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A SIMULATION PROCEDURE FOR MULTICOMPONENT DISTILLATION COLUMNS INCORPORATING PLATE EFFICIENCIES

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Key Words: Distillation Column, Multicomponent Separation, Nonideal Solution, Plate Efficiency, Newton-Raphson Method

The Newton-Raphson method can be a powerful tool in the solution of operating problems for multicomponent distillation columns. In this solution process, however, the stability or converging speed of the Newton-Raphson iterative calculation is greatly dependent on the choice of independent variables and the definition of the functions to be zeroed. Kinoshita *et al.*²⁾ have developed a simulation procedure where liquid mole fractions for $(m-1)$ components are chosen for the independent variables and unique functions to be zeroed are introduced. The Newton-Raphson iterative calculation thus applied to the solution of the resultant nonlinear simultaneous equations shows remarkably high speed in achieving convergence. Stability is also quite high and the procedure tolerates rather wild initial estimates of the independent variables. This feature is very significant because in cases of highly nonideal solutions it is not easy to obtain good initial estimates of the liquid mole fractions. Another advantage is that the independent variables are always liquid mole fractions only, regardless of the incorporation or neglect of the heat balances. This advantage is also significant, because we sometimes wish to simulate the column without incorporating the heat balances. Because of the latter advantage, the procedure contrasts with some other

procedures (e.g. the Naphtali-Sandholm procedure⁵⁾) where the flow rates or component flow rates are included in the independent variables.

The present short communication extends the procedure to cases where the specifications of plate efficiencies need to be taken into account in the simulation.

1. Simulation Procedure

The model column is shown in Fig. 1. In cases of no

Fig. 1. Model column for computer simulation.

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chemical reactions, the component material balances are expressed by

$$\left. \begin{aligned} V_2 y_{i,2} - (L_1 + U_1) x_{i,1} - V_1 y_{i,1} &= 0 \\ L_{j-1} x_{i,j-1} + V_{j+1} y_{i,j+1} + F_j z_{i,j} \\ - (L_j + U_j) x_{i,j} - (V_j + W_j) y_{i,j} &= 0, \\ (j=2, \dots, N-1) \\ L_{N-1} x_{i,N-1} + F_N z_{i,N} - L_N x_{i,N} - V_N y_{i,N} &= 0 \end{aligned} \right\} \quad (1)$$

In the present study, the Murphree plate efficiencies (η_j 's)⁵ are introduced. Then, the relations among the vapor and liquid mole fractions are given by

$$\left. \begin{aligned} y_{i,1} &= y_{i,1}^* \\ y_{i,j} &= (1 - \eta_j) y_{i,j+1} + \eta_j y_{i,j}^*, \\ (j=2, \dots, N-1) \\ y_{i,N} &= y_{i,N}^* \\ y_{i,j}^* &= K_{i,j} x_{i,j}, \quad (j=1, \dots, N) \end{aligned} \right\} \quad (2)$$

The global material balances and heat balances are expressed by the following equations²:

$$\begin{aligned} L_j + V_2 - L_1 &= V_{j+1} + \sum_{k=2}^j (F_k - W_k - U_k) \\ L_j &= \left\{ L_1 h_1 - (L_1 + U_1 + V_1) H_2 + (V_1 + U_1) H_{j+1} \right. \\ &\quad \left. - H_{j+1} \sum_{k=2}^j (F_k - W_k - U_k) \right. \\ &\quad \left. + \sum_{k=2}^j (F_k H_{Fk} - W_k H_k - U_k h_k) \right\} / (h_j - H_{j+1}), \\ (j=2, \dots, N-1) \end{aligned} \quad (3)$$

The calculational procedure proposed is summarized below.

