Separation Science and Technology
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713708471

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To cite this Article Leonard, R. A. , Regalbuto, M. C. , Chamberlain, D. B. and Vandegrift, G. F.(1990) 'A New Model for Solvent Extraction in Columns', Separation Science and Technology, 25: 13, 1689 — 1707
To link to this Article: DOI: 10.1080/01496399008050417
URL: http://dx.doi.org/10.1080/01496399008050417

SEPARATION SCIENCE AND TECHNOLOGY, 25(13-15), pp. 1689-1707 (1990)

A NEW MODEL FOR SOLVENT EXTRACTION IN COLUMNS

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ABSTRACT

A new model is proposed for analyzing solvent extraction processes carried out in any type of column. Each column is treated as a series of well-defined equilibrium stages where the backmixing (other-phase carryover) between stages can be large. It is assumed that mass transfer effects can be modeled by a proper choice for stage height and backmixing. With this model, the same number of stages can be used for all extracted chemical components no matter what their distribution coefficients. Thus, this model greatly simplifies the calculations required when evaluating multicomponent solvent extraction processes and so, is more appropriate than either the Height of an Equivalent Theoretical Stage (HETS) or the Height of a Transfer Unit (HTU). Initial evaluation shows that the new model works as well as the HTU method and better than the HETS method when correlating actual pulse column data.

INTRODUCTION

The TRUEX process is a solvent extraction procedure capable of separating, with high efficiency, small quantities of transuranic elements (i.e., Np, Am, Pu, and Cm) from aqueous nitrate or chloride solutions that are typically generated in nuclear operations, see Horwitz and Schulz (1). The process effluent that contains most of the dissolved solids is sufficiently separated from transuranic (TRU) elements to warrant disposal as a nonTRU waste.

A computer program called the Generic TRUEX Model (GTM) is being developed so that one can easily evaluate the TRUEX process

for removing actinides from nuclear waste streams. The GTM consists of three parts. The first part calculates the distribution coefficients for every chemical component at each stage based on chemical equilibria and thermodynamic activities. The second part uses these D values to calculate the concentration of every chemical component at each stage. The third part estimates the cost and space requirements of installing the process.

The existing GTM algorithm can model solvent extraction processes done in a centrifugal contactor, a mixer settler, or other stagewise equipment. To extend the usefulness of the GTM program, we needed a means for treating solvent extraction in any type of continuous (differential) contact equipment as if it were a stagewise process. If such a column model could be developed, it could fit easily into the GTM and be able to take advantage of the distribution coefficients generated by the GTM. In this paper, we propose such a model and use it to analyze pulsed column data for cerium. The results look very encouraging.

Finally, we looked at some additional topics related to modeling columns. These topics include (1) a model for the separating (disengaging) zone of a solvent extraction column, (2) the conversion of the modeling equations from molar to molal units, and (3) key points to watch for when setting up a column model and comparing model calculations with actual data.

PREVIOUS MODELS

Most previous models for liquid extraction in columns, see Treybal (2), involve use of either the Height Equivalent to a Theoretical Stage (HETS) or the Height of a Transfer Unit (HTU). While the HETS method is simple, since it breaks the column up into the number of theoretical stages required to obtain the observed separation for a component, the value for HETS varies widely with changes in the flow rate and the distribution coefficient, that is, with component type and concentration. The HTU method, introduced to improve on the HETS method, does not have stages that are appropriate for use in the GTM. Conversion techniques to obtain an appropriate stage height, e. g., the HETS, involve the extraction factor for the component, that is, the organic-to-aqueous flow ratio (R) times the distribution factor (D) for a component. As the D values for each component will typically be different, the number of stages required to model each component using the HETS method will also be different. The different number of stages for each component would be hard to handle in the GTM since the concentration of each component in a stage is a part of the calculation to determine the distribution coefficient of every component in the stage.

Two other general problems with the HTU method are as follows. First, the surface area for the dispersed phase and the overall mass transfer coefficient for each component are hard to determine. Second, the conversion of HTU to HETS has only been worked out for components at dilute concentrations with constant D values.

