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An Algorithm for Solving Countercurrent Extraction Processes

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Abstract

A computational algorithm for solving multistage countercurrent extraction processes has been developed. The algorithm is based on correlating liquid–liquid equilibrium data. Solute and solvent balances between the phases are checked on each stage. Excellent agreement between the computation results and that of the graphical method has been obtained. This technique can be used for optimization and determination of the minimum solvent rates.

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1. INTRODUCTION

A separation of components by liquid–liquid extraction depends on the distribution of components (solutes) between two liquid solvents. The two solvents must be immiscible, but the most commonly encountered solvents are partially miscible.

In the most simple case the feed solution containing the solute to be extracted is introduced into a vessel where the extracting solvent is added and mixed with the feed. The solute distributes between the two phases until equilibrium is approached. The dispersion is then transferred into a settling vessel where the phases, extract and raffinate, are separated. Extraction in such a single stage may not be sufficient to remove all solute present in the feed solution. The raffinate may then be introduced into a similar stage or stages, the number of which depends upon the degree of separation required.

The flow of the feed solution and solvent from stage to stage may be countercurrent or cross-current. Computations of such problems are usually performed on triangular coordinates or on solute-free coordinates. Analytical solutions are only possible if some approximations are intro-

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duced, such as using linear distribution relations and assuming constant flow rates throughout the mixer-settlers cascade (*1*).

Graphical methods are usually more accurate than analytical methods, especially in extraction problems dealing with partially miscible solvents since graphical methods take into consideration the balance of all the components in the system whereas analytical methods are usually based on solute balance. Therefore, developing accurate models representing the distribution relations of the solvents in the two phases of an extraction system will allow for simulation and accurate computation of such processes.

Different trials based on thermodynamic principles have been made for correlating these data systems, with varying degrees of success (*2*, *3*). The UNIQUAC equation is considered more accurate than other expressions. However, this correlation is still under continuous development in order to improve its ability to predict and/or to correlate available data systems (*2*). A modified version of the UNIQUAC equation proposed by Anderson and Prausnitz (*4*) and recommended by Perry (*3*) was found to produce an average absolute error in distribution coefficients of 5.9% in correlating some Type 1 systems as reported by Simonetty et al. (*5*). However, Rose and Kyka (*6*) stated that 5% error in the prediction of the activity coefficient can represent a 10% to 50% error in the separation per stage.

In this work a technique has been developed to simulate countercurrent extraction processes based on accurate correlation models for liquid–liquid data system which had been developed earlier by Salem and Sheirah (*7*). Such models can be easily used for any liquid system, especially when graphical methods become difficult in cases of small distribution coefficients or small immiscibility areas.

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2. CORRELATION OF LIQUID–LIQUID DATA

Recently, Salem and Sheirah (*7*) presented an efficient and accurate technique for correlating liquid–liquid data systems in simple models which can be incorporated in computer simulation programs for purposes of comprehensive analysis, optimization, and solvent selection in an extraction process. The technique has been tested by more than 30 different ternary and pseudoternary systems. Excellent agreement has been obtained between the data generated from the correlations and experimental data (*7*). This technique is developed for a ternary system, A-B-C, which contains a carrier solvent, A, a partially miscible extracting solvent, B, and a solute, C, which is totally miscible with both solvents. The basic idea in this technique is to express the solubility data as polynomials of a single pa-

