

BRIEF COMMUNICATION

MULTICOMPONENT EXTRACTION WITH BACKMIXING

L. BOYADZHIEV and G. ANGELOV

Bulgarian Academy of Sciences, Central Laboratory of Chemical Engineering, Sofia 13, Bulgaria

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Investigations concerning multistage counter-current extraction units have shown backmixing to have considerable influence on column performance. Several mathematical models and procedures have been proposed for calculating multistage extractors, taking into account the effect of backmixing (Joung 1957; Miyauchi & Vermeulen 1963; Sleicher 1960; Hartland & Mecklenburgh 1966; Prochazka & Landau 1963; McSwain & Durbin 1966; Prochazka & Landau 1967; Mecklenburgh & Hartland 1969). However, all of them deal with three component systems with only one component distributed between two phases. Multicomponent extraction is a process of great practical importance but has not received so much attention due to its complexity and the lack of equilibrium data (Scheibel 1959; Smith & Brinkley 1960; Hanson *et al.* 1962; Tolic & Miyauchi 1972; Boyadzhiev 1973; Roche 1966; Rod & Vrba 1972; Ingham 1972).

In the present work, a mathematical model and a method for the computation of a multistage multicomponent extraction process is proposed, which considers backmixing in both phases.

Mathematical model

A scheme of a multistage counter-current extraction cascade of NS perfectly mixed stages is shown as figure 1. It is known (Hartland & Mecklenburgh 1968) that, under these conditions, longitudinal mixing and backmixing are practically identical. Each phase, flowing through the stages, takes away a fraction of the other phase and so E_B and R_B may be considered as flows moving backwards to the main flows of the light (E_j) and heavy (R_j) phases. The rate of backmixing from the j th, to the $(j - 1)$ th stage for the heavy phase can be expressed by (Prochazka & Landau 1963; Mecklenburgh & Hartland 1969).

$$r_j = \frac{R_{Bj}}{R_j} \quad [1]$$

and analogously for the light phase

$$e_j = \frac{E_{Bj}}{E_j} \quad [2]$$

The model assumes feed and product flows of each phase at all stages, providing the possibility of introducing recirculation schemes, if necessary.

It is assumed that the stages are perfectly mixed and phase equilibrium is attained, hence

$$Y_{i,j} = k_{i,j}X_{i,j} \quad [3]$$

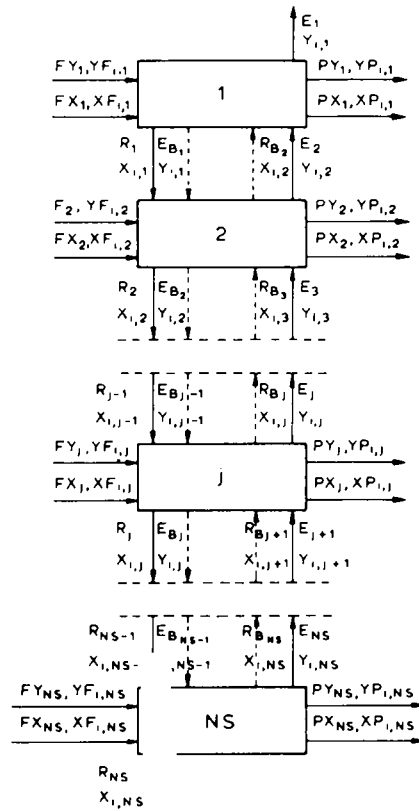


Figure 1. A counter-current extraction cascade.

where Y and X are the heavy phase and light phase concentrations (mole fraction), respectively and k is the dimensionless distribution coefficient.

The concentration of the components is expressed as molar fractions [mol/mol] and can be written

$$\sum_{i=1}^{NC} X_{i,j} = 1 \quad [4]$$

$$\sum_{i=1}^{NC} Y_{i,j} = 1. \quad [5]$$

For each stage, the balance of entering, and leaving, flows is:

$$R_{j-1} + FY_j + FX_j + e_{j-1}E_{j-1} + r_{j+1}R_{j+1} + E_{j+1} \\ = R_j(1 + r_j) + E_j(1 + e_j) + PY_j + PX_j \quad [6]$$

where FY and FX are the feed flows, and PY and PX are the production flows of the heavy phase and light phase, respectively, and the component material balance is

$$R_{j-1}X_{i,j-1} + FY_jYF_{i,j} + FX_jXF_{i,j} + e_{j-1}E_{j-1}Y_{i,j-1} + r_{j+1}R_{j+1}X_{i,j+1} + E_{j+1}Y_{j+1} \\ = R_j(1 + r_j)X_{i,j} + E_j(1 + e_j)Y_{i,j} + PY_jY_{i,j} + PX_jX_{i,j}. \quad [7]$$