More recently, models that include the effects of backmixing, that is, one phase being carried or otherwise transported in the flow direction of the other phase, have been proposed for liquid extraction columns, see Geldard and Beyerlein (3), Nabeshima et al. (4), Misek and Rod (5), King (6), and Sleicher (7). These models reflect a growing recognition that backmixing is important, see Hanson (8). In addition, backmixing of the continuous phase has been observed experimentally, see Godfrey et al. (9), Geier (10), and Ingham (11). However, in the column models that incorporate the effects of backmixing, the area of the dispersed phase and the overall mass transfer coefficient are also included. Thus, the final model is even more complex than the HTU method and still contains the problems that make the HTU method unacceptable for the Generic TRUEX Model.

NEW MODEL

Because of these problems with the existing models for liquid extraction in columns, especially the problem of a different number of stages for each component, we developed a new model based only on backmixing. The new column model treats extraction in a column as a series of well-defined stages where the backmixing (other-phase carryover) for either phase can be large. Since this model applies to all components regardless of their D value, the same number of process stages will be appropriate for all components, greatly simplifying programming for the Generic TRUEX Model. The basic assumption of this new column model is that the concentration profiles in a column can be defined in terms of two parameters, equilibrium stage height (H_s) and backmixing. These two parameters are specific for a particular set of column conditions and are interdependent; however, only one condition of H_s and backmixing will allow the use of equilibrium distribution ratios for all components. The value of H_s can be attributed to mass transfer due to diffusion and droplet coalescence; any additional effects due to the bulk mass transfer are embodied in the backmixing.

Two sets of backmixing equations are given for the new model. A first approximation allows one to estimate the effect that backmixing will have on components with different D values. This approximation works when the backmixing is low. When backmixing is high, a complete set of flow equations must be used. These equations allow one to calculate the appropriate flow rates for any amount of backmixing. Finally, using either of these two backmixing forms, the equations needed to determine the concentration profile for each component are given.

First Backmixing Approximation

As a first approximation to the new model, it was assumed that backmixing (other-phase carryover) was small so that the actual flow of the phase being carried back could be ignored. To compensate for the effect of this flow, an effective D value, D_{eff}, is used in place of the true value. This D_{eff} value is given by

$$D_{eff} = (D + f_{o,i})/(1 + f_{a,i}D) \quad (1)$$

where $f_{o,i}$ is the fraction of aqueous phase in the organic phase leaving the stage, and $f_{a,i}$ is the fraction of organic phase in the aqueous phase leaving the stage. This D_{eff} value is derived from the extraction factor, E, where E is the amount of a component in the organic effluent from stage i divided by the amount of a component in the aqueous effluent from stage i. If stage i is an equilibrium stage and if there is no other-phase carryover, then

$$E = (q_{o,i}y_i)/(q_{a,i}x_i) \quad (2)$$

where $q_{a,i}$ is the volumetric flow rate for the aqueous phase from stage i, $q_{o,i}$ is the volumetric flow rate for the organic phase from stage i, x_i is the molar concentration of the component j in the aqueous phase from stage i, and y_i is the molar concentration of the component j in the organic phase from stage i. Note that the extraction factor, as given by Eq. 2, can also be written as

$$E = RD \quad (3)$$

If the equilibrium stage i has some other-phase carryover, that is, $f_{a,i}$ and $f_{o,i}$ are greater than zero, then an effective extraction factor, E_{eff}, can be written as

$$E_{eff} = (q_{o,i}y_i + q_{o,i}f_{o,i}x_i)/(q_{a,i}x_i + q_{a,i}f_{a,i}y_i) \quad (4)$$

or as

$$E_{eff} = RD_{eff} \quad (5)$$

where D_{eff}, as given by Eq. 1, takes into account the other-phase carryover.

Equation 1 is not recommended for the GTM or other computer models because it does not include the interaction of the other-phase carryover between stages; however, it does give one a quick way to estimate how backmixing will affect the apparent D value for a component. In particular, when the D value for a component is much greater than 1.0, the backmixing of the organic phase in the aqueous phase ($f_{a,i}$) is important to D_{eff} (and, hence, component separation). Also, when the D value for a component is much less than 1.0, the backmixing of the aqueous phase in the organic phase ($f_{o,i}$) is important to D_{eff} (and, hence, component separation).