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rameter Z. Given the solute concentration, W_C, one can express the parameter Z in the form

$$Z = P(W_C) \tag{1}$$

The value of Z obtained is then used to correlate the concentration of solvent A or B in the system by the polynomials

$$W_A = PA(Z) = \sum_i a_i Z^i \tag{2}$$

and

$$W_B = PB(Z) = \sum_i b_i Z^i \tag{3}$$

where the coefficients of the polynomials, a_i and b_i, are obtained by least-squares techniques. The parameter Z is defined in such a way as to make it a single-valued function of W_C that falls in the range 0 to 1. A suitable expression for Z is

$$Z = \frac{W_B + KW_C - W^\circ_{BA}}{W^\circ_{BB} - W^\circ_{BA}} \tag{4}$$

where K is a constant chosen to minimize the error variance in the fitting of the data by Eq. (2); W_B and W_C are the mass fractions of Components B and C, respectively; W°_{BB} is the mass fraction of Component B saturated with A; and W°_{BA} is the mass fraction of Component B in Phase A saturated with B. W°_{BA} and W°_{BB} are thus the $W_C = 0$ end-points of the binodal curve.

From Eqs. (1), (2), and (3) the concentrations of the components in a liquid system or phase can be estimated. This model will be incorporated in the extraction algorithm proposed here.

3. DEVELOPING THE COUNTERCURRENT EXTRACTION COMPUTATION MODEL

Refer to Fig. 1, which shows the flow sheet for a multistage countercurrent cascade. In this process the feed solution R_0, composed of the carrier solvent, A, and the solute, C, is brought into contact with the selective solvent, B, in a number of stages, N. The raffinate and extract

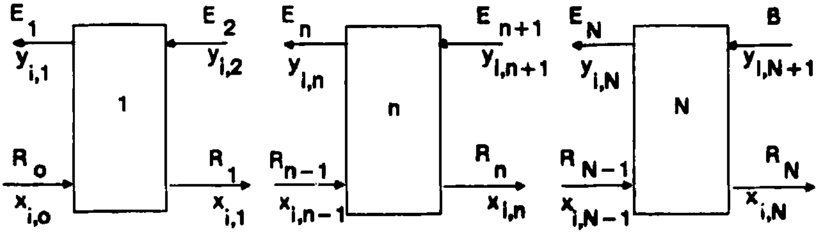

FIG. 1. Flow in a countercurrent extraction system.

phases coming out of each stage, n, are given by R_n and E_n, respectively. Applying total and solute material balances on the cascade gives

$$R_0 + B = R_N + E_1 \tag{5}$$

$$R_0 x_{C,0} + B y_{C,N+1} = R_N x_{C,N} + E_1 y_{C,1} \tag{6}$$

R_0, B, $x_{C,0}$ and $y_{C,N+1}$ are usually specified in such problems. A target value for $x_{C,N}$ is also assumed. The values of R_N, E_1, and $y_{C,1}$ have to be estimated. One of these unknowns has to be assumed in order to solve Eqs. (5) and (6). Therefore, assuming a value for E_1:

$$E_1 = B + R_0(x_{C,0} - x_{C,N}) \tag{7}$$

and using this value of E_1 in Eqs. (5) and (6) gives

$$R_N = R_0 + B - E_1 \tag{8}$$

and

$$y_{C,1} = (R_0 x_{C,0} + B y_{C,N+1} - R_N x_{C,N})/E_1 \tag{9}$$

The solute concentration in the extract stream from Stage 1 is calculated from Eq. (9). This has to be checked by estimating the solvents concentrations in the same streams by using Eqs. (2) and (3), and then applying a solvent balance on the whole system.

This is done by calling a subroutine, "solubility," which is based on the model discussed before. However, another polynomial representing the distribution relation will be added to reduce the number of trials. Hence, given a solute concentration of a raffinate stream from a certain stage x_{CA},

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the solvents concentrations associated with it can be obtained from Eqs. (1) and (2) written for the raffinate phase as

$$Z1 = P1(x_{\mathrm{CA}}) \tag{10}$$

$$x_{\mathrm{AA}} = PA(Z1) \tag{11}$$

and then

$$x_{\mathrm{BA}} = 1 - (x_{\mathrm{AA}} + x_{\mathrm{CA}}) \tag{12}$$

Similarly, for a solute concentration of an extract stream from a certain stage, y_{CB}, the solvent concentrations associated with it are calculated from Eqs. (1) and (2) written for the extract phase as

