"SIMULATION OF CROSS-CURRENT EXTRACTION PROCESSES"

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ABSTRACT

Extraction processes dealing with partially miscible solvents are usually calculated by graphical methods to estimate the number of stages required, flow rates and compositions of the streams. Such procedures may be lengthy. Alternative calculation procedures are usually based on such simplifying assumptions as constant flow rates and linearization of the distribution relations.

An algorithm for simulating multiple contact cross-current extraction processes has been developed. The algorithm is based on correlating liquid-liquid equilibrium data. No simplifying assumptions are introduced. Excellent agreement between the simulation results and that of the graphical methods has been obtained.

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 attained.

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 the 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 counter current or cross-current. In multi-stage cross current extraction the raffinate is successively contacted with fresh solvent as shown in Figure 1. Computations of such problems are usually performed on triangular coordinates, or on solute free coordinates. Analytical solutions are only possible if some approximations are introduced as using linear distribution relations and assuming constant flow rates throughout the mixer-settlers cascade (1).

Simulation of such processes requires that the equilibrium data should be represented by fairly accurate mathematical models.

In this work a technique has been developed for simulating multiple contact cross-current extraction processes. No simplifying assumptions have to be introduced.

2. CROSS-CURRENT CONTACT EXTRACTION WITH PARTIALLY MISCIBLE SOLVENTS

In these processes the feed solution, R_o, composed of the carrier solvent A and the solute C, is brought into contact with the selective solvent S_1, containing the extracting solvent B, to give raffinate, R_1, and an extract, E_1. If multiple contact is used the flow of the streams will be as shown in Figure 1. X and y are the concentrations of the solute in the raffinate and extract streams, mass fractions, respectively. Computations of such problems are usually performed on triangular coordinates, or on solvent-free coordinates, (1) in order to get fairly accurate results. Equal amounts of solvent may be used in the various stages. In case of a temperature profile being used on the different stages, each stage must be computed with the help of a phase diagram at the appropriate temperature.

3. CORRELATION OF LIQUID-LIQUID DATA

Stage-wise extraction problems are represented by non-linear finite difference equations. Accurate solution of these equations by computer requires that the equilibrium data should be represented by mathematical models. Recently, Salem and
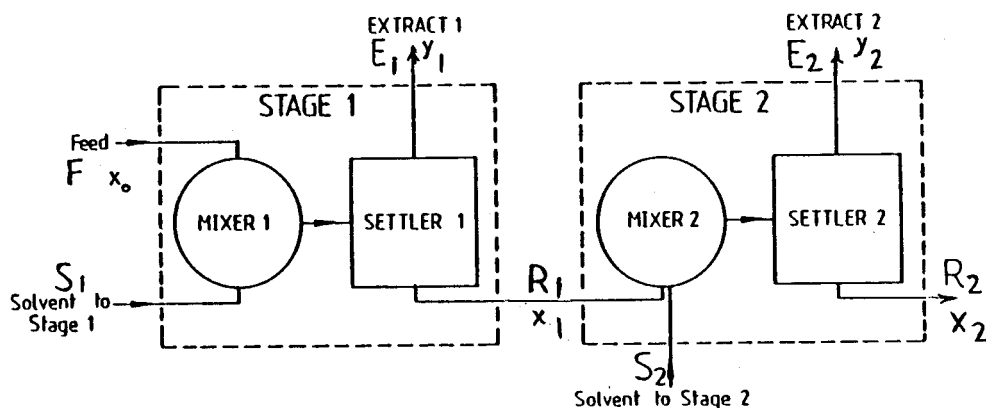
Figure 1: Multi-Stage Crossflow Extraction.

Sheirah (2) presented an efficient and accurate technique for correlating liquid-liquid data in simple models which can be easily computerized for purposes of comprehensive analysis of extraction processes and selection of solvents. The technique has been tested with different ternary and quaternary systems and excellent agreement has been obtained between the computation results and experimental data. The solubility data for a ternary system A-B-C which are usually displayed in tables or in triangular diagrams can be represented on a rectangular diagram as shown in Figure 2, where the concentration of each component is plotted against a parameter Z, defined as:

$$Z = \frac{W_B + KW_C - W^0_{BA}}{W^0_{BB} - W^0_{BA}} \tag{1}$$

W^0_{BB} is the mass percent of component B saturated with A. W^0_{BA} is the mass percent of component B in the co-existing phase A saturated with B. W^0_{BA} and W^0_{BB} are the $W_c = 0$ end-points of the binodal curve. K is a constant obtained by trial and error. A recursive least squares technique has been used for correlating the data required in any extraction, azeotropic or extractive distillation computations.
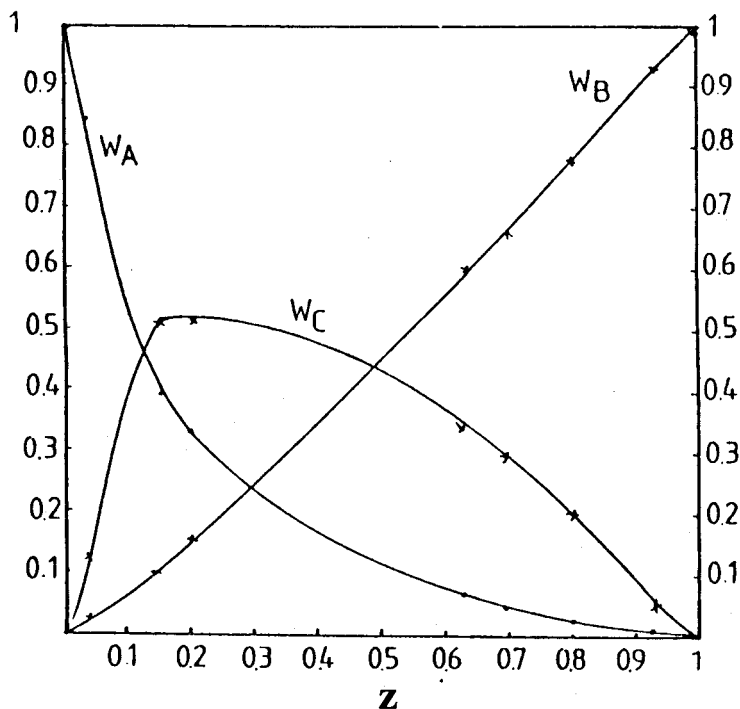
Figure 2: Representation of n-heptane, sulfolane + 10% 2-propane, toluene system at 30°C on a rectangular coordinates against z (1).

This technique has been used to simulate the system water (A)-isopropyl ether (B)-acetic acid (C) (1). The correlations developed (2) were:

$$W_A = P_1(Z) \tag{2}$$
$$W_B = P_2(Z) \tag{3}$$
$$W_{cB} = P_3(W_{CA}) \tag{4}$$
$$W_{BB} = P_4(W_{BA}) \tag{5}$$

P_1, P_2, P_3 and P_4 are polynominals of degree n, where n = 3 or 4.

The data obtained for this system are displayed in Table 1. These four polynominals provide the mathematical representation of liquid-liquid equilibrium data required for computer solution of extraction processes.

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Table 1: Water System (A)- Isopropyl ether (B)- Acetic acid (C) at 20⁰C (2).

No.	Polynomial	n	Coefficients					K	Variance
			a_0	a_1	a_2	a_3	a_4		
1	$W_A = P_1(Z)$	3	99.2827	−98.5085	−0.6481	0.3628	—	1	0.001
2	$W_B = P_2(Z)$	4	0.6704	93.8379	14.0867	−13.6207	4.5674	0.01	0.0027
3	$W_{CB} = P_3(W_{CA})$	3	−0.00123	0.2567	0.0058	0.00012	–	–	0.7365
4	$W_{BB} = P_3(W_{BA})$	4	90.963	14.575	−7.49	0.8459	−0.0276	–	3.3036

4. SIMULATING MULTIPLE CONTACT CO-CURRENT EXTRACTION

Applying total and solute material balances on stage 1 in Figure 1 gives

$$R_o + S_1 = R_1 + E_1 \tag{6}$$
$$R_o x_o + S_1 y = R_1 x_1 + E_1 y_1 \tag{7}$$

For pure solvent, $y = o$

From the equilibrium relation,

$$y_1 = m_1 x_1 \tag{8}$$

m = distribution coefficient.

Solving these equations:

$$x_1 = \frac{R_o x_o}{R_1 + (R_o + S_1 - R_1)m_1} \tag{9}$$

rearranging this equation gives:

$$\frac{R_1}{R_o} = \left(\frac{1}{1-m_1}\right)\left(\frac{x_o}{x_1}\right) - \left(\frac{m_1}{1-m}\right)\left(1+\frac{S_1}{R_o}\right) \tag{10}$$

This equation contains two unknowns, R_1 and x_1.