Flow Equations for High Backmixing

To solve the flow equations for high amounts of backmixing, the input data indicated on the schematic of a column stage for the new model (see Fig. 1) must be specified. Besides the $f_{o,i}$ and $f_{a,i}$ quantities already defined for stage i, one needs to specify (1) the

volumetric flow rate for the organic and aqueous feeds to stage i, $q_{f,o,i}$ and $q_{f,a,i}$, respectively, and (2) the fraction of the organic and aqueous streams from stage i that is taken as an effluent, $f_{e,o,i}$ and $f_{e,a,i}$, respectively. In this model, it is assumed that $f_{o,i}$ and $f_{a,i}$ apply only to that part of the exiting stage stream which is not taken as an effluent. If an effluent does have some of the other phase dispersed in it, this other phase is modeled by including it as part of the main effluent for the other phase.

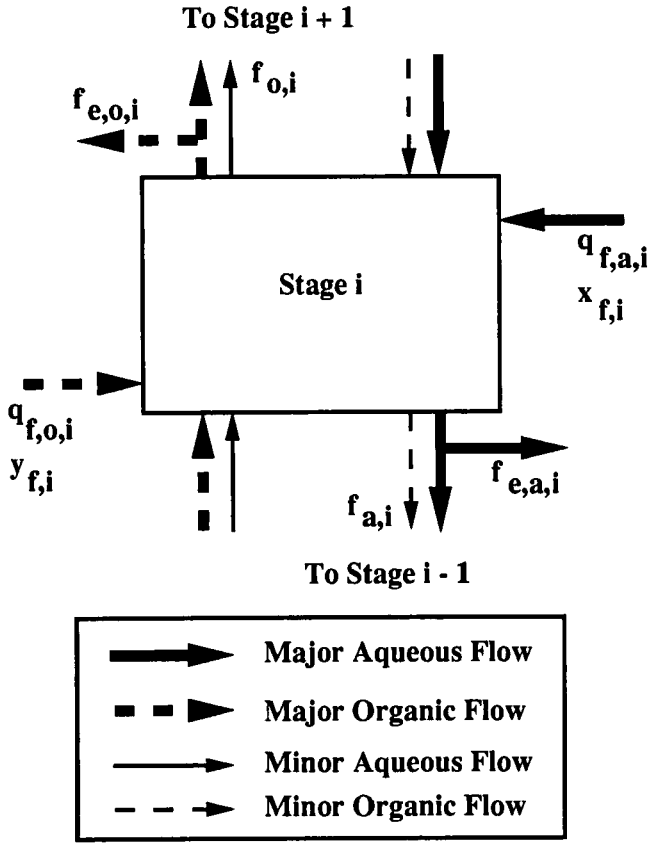

Fig. 1. Schematic for Stage i with User-Specified Quantities Shown

Based on the known (input) data shown in Fig. 1 and the unknown flows, $q_{o,i}$, the organic flow rate out of stage i in the expected direction, and $q_{a,i}$, the aqueous flow rate out of stage i in the expected direction, the various flow rate terms into and out of stage i are as shown in Fig. 2. Writing material balance equations for these flows in the general stage i, the organic flow rate is