$$Z2 = P2(y_{\mathrm{CB}}) \tag{13}$$

$$y_{\mathrm{AB}} = PA(Z2) \tag{14}$$

and then

$$y_{\mathrm{BB}} = 1 - (y_{\mathrm{AB}} + y_{\mathrm{CB}}) \tag{15}$$

If the extract solute concentration in a stage n, y_{CB}, is given, the composition of the raffinate phase in equilibrium with this extract phase can be estimated from the equilibrium relation

$$x_{\mathrm{CA}} = P3(y_{\mathrm{CB}}) \tag{16}$$

Equations (10), (11), and (12) are then used to estimate the associated solvents in the raffinate stream.

Now, using the values for $x_{\mathrm{C},0}$, $x_{\mathrm{C},N}$, and $y_{\mathrm{C},1}$—estimated from Eq. (9)—in the solubility subroutine gives the corresponding solvents concentrations $x_{\mathrm{A},0}$, $x_{\mathrm{A},N}$, $x_{\mathrm{B},N}$, $y_{\mathrm{A},1}$, and $y_{\mathrm{B},1}$. Considering that $y_{\mathrm{C},N+1} = 0$, then $y_{\mathrm{B},N+1} = 1$ and also $x_{\mathrm{B},0} = 0$. Applying a Solvent A balance on the system gives

$$R_0 x_{\mathrm{A},0} + \mathrm{B} y_{\mathrm{A},N+1} = R_N x_{\mathrm{A},N} + E_1 y_{\mathrm{A},1} \tag{17}$$

$$R_N = (R_0 x_{\mathrm{A},0} - E_1 y_{\mathrm{A},1})/x_{\mathrm{A},N} \tag{18}$$

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Similarly, a Solvent B balance gives

$$R_0x_{B,0} + By_{B,N+1} = R_Nx_{B,N} + E_1y_{B,1} \tag{19}$$

Then from Eqs. (18) and (19):

$$E_1 = \frac{(By_{B,N+1} - R_0x_{A,0}x_{B,N}/x_{A,N})}{(y_{B,1} - y_{A,1}x_{B,N}/x_{A,N})} \tag{20}$$

The value of E_1 estimated from Eq. (20) is compared with that of Eq. (7). If the comparison is not within a certain convergence limit, then E_1 of Eq. (20) is used to reevaluate Eqs. (8) and (9). The previous steps are repeated until the correct values of E_1 and R_N are obtained. The composition of the extract stream E_1 is also recalculated; $y_{i,1}$. The composition of the raffinate stream from Stage 1, $x_{i,1}$, can be calculated from the solubility correlations (16), (10), (11), and (12).

Rearranging Eq. (5) gives

$$E_1 - R_0 = B - R_N = \Delta \tag{21}$$

from which Δ can be estimated.

Applying material balance for Stages n through N gives

$$E_{n+1} - R_n = B - R_N = \Delta \tag{22}$$

R_N can be roughly estimated by assuming total immiscibility of solvents. Therefore,

$$R_N = R_0(1 - (x_{C,0} - x_{C,N})) \tag{23}$$

and since for any Stage n,

$$R_N = R_n(1 - (x_{C,n} - x_{C,N})) \tag{24}$$

then R_n can be calculated from Eq. (24) as

$$R_n = R_N/(1 - (x_{C,n} - x_{C,N})) \tag{25}$$

and E_n can be estimated from Eq. (22) as

$$E_n = R_{n-1} + \Delta \tag{26}$$

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Applying a solute balance on any Stage n gives

$$R_{n-1}x_{C,n-1} + E_{n+1}y_{C,n+1} = R_n x_{C,n} + E_n y_{C,n} \tag{27}$$

R_n and E_{n+1} are calculated from Eqs. (25) and (26). Then, from Eq. (27):