To make the computational procedure easier, the flows R_0 and E_{NS+1} are assumed to be equal to zero. A complete phase separation is presumed to take place at the first, and the last, stage, so the flows E_1 and R_{NS} leaving the end stages remove none of the other phase. These circumstances change the flow balance equations. For the first stage it is:

$$FY_1 + FX_1 + r_2R_2 + E_2 = R_1 + E_1(1 + e_1) + PY_1 + PX_1 \quad [8]$$

and for the NS -stage

$$R_{NS-1} + FY_{NS} + FX_{NS} + e_{NS-1}E_{NS-1} = PX_{NS} + PY_{NS} + E_{NS} + R_{NS}(1 + r_{NS}) \quad [9]$$

The component material balance for the first stage, is:

$$\begin{aligned} FY_1YF_{i,1} + FX_1XF_{i,1} + r_2R_2X_{i,2} + E_2Y_{i,2} \\ = R_1X_{i,1} + E_1(1 + e_1)Y_{i,1} + PY_1Y_{i,1} + PX_1X_{i,1} \end{aligned} \quad [10]$$

and for the NS -stage

$$\begin{aligned} R_{NS-1}X_{i,NS-1} + FY_{NS}YF_{i,NS} + FX_{NS}XF_{i,NS} + e_{NS-1}E_{NS-1}Y_{i,NS-1} \\ = PX_{NS}X_{i,NS} + PY_{NS}Y_{i,NS} + E_{NS}Y_{i,NS} + R_{NS}(1 + r_{NS})X_{i,NS} \end{aligned} \quad [11]$$

Computational procedure*

Equations [1]–[11] lead to the concentration profiles of each component ($X_{i,j}$, $Y_{i,j}$) and the interstage flows (R_j and E_j) through the stages of the cascade. An iteration method, developed earlier (Boyadzhiev 1973), is used to compute these values. The procedure is modified to fit the requirements of the new model. The flow diagram of the computational procedure is shown by figure 2.

The principal way of the computation is:

(1) The feed (FX_j , FY_j) and production (PX_j , PY_j) flowrates, the known concentrations ($XF_{i,j}$, $YF_{i,j}$), the backmixing factors (r_j , e_j) and the initial assumptions for the concentrations ($X_{i,j}$, $Y_{i,j}$) and the internal flowrates (R_j and E_j) are set.

(2) The distribution coefficient $k_{i,j}$ is computed using the initial assumptions for the concentrations ($X_{i,j}$, $Y_{i,j}$).

(3) From [1], [2], [3], [6] and [7] one obtains:

$$X_{i,j} = \frac{BX_{i,j}}{k_{i,j}B_j + (1 - k_{i,j})[R_j(1 + r_j) + PX_j]} \quad [12]$$

where

$$\begin{aligned} BX_{i,j} = R_{j-1}X_{i,j-1} + FY_jYF_{i,j} + FX_jXF_{i,j} \\ + e_{j-1}E_{j-1}Y_{i,j-1} + r_{j+1}R_{j+1}X_{i,j+1} + E_{j+1}Y_{i,j+1} \end{aligned} \quad [13]$$

$$B_j = R_{j-1} + FY_j + FX_j + e_{j-1}E_{j-1} + r_{j+1}R_{j+1} + E_{j+1} \quad [14]$$

$$i = 1, 2, \dots, NC$$

$$j = 2, 3, \dots, NS - 1.$$

For the first, and the last stage, according to [8]–[11], the terms $BX_{i,j}$ and B_j are:

$$BX_{i,1} = FY_1YF_{i,1} + FX_1XF_{i,1} + r_2R_2X_{i,2} + E_2Y_{i,2} \quad [15]$$

$$B_1 = FY_1 + FX_1 + r_2R_2 + E_2 \quad [16]$$

$$BX_{i,NS} = R_{NS-1}X_{i,NS-1} + FY_{NS}YF_{i,NS} + FX_{NS}XF_{i,NS} + e_{NS-1}E_{NS-1}Y_{i,NS-1} \quad [17]$$

$$B_{NS} = R_{NS-1} + FY_{NS} + FX_{NS} + E_{NS-1}e_{NS-1} \quad [18]$$

where

$$i = 1, 2, \dots, NC.$$

* A Fortran IV program is available on request.