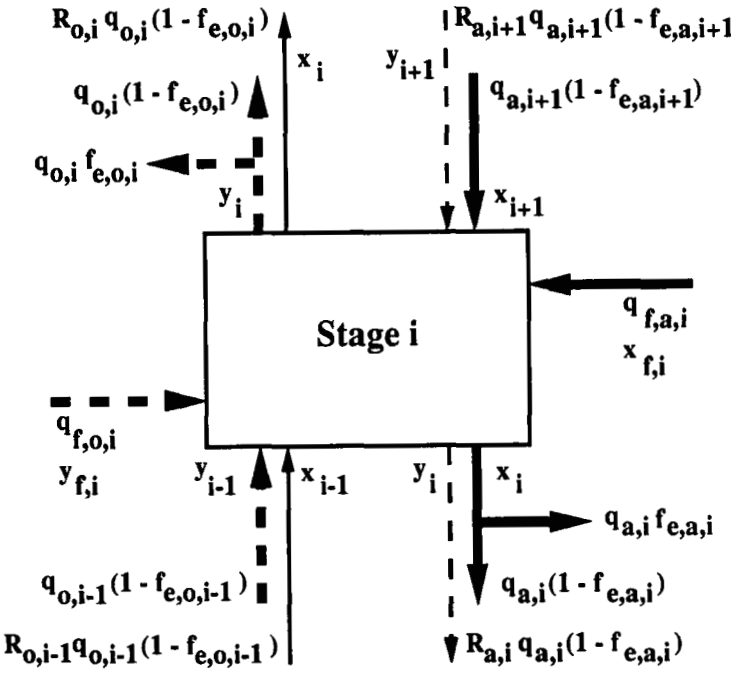

Fig. 2. Schematic for Stage i with Flow Rates and Concentrations Shown

$$q_{o,i} = q_{f,o,i} + (1-f_{e,o,i-1})q_{o,i-1} + R_{a,i}(1-f_{e,a,i+1})q_{a,i+1} - R_{a,i}(1-f_{e,a,i})q_{a,i}, \qquad 2 \le i \le m-1 \tag{6}$$

where m is the total number of stages in the column. For the corresponding aqueous flow rate

$$q_{a,i} = q_{f,a,i} + (1-f_{e,a,i+1})q_{a,i+1} + R_{o,i-1}(1-f_{e,o,i-1})q_{o,i-1} - R_{o,i}(1-f_{e,o,i})q_{o,i}, \qquad 2 \le i \le m-1 \tag{7}$$

In these two equations, the quantities $R_{o,i}$ and $R_{a,i}$ are the ratios of the other phase to the main phase. These ratios, which are related to the amount of backmixing, are given by

$$R_{o,i} = f_{o,i}/(1-f_{o,i}) \tag{8}$$

and

$$R_{a,i} = f_{a,i}/(1-f_{a,i}) \tag{9}$$

Note that $R_{o,i}$ and $R_{a,i}$ are equivalent to the fraction of other phase carried along with the main phase, $f_{o,i}$ and $f_{a,i}$, respectively. When i=1, the material balance equations for these flows become

$$q_{o,i} = q_{f,o,i} + R_{a,i}(1-f_{e,a,i+1})q_{a,i+1} \tag{10}$$

and

$$q_{a,i} = q_{f,a,i} + (1-f_{e,a,i+1})q_{a,i+1} - R_{o,i}(1-f_{e,o,i})q_{o,i} \tag{11}$$

since the i-1 terms of Eqs. 6 and 7 disappear and $f_{e,a,i}$ becomes 1.0. When i=m, the material balance equations for these flows become

$$q_{o,i} = q_{f,o,i} + (1-f_{e,o,i-1})q_{o,i-1} - R_{a,i}(1-f_{e,a,i})q_{a,i} \tag{12}$$

and

$$q_{a,i} = q_{f,a,i} + R_{o,i-1}(1-f_{e,o,i-1})q_{o,i-1} \tag{13}$$

since the i+1 terms of Eqs. 6 and 7 disappear and $f_{e,o,i}$ becomes 1.0.

Thus, for a column with m stages, there are 2m linear equations with 2m unknowns ($q_{o,i}$ and $q_{a,i}$, i=1,...,m). These equations can be solved for $q_{o,i}$ and $q_{a,i}$ by a number of standard techniques. One such technique is the method of determinants commonly called Cramer's rule, see Hohn (12). A second such technique is matrix inversion, see Hohn (12) or Hildebrand (13). Also available is a series of Gauss elimination techniques including the Gauss, Gauss-Jordan, and Crout reductions, see Hildebrand (13). These flow rates are then used to calculate the concentration of each component for both phases in every stage. These concentration calculations are described next.