$$y_{C,n+1} = (R_n x_{C,n} + E_n y_{C,n} - R_{n-1}x_{C,n-1})/E_{n+1} \tag{28}$$

Using the values of $x_{C,n}$ and $y_{C,n+1}$ in the solubility correlations gives $x_{A,n}$, $x_{B,n}$, $y_{A,n+1}$, and $y_{B,n+1}$. Therefore, a Solvent A balance can be applied on Stage n:

$$R_{n-1}x_{A,n-1} + E_{n+1}y_{A,n+1} = R_n x_{A,n} + E_n y_{A,n} \tag{29}$$

Substituting from Eq. (26) into Eq. (29) and rearranging, we get

$$R_n = (R_{n-1}x_{A,n-1} + \Delta y_{A,n+1} - E_n y_{A,n})/(x_{A,n} - y_{A,n+1}) \tag{30}$$

This value of R_n is compared with that calculated from Eq. (25). If they do not agree, the estimated R_n from Eq. (30) is used in Eq. (26) to get E_{n+1}, which is used in Eq. (28), and the procedure is iterated until convergence occurs. The above steps are first applied with $n = 1$, and then n is incremented and the procedure repeated in the same way until the resulting value of $x_{C,n}$ is less than or equal to the specified $x_{C,N}$. This determines the number of stages, the flow rates from each stage, and the total composition of each stream. A flow chart showing the steps of the algorithm is given as Fig. 2.

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4. EXAMPLE

This computation technique has been used to solve the problem of extracting acetic acid, C, from water, A, by isopropyl ether, B, using the data given by Treybal (*1*), where R_0 = 8000 kg/h, B = 20,000 kg/h, $x_{C,0}$ = 0.3 mass fraction, and $x_{C,N}$ = 0.02 mass fraction. The data for this system have been correlated by the polynomials shown in Table 1. A program has been written in Pascal for solving this problem on an IBM PC.

The computation results are given in Table 2. This table shows that for the specified $x_{C,N}$ = 0.02, 8.2 theoretical stages are required. Graphical calculations by Treybal gave N = 7.6. These calculations have been checked graphically many times and found to be 8. E_1 and R_N estimated by this technique are 22,923.7 and 5076.33 kg/h compared with 23,000 and

