, *i.e.* strong dependency of m on phase composition. For matrix $\mathbf{C}$ inversion Gauss–Seidel elimination procedure is used. The values of x, y are determined by the formulas

$$x_N = U_N \tag{33}$$

$$x_k = (U_k + f x_{k+1})/(1 + f); \quad k = N - 1, \ldots, 1 \tag{34}$$

$$y_1 = Z_1 \tag{35}$$

$$y_k = (Z_k + s y_{k-1})/(1 + s); \quad k = 2, \ldots, N. \tag{36}$$

The calculation procedure can be summarized as follows:

A) Given $N, Q, t, f, s, m = m(x, y), \delta, x_0, y_{N+1}$.

B) Find the starting approximation of x, y using formulas (*30*), (*31*) and let $x = x_k^{(0)}$, $y = y_k^{(0)}$ for $k = 1, \ldots, N$. Set $n = 1$. Compute coefficients α, β from Eqs (*18*)–(*20*).

C) Calculate $m_k = m(x_k, y_k)$ for $k = 1, \ldots, N$.

D) Calculate elements of $\mathbf{C}$ from Eq. (*28*) and elements of $\mathbf{A}$ from Eqs (*26*), (*27*).

E) Calculate elements of $\mathbf{C}^{-1}$ using Gauss–Seidel procedure.

F) Calculate elements of vectors **U** (Eq. (*29*)) and **Z** (Eq. (*23*)).

G) Calculate $x_k^{(n)}$ and $y_k^{(n)}$ using formulas (*33*)–(*36*).

H) If $|x_k^{(n)} - x_k^{(n-1)}| < \delta$ and $|y_k^{(n)} - y_k^{(n-1)}| < \delta$ for all k stop the calculation. Otherwise let $x_k = x_k^{(n)}$, $y_k = y_k^{(n)}$, set $n + 1 \rightarrow n$ and go back to the step *C*.

Example. The results of all particular approximations of the solution for $N = 10$, $Q = 0{\cdot}4$, $t = 5{\cdot}0$, $f = 1{\cdot}0$, $s = 0{\cdot}5$, $m = 1/(1 + 0{\cdot}2y)$, $\delta = 0{\cdot}00005$, $x_0 = 4{\cdot}0$, $y_{N+1} = 0{\cdot}0$ are summarized in Table I.

A sufficiently large set of problems has been solved using HP 9821A calculator in order to check the convergence of the proposed method. The range of the parameters has been: number of stages 4—20, back-flow coefficients 0—10, mass transfer number 0·1—100. The analysis of computation results of particular problems has shown that the number of iterations is for the given accuracy δ practically independent of the dimensionality of the problem and amounts to 4—6 (for $\delta = 0{\cdot}00005$). The computing time increases with the number of stages N and amounts in average to 1 second per iteration and $N^{2.4}$.

LIST OF SYMBOLS

a	specific interfacial area
E	back-flow in feed phase
f	back-flow coefficient in feed phase
F	flow of feed phase
k	stage number counted from feed phase inlet
K	mass transfer coefficient related to feed phase
m	distribution coefficient characterizing equilibrium between phases
N	number of stages of countercurrent separation cascade
Q	phase ratio
R	back-flow in solvent phase
s	back-flow coefficient in solvent phase
S	flow of solvent phase
t	mass transfer number
U	modified solute concentration in feed phase
V	volume of a stage
x	solute concentration in feed phase
x^+	solute concentration in feed phase in equilibrium
y	solute concentration in solvent phase
Z	modified solute concentration in solvent phase
δ	positive number characterizing the accuracy of the calculation

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