Component Concentration Equations

With (1) $q_{o,i}$ and $q_{a,i}$ calculated for all m stages and (2) the molar concentration of component j given for any aqueous or organic feed to each stage i ($x_{f,i}$ and $y_{f,i}$, respectively), the unknown concentrations for the aqueous and organic phases in stage i (x_i and y_i, respectively, i=1,...,m) can now be determined. Note that, while this derivation is done for component j, it applies to each of the n components with j = 1,..., n. The subscript j is not shown here as a matter of convenience.

First it is assumed that one knows or can determine the distribution coefficient D_i for each stage i. Then, since these are assumed to be equilibrium stages,

$$D_i = y_i/x_i \tag{14}$$

Thus, all y_i values for component j can be replaced by $D_i x_i$ in the material balance equations for component j. The final material balance equation for stage i is

$$a_i x_{i-1} + b_i x_i + c_i x_{i+1} = d_i \tag{15}$$

where

$$a_1 = 0 \tag{16}$$

$$a_i = -(1 - f_{e,o,i-1})(d_{i-1} + R_{o,i-1})q_{o,i-1}, \quad 2 \leq i < m \tag{17}$$

$$b_i = [D_i + R_{o,i}(1 - f_{e,o,i})]q_{o,i} + [1 + R_{a,i}(1 - f_{e,a,i})D_i]q_{a,i}, \quad 1 \leq i \leq m \tag{18}$$

$$c_i = -(1 - f_{e,a,i+1})(1 + R_{a,i+1}D_{i+1})q_{a,i+1}, \quad 1 \leq i \leq m-1 \tag{19}$$

$$c_m = 0 \tag{20}$$

and

$$d_i = x_{f,i}q_{f,a,i} + y_{f,i}q_{f,o,i}, \quad 1 \leq i \leq m \tag{21}$$

In addition, since all of the aqueous phase is taken as effluent at stage 1 and all of the organic phase is taken as effluent at stage m,

$$f_{e,a,1} = 1 \tag{22}$$

and

$$f_{e,o,m} = 1 \tag{23}$$

This forms the set of m equations for component j.

Thus, for a column with m stages, there are m linear equations with m unknowns (x_i, i=1,...,m) for component j. To solve this set of linear equations, the techniques cited above for the flow rate equations can be used. However, because the coefficients for this set of equations form a tridiagonal matrix, see Walas (14), the Thomas algorithm can also be used, see King (6) or Carnahan et al. (15). After the x_i values for component j are determined at every stage, the y_i values can be calculated from Eq. 14. Since this procedure can be applied to each of the n components, this completes the solution of the component concentration equations.

One further note on the choice of $q_{o,i}$'s and $q_{a,i}$'s to be used in the concentration calculations. Normally, one would use the flow equations for high backmixing. However, if one does use D_{eff} to give an approximation to backmixing, then the $f_{o,i}$'s and $f_{a,i}$'s (actually the $R_{o,i}$'s and $R_{a,i}$'s) in the a_i's, b_i's, and c_i's (see Eqs. 17, 18, and 19) become zero while the D_i's are replaced with $D_{eff,i}$'s. For this approximation, the concentration of an exiting

stream reflects the average concentration of both phases in the stream. This can sometimes cause problems when calculated stage concentrations are being compared with actual concentrations. For example, this problem will occur when components have high D values in the extraction section or low D values in the stripping section. Thus, even when the other-phase carryover is low, the use of the flow equations for high backmixing is still recommended.

Spreadsheet Use

The above equations can be solved in a number of ways. One way that we have found to be very convenient is the use of spreadsheets (electronic worksheets). A previous article, see Leonard (16), has already discussed the use of electronic worksheets for solvent extraction calculations. Since that article was written, we have rearranged the worksheet, as shown schematically in Fig. 3, and