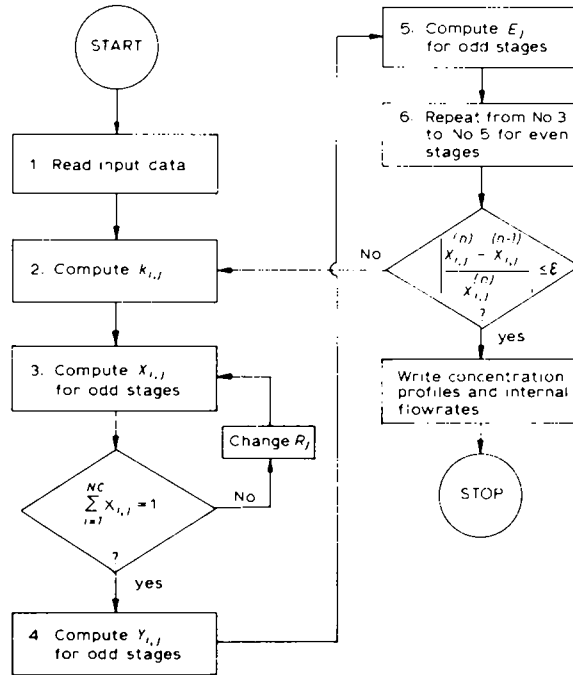


Figure 2. Flow diagram of computational procedure.

The concentrations $X_{i,j}$ for the odd numbered stages are obtained from [12], using initial assumptions for the even stages. A check as to whether the condition of [4] is fulfilled is carried out. If it is not, the values of R_j in [12] are varied according to a trial and error procedure and the concentrations $X_{i,j}$ are recalculated until this condition is attained.

(4) The concentrations $Y_{i,j}$ for the odd stages are obtained from equilibrium equations [3].

(5) The flowrates E_j for the odd stages are computed from [6].

(6) The operations from point 3 to point 5 are repeated for the even stages using the values just obtained of $X_{i,j}$, $Y_{i,j}$, E_j and R_j for the odd stages.

The computational procedure is reiterated from point 2 to point 6 until a negligible difference between two consecutively computed concentration values of each component is reached.

The expression:

$$\left| \frac{X_{i,j}^{(n)} - X_{i,j}^{(n-1)}}{X_{i,j}^{(n)}} \right| \leq \varepsilon \quad [19]$$

where n is the number of iterations, can be used as a criterion for stopping the iterations. ε ranges are usually taken from 10^{-3} to 10^{-6} .

The proposed model and the computational procedure are illustrated by the following example, also used to show the influence of backmixing on the efficiency of a counter-current extraction process.

*Example**. Acetone-ethanol mixture (molar ratio 1:1) is to be separated by means of two solvents: chloroform (heavy phase) and water (light phase). The separation is to take place in a 15-stage extraction cascade. The number of components is four, viz. (1) Acetone; (2) ethanol; (3) chloroform; and (4) water.

* This example is taken from Hanson *et al.* (1962); Roche (1966).

The concentrations of light and heavy phases leaving the apparatus, and the concentration distribution and internal flowrates through the stages are to be computed.

Stage	Feed Flowrate [mol/s]	Composition [mol/mol]			
I	$FX_1 = 80$	$XF_{1,1} = 0.0$	$XF_{2,1} = 0.0$	$XF_{3,1} = 1.0$	$XF_{4,1} = 0.0$
VI	$FX_6 = 20$	$XF_{1,6} = 0.5$	$XF_{2,6} = 0.5$	$XF_{3,6} = 0.0$	$XF_{4,6} = 0.0$
XV	$FY_{15} = 100$	$YF_{1,15} = 0.0$	$YF_{2,15} = 0.0$	$YF_{3,15} = 0.0$	$YF_{4,15} = 1.0$

with the initial assumptions $R_j = FX_1$, $E_j = FY_{15}$, $X_{i,j} = XF_{i,1}$, $Y_{i,j} = YF_{i,15}$, $j = 1, 2, \dots, NS$, $i = 1, 2, \dots, NC$.