(1) If $x_{i,j}$'s ($i=1, \dots, m-1$; $j=1, \dots, N$) are given, $x_{m,j}$'s are also determined from

$$x_{m,j} = 1 - \sum_{k=1}^{m-1} x_{k,j} \quad (4)$$

(2) Then, $y_{i,j}^*$'s can be calculated by solving the following nonlinear equation for T_j by the Newton method:

$$\sum_{i=1}^m y_{i,j}^* = 1 \quad (5)$$

(3) By using Eq. (2) successively from $j=N$ to $j=1$, the vapor mole fractions, $y_{i,j}$'s, are all determined.

(4) The vapor and liquid enthalpies are now calculable, and by using Eqs. (4) and (3) alternately, V_j 's and L_j 's are all determined. In cases where the heat balances are not considered, this step is skipped.

(5) Equation (1) cannot be arranged in the tri-

diagonal matrix form because vapor mole fractions are not in equilibrium with liquid mole fractions. To recalculate liquid mole fractions, $X_{i,j}$'s, Eq. (1) is treated in the following prudent manner:

$$\left. \begin{aligned} X_{i,1} &= (V_2 y_{i,2} - V_1 y_{i,1}) / (L_1 + U_1) \\ X_{i,j} &= \{ F_j z_{i,j} + L_{j-1} X_{i,j-1} + V_{j+1} y_{i,j+1} \\ &\quad - (V_j + W_j) y_{i,j} \} / (L_j + U_j), \\ (j=2, \dots, N-1) \\ X_{i,N} &= (L_{N-1} X_{i,N-1} - V_N y_{i,N}) / L_N \end{aligned} \right\} \quad (6)$$

The above equations are used successively from $j=1$ to $j=N$. Thus, even in cases of 100% efficiencies, the present procedure is not identical with the previous one.²

(6) After normalizing $X_{i,j}$'s, the functions, $f_{i,j}$'s, are determined:

$$f_{i,j} = x_{i,j} - X_{i,j}, \quad (i=1, \dots, m-1; j=1, \dots, N) \quad (7)$$

Thus, $f_{i,j}$'s are treated as functions of $x_{i,j}$'s, and the following set of nonlinear equations are solved by using the Newton-Raphson method²:

$$\left. \begin{aligned} f_{1,1}(x_{1,1}, \dots, x_{m-1,N}) &= 0 \\ &\vdots \\ f_{m-1,N}(x_{1,1}, \dots, x_{m-1,N}) &= 0 \end{aligned} \right\} \quad (8)$$

The Jacobian matrix is numerically evaluated. It is obvious that the procedure can readily be extended to cases where chemical reactions are promoted.²

The initial estimates of the liquid mole fractions are obtained either from

$$x_{i,j}^0 = \sum_{j=1}^N z_{i,j} F_j / \sum_{j=1}^N F_j \quad (9)$$

or by using the successive approximation of the tridiagonal matrix algorithm (assuming 100% plate efficiencies)⁶ twice. The new values of the independent variables are calculated from

$$x_{i,j}^{r+1} = x_{i,j}^r + \Delta x_{i,j} \quad (10)$$

If any of the liquid mole fractions becomes minus, its value is changed to an infinitesimal one (e.g. $1.0E-10$) and the mole fractions are normalized.

2. Numerical Experiments

The preliminary computer program used in ref. 2 was first elaborated to shorten the computation time to a large extent. Then, the program was modified so that it can permit the specifications of Murphree plate efficiencies. Numerical experiments were then made by means of the FACOM M-380 SYSTEM at Japan Atomic Energy Research Institute (JAERI), for a