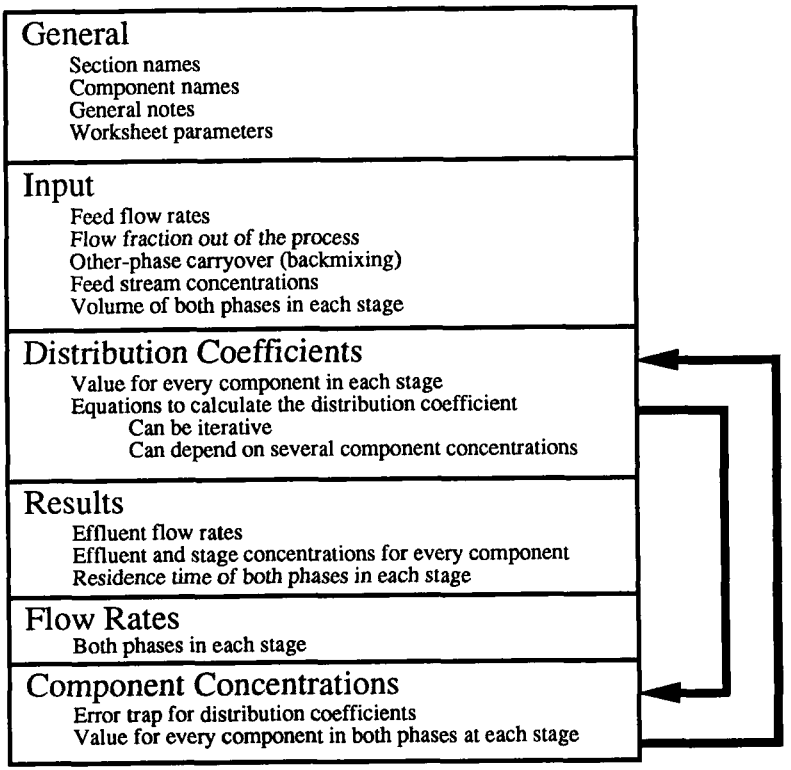

Fig. 3. Schematic Showing Spreadsheet Layout for Stagewise Process Calculations

taken advantage of new spreadsheet features such as iterative calculations and matrix inversion. The aqueous phase concentrations, x_i's, and the organic phase concentrations, y_i's, are both found in the component concentration section. Because the distribution coefficient section has a D value for each component at every stage, one is not limited to a constant D value for each component. In fact, one can use equations to calculate D values for one or more components (as we do in the Generic TRUEX Model). These equations can be iterative and can depend on the concentration of one or more components in the stage, including the component whose D value is being calculated. The arrows between the distribution coefficient section and the component concentration section in Fig. 3 are there to indicate this type of iterative calculation. Thus, this spreadsheet algorithm for stagewise solvent extraction, which we call SASSE, is very powerful and yet very easy to set up and use.

In the modeling of test results reported below, the matrix inversion technique was used on the 2m linear equations for high backmixing (Eqs. 2 through 9) to obtain the $q_{o,i}$'s and $q_{a,i}$'s. On the spreadsheet layout shown in Fig. 3, the matrix inversion was done below the layout so that it was out of the way. The time to run this SASSE worksheet using Microsoft Excel 2.2 on a Macintosh II personal computer with 14 process (column) stages, 5 components, and the D values given rather than calculated is 20 seconds. When D values must be calculated through an iterative process, the calculational time is around 60 seconds. Because Excel has excellent charting capabilities, one can set up a chart to see immediately the change in concentration profile for one or more of the components.

DATA ANALYSIS

Extraction column data are used as follows to calculate the stage height, H_s, and the fraction of continuous phase carried out of stage i with the dispersed phase, $f_{d,i}$, for the new model. Note that, if the aqueous phase is the continuous phase, then $f_{d,i}$ is $f_{o,i}$. Conversely, if the organic phase is the continuous phase, then $f_{d,i}$ is $f_{a,i}$. For a component to be analyzed, one must know its D value throughout the column and its concentration in all feed and effluent streams. In addition, one needs to know the O/A flow ratio in the column, the continuous phase in the column, and the height of the column section where contact between the two phases occurred.