To obtain equilibrium data the Margules equation is used (Roche 1966)

$$\begin{aligned} \ln \gamma_{i,j} = & 2C_{i,j} \sum_{K=1}^{NC} C_{K,j} A_{K,i} + \sum_{K=1}^{NC} C_{K,j}^2 A_{i,K} \\ & + \sum_{K=1}^{NC} \sum_{L=1}^{NC} C_{K,j} C_{L,j} A_{S_{i,K,L}} - 2 \sum_{i=1}^{NC} C_{i,j}^2 \sum_{K=1}^{NC} C_{K,j} A_{i,K} \\ & - 2 \sum_{i=1}^{NC} \sum_{K=2}^{NC} \sum_{L=3}^{NC} C_{i,j} C_{K,j} C_{L,j} A_{S_{i,K,L}} \end{aligned} \quad [20]$$

for $K \neq i$ $L \neq i$ $K < L$ and where

$$A_{S_{i,K,L}} = \frac{1}{2}(A_{i,K} + A_{K,i} + A_{i,L} + A_{L,i} + A_{K,L} + A_{L,K}). \quad [21]$$

Equation [20] gives the activity coefficient $\gamma_{i,j}$ of the component i in a mixture of NC components. It gives the activity coefficients in the heavy ($\gamma_{i,j}^{(R)}$) and light ($\gamma_{i,j}^{(E)}$) phases and hence the values of $k_{i,j} = \gamma_{i,j}^{(R)}/\gamma_{i,j}^{(E)}$.

The values of the constants A are those used in Roche (1966). For the system considered they are:

$A_{11} = 0.0$	$A_{12} = 0.5446$	$A_{13} = -0.9417$	$A_{14} = 1.872$
$A_{21} = 0.599$	$A_{22} = 0.0$	$A_{23} = 1.61$	$A_{24} = 1.46$
$A_{31} = -0.674$	$A_{32} = 0.501$	$A_{33} = 0.0$	$A_{34} = 5.91$
$A_{41} = 1.338$	$A_{42} = 0.877$	$A_{43} = 4.76$	$A_{44} = 0.0$

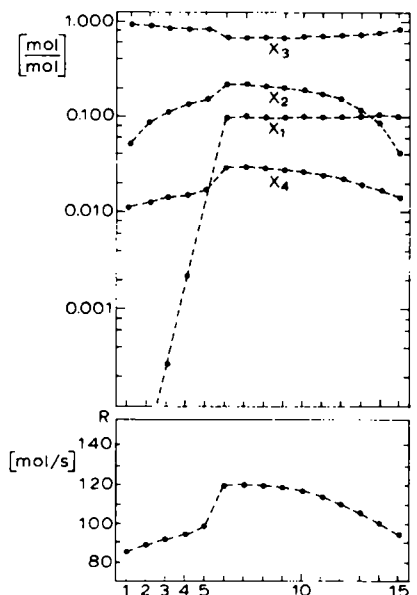


Figure 3. The change of the internal flowrates of the heavy phase and the concentrations of its components through the stages ($r_j = e_j = 0$).

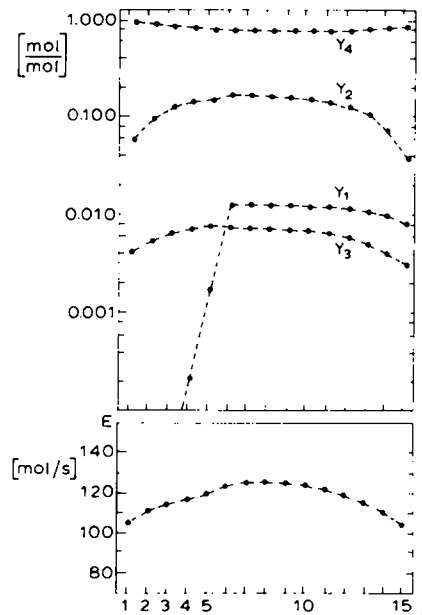


Figure 4. The change of the internal flowrates of the light phase and the concentrations of its components through the stages ($r_j = e_j = 0$).

To simplify the computation in the example, the backmixing factors are assumed to be constant through the stages. The model and procedure allow arbitrarily chosen values of the factors r_j and e_j to be used. Similarly, the computation of equilibrium by the Margules equation can be easily replaced by any other useful correlation.