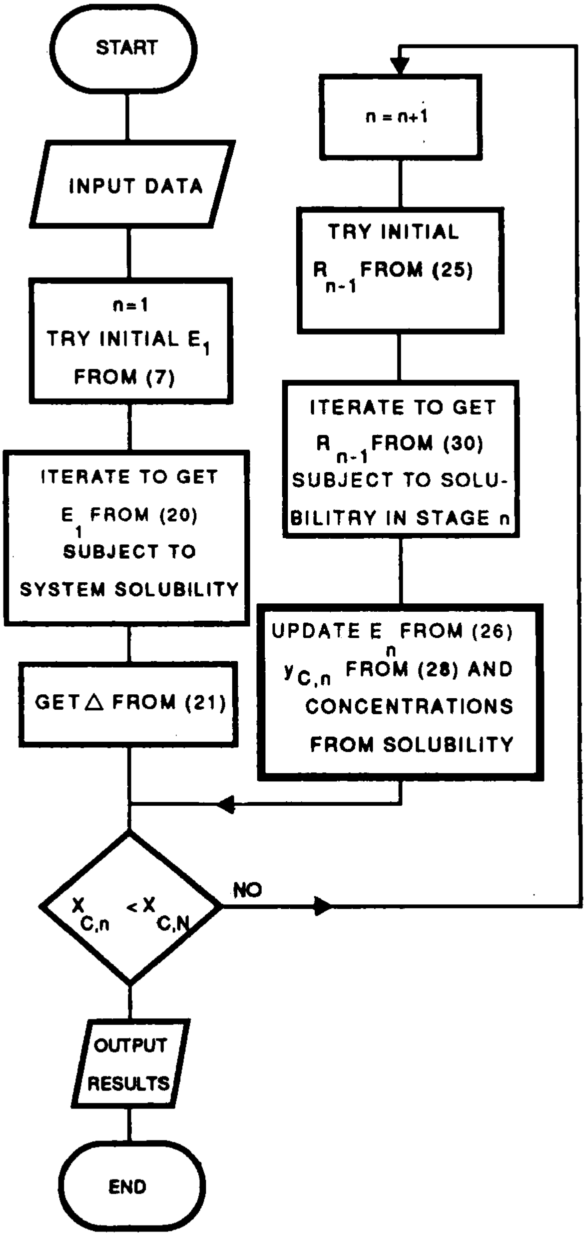

FIG. 2. General flow chart of the algorithm.

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TABLE 1

Coefficients of Polynomials for the Solubility Subroutine of the System Water (A)–Isopropyl Ether (B)–Acetic Acid (C) at 20°C[a]

No.	Polynomial	n	a_0	a_1	a_2	a_3	a_4	K	Variance
1	$x_A = PA(Z1)$	3	99.283E-2	−98.5085E-2	−0.6481E-2	0.3628E-2	0	1	0.001
2	$Z1 = P1(x_C)$	3	−15.767E-4	15,225.4E-4	−345,175E-4	65,246.7E-4	0	—	0.0008
3	$Z2 = P2(y_C)$	3	0.9994519	−0.28728867	0.6026306	−0.2522628	0	—	0.0005
4	$x_C = P3(y_C)$	4	5.309E-3	3.181	−11.61	27.7	−2.818	—	0.012

[a] The mutual solubility of the solvents at zero solute concentrations for this system are not given in the published data (7). They were estimated by extrapolation; therefore $W^{\circ}_{BA} = 0.007$ mass fraction and $W^{\circ}_{BB} = 0.995$ mass fraction.

TABLE 2

Simulation Results for $X_{C,0}$ = 0.3, $X_{C,N}$ = 0.02, R = 8000, and B = 20,000 kg/h

I	E	R	x_C	y_C
1	2.292367E+04	7.284943E+03	2.352349E−01	1.003026E−01
2	2.220861E+04	6.715563E+03	1.856322E−01	7.262842E−02
3	2.163923E+04	6.318837E+03	1.452953E−01	5.295607E−02
4	2.124251E+04	6.013896E+03	1.120937E−01	3.847951E−02
5	2.093757E+04	5.764989E+03	8.428727E−02	2.738733E−02
6	2.068866E+04	5.554981E+03	6.069196E−02	1.861982E−02
7	2.047865E+04	5.375154E+03	4.053170E−02	1.154601E−02
8	2.029883E+04	5.220558E+03	2.328875E−02	5.772160E−03
9	2.014423E+04	5.076329E+03	8.594399E−03	1.036733E−03

I	x_A	x_B	y_A	y_B
1	7.457087E−01	1.905638E−02	3.040677E−02	8.692906E−01
2	7.917807E−01	2.258707E−02	2.384518E−02	9.035264E−01
3	8.283654E−01	2.633928E−02	1.915090E−02	9.278930E−01
4	8.598208E−01	2.808543E−02	1.560445E−02	9.459160E−01
5	8.882025E−01	2.751021E−02	1.280238E−02	9.598103E−01
6	9.144011E−01	2.490690E−02	1.052065E−02	9.708595E−01
7	9.387285E−01	2.073982E−02	8.629130E−03	9.798249E−01
8	9.612074E−01	1.550386E−02	7.047752E−03	9.871801E−01
9	9.817363E−01	9.669314E−03	5.723469E−03	9.932398E−01

5000 kg/h by Treybal (*1*), with percentage errors of 0.33 and 1.5%. However, an average Murphree Efficiency for the unit has to be assumed (say 0.8) and then the actual number of stages required can be estimated by dividing the number of equilibrium stages calculated from the model by the efficiency (8.2/0.8 = 10 in this example). This program can be used to optimize the process by using different values of Solvent B to get the number of stages required for each solvent rate and, hence, the optimum number of stages can be determined. This is shown in Table 3 and Fig. 3. Figure 3 shows that the minimum number of stages required is around 4 and the minimum phase ratio is 1.6875 compared with 1.63 obtained by the graphical method given by Treybal (*1*).