Given this information, one sets up a SASSE worksheet with a small number of stages and a small amount of backmixing for each phase, typically, 0.5%. If the calculated concentration is less than the observed separation in the column (this separation is the ratio of the concentrations of a component entering and leaving the column), the number of model stages is increased. This is continued until the calculated separation is greater than the observed separation. Then, for this number of stages, the amount of

backmixing of continuous phase with the dispersed phase is increase until the calculated and observed separations match. Because the section height is known, the stage height can be determined for the calculated $f_{d,i}$ value. The number of stages is increased again, an new values for H_s and $f_{d,i}$ are calculated. This process is repeate several times so that one obtains a continuum, any point of which could characterize the column behavior for this component. For example, for run 11 shown in Fig. 4, the column separation could be characterized equally well by (1) a stage height of 0.72 m and backmixing of 0.05 or (2) a stage height of 0.42 m and backmixing o 0.73 m. To determine which point of all these points is the appropriate one to use in the model, curves showing the locus of possible operating points are generated for several components that span the range of D values in the column. The common intersection point of all these curves gives the appropriate H_s and $f_{d,i}$ values to be used in the model.

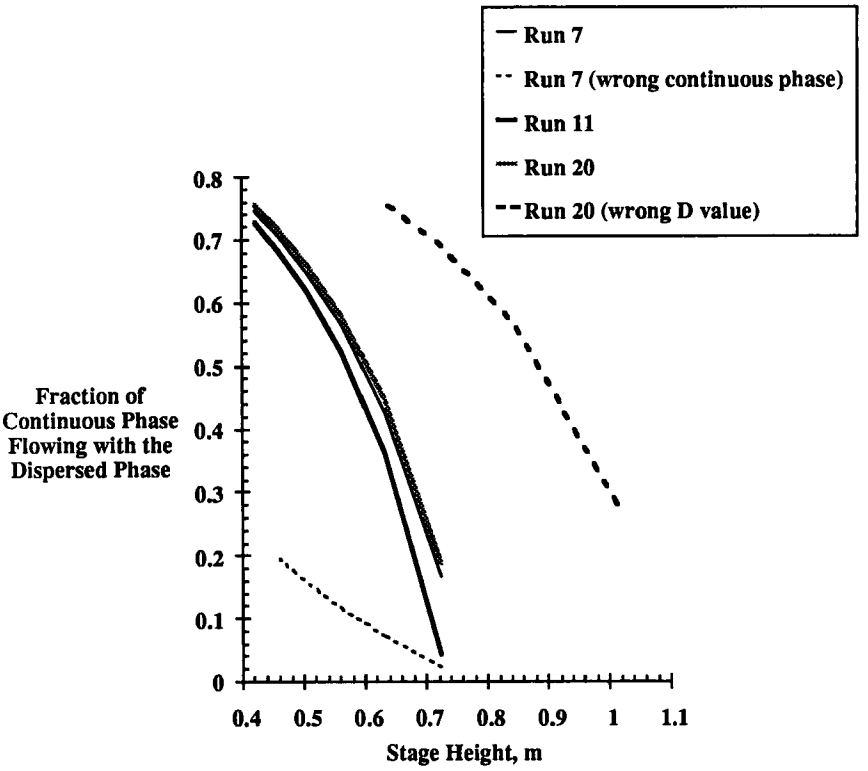

Fig. 4. Locus of Operational Points for Three Extraction/Scrub Runs

When, as is the case for the test of the new model discussed below, the data are from two different columns, the operating conditions with respect to plate geometry, plate spacing, pulse amplitude, and pulse frequency should be the same. In addition, the extraction factor (RD) should be sufficiently different so that the locus of possible operating points for the various cases will intersect rather than form a series of overlapping or parallel curves.

In analyzing column data as well as modeling columns, one should note carefully where the individual columns are. While backmixing can be quite high within a column, the separating zone at each end of a column limits the amount of other-phase carryover between columns in a multi-column process. If the amount of other-phase carryover between columns is not known, a small value, e. g., 0.5% or 0.1%, should be used. Because of the way that the flow equations are set up with the backmixing (other-phase carryover) specified at each stage for both phases, this modeling of distinct columns within an overall system is easy to implement.