The change of the internal flowrates of the heavy phase and the concentration of its components through the stages are given in figure 3. Analogous data for the light phase are given in figure 4. These results are obtained without backmixing ($r_j = e_j = 0$) so that a comparison may be made with other computational methods (Hanson *et al.* 1962; Roche 1966) which do not take into account the backmixing effect. The good agreement with these rigorous methods (see table 1) and the simplicity of the proposed method (Boyadzhiev 1973) allow it to be considered as very useful and applicable to multicomponent computations.

Table 1. Comparison with a rigorous solution (Roche 1966) in the case of no backmixing

Stage number	Concentration of component 1 (acetone)			
	In the heavy phase		In the light phase	
	This work	Roche (1966)	This work	Roche (1966)
1	0.000003	0.000003	0.000000 ²	0.000000 ²
2	0.000031	0.000031	0.000003	0.000003
3	0.000272	0.000273	0.000025	0.000025
4	0.002189	0.002192	0.000214	0.000215
5	0.016263	0.016272	0.001732	0.001735
6	0.096346	0.096312	0.012988	0.012992
7	0.096439	0.096414	0.012974	0.012986
8	0.096697	0.096636	0.012965	0.012973
9	0.097193	0.097102	0.012923	0.012940
10	0.098180	0.098007	0.012843	0.012860
11	0.099844	0.099588	0.012632	0.012675
12	0.102307	0.101985	0.012242	0.012303
13	0.105426	0.105096	0.011592	0.011676
14	0.108439	0.108176	0.010682	0.010750
15	0.105293	0.105163	0.008983	0.009025

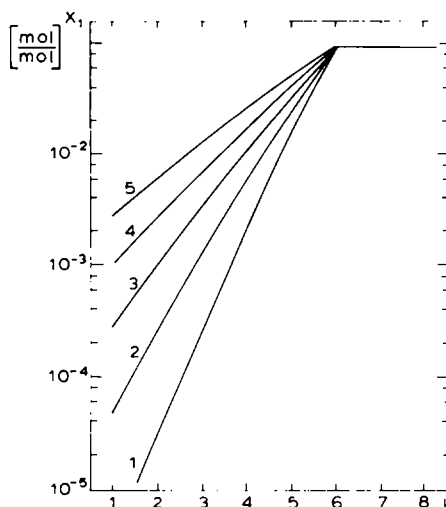


Figure 5. The influence of the backmixing in the heavy phase (r_j) on the component (1)—acetone—concentration in the same phase ($e_j = \text{const.} = 0$).

The influence of backmixing in the heavy phase (r_j) on the component (1)—acetone—concentration in the same phase is shown in figure 5. The tendency for concentration smoothing throughout the stages, as the backmixing factor increases, is evident. Taking into account the fact that acetone is fed into stage 6 and is soluble mainly in the heavy phase, it is evident that the increase in acetone concentration in stages 1–6 due to backmixing reduces the apparatus efficiency. This conclusion is confirmed by figure 6, which shows acetone concentration in the light phase outlet upon rise of the backmixing factors. In this case, the influence of backmixing in the heavy phase (curve 1 of figure 6) is greater than those in the light phase (curve 2).

CONCLUSIONS

The proposed model and computational method allow the concentration profiles and internal flowrates through the stages of a multistage cascade in the case of multicomponent liquid–liquid extraction to be obtained. The model deals with the general case when fractions of the two phases are flowing backwards and the equilibrium dependence is an arbitrary function of the concentrations of all components. The model and the procedure are limited by the restriction that equilibrium is reached in all stages. Nevertheless, the results obtained are in agreement with the basic concept of the influence of backmixing on the process efficiency.

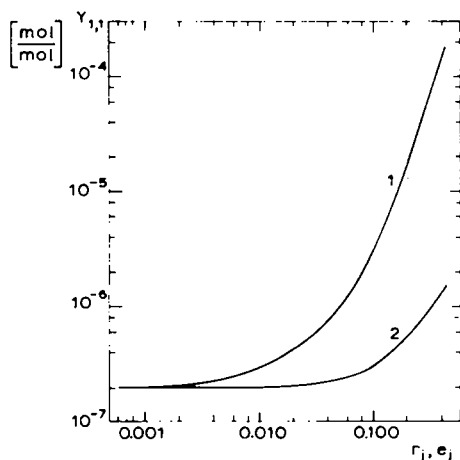


Figure 6. The influence of backmixing on the component (1)—acetone—concentration in the light phase outlet. Curve 1 $Y_{1,1} = f(r_j)$, ($e_j = 0$); Curve 2 $Y_{1,1} = f(e_j)$, ($r_j = 0$).

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