Assuming a value for x_1 ($< x_o$) the value of $m_1(x_1)$ can be obtained from Equation 4, and R_1 calculated. Generally (R_1/R_o) should be less than 1, otherwise another value for x_1 should be assumed. As R_1 is calculated, E_1 and y_1 can be computed using Equations 6 and 7 respectively.

A mass balance on the solvent components A and B in this stage proves that the

assumed value of x_1 is correct within a certain convergence criterion. Otherwise another value should be tried. To do so, the total composition of the raffinate R_1 and extract E_1 is determined. Noting that the raffinate is phase A and the extract is phase B. In phase A the solute concentration $x_1 = W_{CA}$ is known. To determine the other two components assuming a value for Z, then from equation 1:

$$W_{BA} = Z (W°_{BB} - W°_{BA}) + W°_{BA} - KW_{CA} \tag{11}$$

using the parameters of the polynomial P_1 from Table 1, then

$$W_{AA} = P_1 (Z) \tag{12}$$

Now if

$$W_{CA} + W_{BA} + W_{AA} = 100 \tag{13}$$

The assumed value of z is correct. Otherwise another value is to be tried. The composition of the extract phase B is calculated. Since W_{CB} is known ($W_{CB} = y_1$) so to calculate W_{BB} and W_{BA}:

$$W_{BB} = P_4 (W_{BA}) \tag{14}$$

$$W_{AB} = 100 - (W_{BB} + W_{CB}) \tag{15}$$

Checking for the solvent balance:

$$S_1 = R_1(W_{AB}) + E_1(W_{BB}) \tag{16}$$

$$R_o(1-x_o) = R_1(W_{AA}) + E_1(W_{AB}) \tag{17}$$

If these two equalities are satisfied then all the assumptions are correct. Otherwise another value for x_1 is to be tried. This procedure is followed from stage-to-stage to the final required raffinate concentration. The general formula applied for any stage n is given by:

$$\frac{R_n}{R_{n-1}} = \left(\frac{1}{1-m_n} \cdot \frac{x_{n-1}}{x_n} \right) - \left[\frac{m_n}{1-m_n} \cdot \left(1+\frac{S_n}{R_{n-1}} \right) \right] \tag{18}$$

This algorithm has been used to solve the extraction of acetic acid from water solution by isopropyl ether (1). A numerical example — similar to that used by Treybal (1) is used in this study for illustration and to compare the results of the developed technique with the graphical one. It is required to reduce the concentration of acetic acid (C) in a 100 Kg/hr water (A) solution containing 30% acid to 20% acid using a multi-stage cross current unit. Solvent was introduced at a rate of 40 Kg/hr to each stage. Determine the number of stages, rates and compositions of various streams. The results are given in Table 2 . Excellent agreement has been obtained between the simulation results and the graphical computations.

Table (2): Computation Results Using The Rigorous Simulation .

n	Raffinate Phase					Extract Phase				
	X_C	Z	X_B	X_A	R	Y_C	Z	Y_B	Y_A	E
	0.254	0.2834	0.0330	0.713	100.9	0.1107	0.9658	0.8505	0.0388	39.1
1	0.256	0.287	0.0342	0.7098	98.15	0.1155	0.964	0.844	0.0405	41.85
	0.258	0.289	0.0345	0.7075	96.4	0.117	0.9635	0.842	0.041	43.6
2	0.2263	0.2523	0.03	0.7437	90.975	0.0943	0.971	0.8707	0.035	45.425
	0.227	0.255	0.0315	0.7415	90.32	0.0948	0.9689	0.8695	0.0357	46.08
3	0.2	0.2247	0.029	0.771	84.85	0.0776	0.9768	0.8945	0.0279	45.47

5. CONCLUSION

A computation technique has been developed to replace lengthy graphical methods used in solving extraction problems. This technique is based on correlating liquid-liquid data. Data systems can be handled without any simplifying assumptions.

The technique can be used for optimising such processes. Similar procedures may be used in the case of counter current extraction.

NOMENCLATURE

A	= Carrier solvent, raffinate phase
B	= Extracting solvent, extract phase
C	= Solute
E	= Extract phase, flow rate, kg/hr
K	= Constant, Equation 1
m	= Distribution coefficient
n	= Stage number
P	= Polynomial
R	= Raffinate stream, flow rate, kg/hr
S	= Solvent input stream flow rate, kg/hr
x	= Solute concentration in the raffinate phase, mass fraction
y	= Solute concentration in the extract phase, mass fraction
Z	= Parameter defined by Equation 1, its value ranges from 0-1
W	= Weight, kg/100kg
W°	= Weight at zero solute concentration, kg/100kg

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