Table 1. Calculation conditions for numerical experiments

—Case 1—		
Water–furfural–acetone (Wilson's equation):		
$N=15$; $N_F=8$; feed mole fractions, (0.45, 0.05, 0.5);		
$R=2.5$; $D/F=0.5$; $\eta_j=1.0$ ($j=2, \dots, N-1$).		
—Case 2—		
Acetone–methanol–chloroform (Wilson's equation):		
$N=20$; $N_F=10$; feed mole fractions, (0.45, 0.22, 0.33);		
$R=3.0$; $D/F=0.7$; $\eta_j=0.9$ ($j=2, \dots, N-1$).		
—Case 3—		
Acetone–methanol–water (Wilson's equation):		
$N=22$; $N_F=10$; feed mole fractions, (0.3, 0.3, 0.4);		
feed temperature = 323.15 K; $R=2.0$; $D=30$ mol/h;		
$F=100$ mol/h; $B=50$ mol/h; $N_{SV}=15$; $N_{SL}=5$;		
$U_s=W_s=10$ mol/h; $\eta_j=0.8$ ($j=2, \dots, N-1$).		
—Case 4—		
Methanol–ethanol–water (Margules 3-equation):		
$N=30$; $N_F=15$; feed mole fractions, (0.5, 0.2, 0.3);		
feed temperature = 345.0 K; $R=3.5$; $D/F=0.5$;		
$\eta_j=0.7$ ($j=2, \dots, N-1$).		

In all cases, the operating pressure is 101.3 kPa, and the feed is supplied in liquid state. Total condensers are used except in case 3. Heat balances are incorporated in cases 3 and 4. The physicochemical properties are given in ref. 2.

Table 2. Number of total iterations and computation time needed

Case	r_i	t [s]
1	3	0.15
2	2	0.19
3	4	0.42
4	3	0.67

The simplest method of Eq. (11) is used in all cases. In cases 2 and 3 only, the liquid mole fractions obtained by using the tridiagonal matrix algorithm twice are regarded as initial estimates. However, even if Eq. (10) is used in cases 2 and 3, the converged solutions are obtained in fourteen and eight iterations, respectively, in which case Eq. (11) is used with no damping factor.

total of four cases as summarized in **Table 1**. The problem was considered solved once the following criterion was satisfied:

$$J = \sum_{j=1}^N \sum_{i=1}^{m-1} |f_{i,j}| / \{(m-1)N\} < 1.0E-4 \quad (12)$$

As given in **Table 2**, the converged solutions were obtained in two to four iterations. The computation time is quite short. For cases 1 and 4, the wild initial estimates by Eq. (10) and the simplest form expressed by Eq. (11) with no damping factor are used, yet the solutions are obtained in only three iterations. The convergence characteristics are shown in **Fig. 2**. It should be noted that the authors^{2,3)} have used absolute values of $f_{i,j}$'s rather than squares of the residuals which have frequently been used by other workers, because the use of the latter exaggerates the

Fig. 2. Convergence characteristics observed in numerical experiments.

converging speed unnecessarily. Nevertheless, **Fig. 2** indicates remarkably high speed in achieving convergence. Another significant result is that the manner expressed by Eq. (7) is essential, and if $X_{i,j}$'s on the right side are replaced by $x_{i,j}$'s, the convergence characteristics are greatly deteriorated. The great stability is not vitiated at all, even in cases where the efficiency varies from stage to stage. In case 4, for example, η_2 and η_{N-1} are assumed to be 0.5 and 0.9, respectively, and the other efficiencies are determined by using the assumption of linear variation. The solutions are readily obtained in only three iterations. It is obvious that the simulation procedure can also be used in cases of ideal solutions. As an example, the simulation problem on page 78 in ref. 1 is solved by using Eqs. (10) and (11) with no damping factor. The solutions are readily obtained in only four iterations.

The procedure now permits the specifications of Murphree plate efficiencies in the simulation. Its great stability and high converging speed are verified. The computation time may further be shortened by using the hybrid method⁴⁾ in the solution of Eq. (9).