TABLE 3

Results of Using Different Solvent Rates, B kg/h, for a Certain Feed Flow Rate R_0 = 8000 kg/h and $x_{C,N}$ = 0.02

B (kg/h)	B/R_0	N	E_1	R_N	$y_{C,1}$
20,000	2.5	9	22,923.7	5076.33	0.100303
17,500	2.1875	13	20,408.2	5091.81	0.112675
15,000	1.875	33	17,892.0	5108	0.128407

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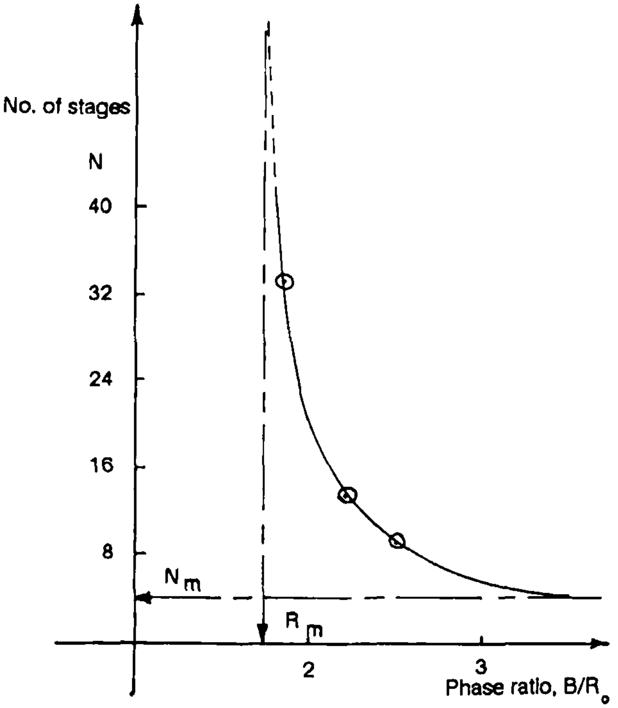

FIG. 3. Determination of minimum phase ratio and number of stages.

The minimum solvent rate can be accurately calculated by this program. As the minimum rate is approached, the number of stages increases rapidly and some arbitrary number, such as 50, may be chosen to approximate the case of an infinite number of stages.

5. CONCLUSIONS

An iterative computation technique is developed for calculating the number of stages required in countercurrent extraction problems. The minimum phase ratio and minimum number of stages can also be calculated. Total composition and flow rates of the streams from each stage can also be estimated. The results of this computation are more accurate than those obtained by graphical techniques. This technique requires correlating the equilibrium data of the system by accurate models which can generate the concentrations of all the components involved in the system. A similar computation technique can be developed for cross-current extraction problems.

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NOMENCLATURE

A	carrier solvent, raffinate phase, flow rate of Solvent A (kg/h)
a_i	coefficients of the Polynomial 2
B	extracting solvent, extract phase, flow rate of Solvent B (kg/h)
b_i	coefficients of Polynomial 3
C	solute
E	extract phase flow rate (kg/h)
K	constant in Eq. (1) obtained by trial and error
N	total number of stages
n	stage number
P	polynomial
R	raffinate phase flow rate (kg/h)
W_i	mass fraction of Component *i* in the system
W°_{AB}	mass fraction of A in B at zero concentration of Solute C
W°_{BA}	mass fraction of B in A at zero concentration of Solute C
x, y	concentration of Component A, B, or C in raffinate and extract phases, respectively, mass fraction
Z	parameter defined by Eq. (1); its value ranges from 0 to 1
Δ	constant defined by Eq. (21)

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