Nomenclature

B	= flow rate of bottom product	[mol/h]
D	= flow rate of top product	[mol/h]
F_j	= flow rate of feed stream supplied to j -th stage	[mol/h]
$f_{i,j}$	= function to be zeroed defined by Eq. (8)	[—]
H_j	= molar enthalpy of vapor stream leaving j -th stage	[J/mol]
H_{Fj}	= molar enthalpy of feed stream supplied to j -th stage	[J/mol]
h_j	= molar enthalpy of liquid stream leaving j -th stage	[J/mol]
J	= average value of absolute of residual functions defined by Eq. (12)	[—]
$K_{i,j}$	= vapor-liquid equilibrium ratio for component i on j -th stage	[—]

L_j	= flow rate of liquid stream leaving j -th stage	[mol/h]	η_j	= Murphree plate efficiency	[—]
m	= total number of components	[—]	<Subscripts>		
N	= number of total stages	[—]	i	= component index ($= 1, \dots, m$)	
N_F	= feed stage number	[—]	j	= stage index ($= 1, \dots, N$)	
N_{SL}	= liquid sidestream stage number	[—]	<Superscript>		
N_{SV}	= vapor sidestream stage number	[—]	r	= iteration number	
R	= reflux ratio	[—]	Literature Cited		
r_i	= number of total iterations	[—]			
T_j	= temperature on j -th stage	[K]	1)	Hirose, Y.: "Joryu Keisanho No Kiso," Baifukan, Tokyo (1975).	
t	= computation time needed	[s]	2)	Kinoshita, M., I. Hashimoto and T. Takamatsu: <i>J. Chem. Eng. Japan</i> , 16 , 370 (1983).	
U_j	= flow rate of liquid sidestream from j -th stage	[mol/h]	3)	Kinoshita, M., I. Hashimoto and T. Takamatsu: <i>J. Chem. Eng. Japan</i> , 16 , 513 (1983).	
U_S	= flow rate of liquid sidestream	[mol/h]	4)	Mah, R. S. H. and T. D. Lin: <i>Computers and Chem. Eng.</i> , 4 , 75 (1980).	
V_j	= flow rate of vapor stream leaving j -th stage	[mol/h]	5)	Naphtali, L. M. and D. P. Sandholm: <i>AIChE J.</i> , 17 , 148 (1971).	
W_j	= flow rate of vapor sidestream from j -th stage	[mol/h]	6)	Wang, J. C. and G. E. Henke: <i>Hydrocarbon Processing</i> , 45 , 155 (1966).	
W_S	= flow rate of vapor sidestream	[mol/h]			
$X_{i,j}$	= liquid mole fraction calculated from Eq. (7)	[—]			
$x_{i,j}$	= liquid mole fraction	[—]			
$y_{i,j}$	= vapor mole fraction	[—]			
$y_{i,j}^*$	= vapor mole fraction in equilibrium with $x_{i,j}$	[—]			
$z_{i,j}$	= feed mole fraction	[—]			

A TWO-DIMENSIONAL MODEL FOR THE SECONDARY FLOW IN AN AGITATED VESSEL WITH ANCHOR IMPELLER

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Key Words: Agitation, Anchor Agitator, Secondary Flow, Numerical Analysis, Laminar Flow

The primary flow produced by an anchor impeller has been studied by many investigators.^{1,2,4-6)} This work has provided significant information about mixing, heat transfer and especially power consumption. However, the temperature or concentration profile in an anchor-agitated vessel is mainly controlled by the secondary flow in the axial direction.

In this work, a two-dimensional model for the secondary flow was proposed to express the flow field in the vertical plane of an anchor-agitated vessel and a numerical study was conducted for a Newtonian fluid.

1. Model Description

A two-dimensional model for a flow-through anchor-agitated vessel is shown in Fig. 1. In this

model, in order to eliminate the velocity gradients in the θ -direction, a cylinder identical in thickness to the width of the blade is placed at the blade position to rotate with a constant angular velocity ω instead of an actual anchor impeller. A Newtonian fluid flows into the vessel from the bottom and passes out from the top. The fluid can pass freely through the rotating cylinder in both the z - and r -directions but not in the θ -direction.

With these assumptions, the governing equations and the boundary conditions for a fully developed laminar flow are as follows:

continuity equation

$$\frac{v_r}{r} + \frac{\partial v_r}{\partial r} + \frac{\partial v_z}{\partial z} = 0 \quad (1)$$

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