Once values for H_s and $f_{d,i}$ have been obtained for a column, they can be used to determine the behavior of other components as well as the effect of various O/A flow ratios and flow rates on the components used to determine H_s and $f_{d,i}$. The procedure used is much like the above procedure for data analysis. Note, however, that (1) this is no longer a trial-and-error procedure when the column height is specified, and (2) only the feed concentrations are required.

TEST OF THE NEW MODEL

To test the new model, data from pulsed column tests at the Idaho Chemical Processing Plant (ICPP), see Maxey et al. (17), were used. The pulsed columns had sieve plates (3.2 mm dia holes with 25% free area) with a spacing of 50.8 mm in a column. Each column had a diameter of 50.8 mm. The heights of the extraction and scrub sections in the extraction/scrub column were 5.06 and 1.56 m, respectively. The height of the stripping section in the stripping column was 2.86 m. Both columns were operated in the aqueous-continuous mode. Except as noted, the pulse frequency was 40 cycles per minute. In all cases, the pulse amplitude was 25.4 mm. The organic solvent consisted of 20% dihexyl-N,N-diethylcarbamoylmethylphosphonate (DHDECMP) in a diluent that is a 2:1 mixture of decalin and diisopropylbenzene. The aqueous phase consisted of HNO_3, $Ce(NO_3)_3$, and other nitrate salts.

Ce Extraction/Scrub Runs

Two extraction/scrub runs were analyzed with the new model. Since the extraction factors for both runs were close (D values are 4.5 ± 0.5, and O/A flow ratios are 0.41 ± 0.05 in the extraction section of the column), the locus of operating points forms parallel

curves. This is seen for Runs 11 and 20 in Fig. 4. A third run, Run 7, made at the same conditions, but with a pulse frequency of 30 cycles per minute, also lies within this family of curves. Also shown in Fig. 4 is the curve obtained if the organic phase is wrongly assumed to be the continuous phase for Run 7. As can be seen, this curve is very different from the aqueous-continuous curve for Run 7. This comparison shows how important it is to know which phase is the continuous phase when using the new model.

For Run 20, the concentration of Ce in the aqueous feed is 10 times that for Runs 7 and 11, that is, 2.2 g/L rather than 0.22 g/L. Because of this, the D value in the extraction section is 4 rather than the 5 used for Runs 7 and 11. In all three runs, the D value in the scrub section is 4. Figure 4 shows the curve obtained when a D value of 5 is wrongly used for the extraction section of Run 20. As can be seen, this curve, which is displaced far to the right, is very different from the proper curve for Run 20 and the appropriate curves for the other two runs. This comparison shows how important it is to have accurate D values when a component is being analyzed.

Ce Stripping Runs

Two stripping runs were also analyzed with the new model. Since the extraction (stripping) factors for both runs were close (D values are about 0.1, and O/A flow ratio is 1.0), the locus of operating points forms parallel curves. This is seen for Runs 3 and 5 in Fig. 5. Since the concentration of Ce in the organic feed was essentially identical, 0.45 g/L for Run 3 and 0.46 g/L for Run 5, the only variation in modeling these two runs is the Ce concentration in the organic product effluent, which was 0.020 g/L for Run 3 and 0.015 g/L for Run 5. As can be seen in Fig. 5, there is a considerable distance between these two curves because of this difference in the effluent concentrations. This comparison shows how important it can be to have accurate effluent (and influent) concentrations when a component is being analyzed.

Column-Specific Model

Once these two sets of runs were analyzed, their average values were plotted on a single chart, shown in Fig. 6. Since each curve represents the locus of points that would be satisfactory for modeling each section, the intersection of these two curves gives a single stage height, H_s, and a single backmixing (other-phase carryover) fraction of the dispersed phase, $f_{d,i}$, which should be appropriate for modeling all components in these and other sieve plate columns with the same plate geometry, plate spacing, pulse frequency, and pulse amplitude. In this case, the results show that a stage height of 0.65 m and a fraction (backmix ratio) of 0.35 (35%) for the continuous aqueous phase being carried up the dispersed organic phase are the appropriate values for this two-parameter model. As mentioned above, a small fraction of 0.005 (0.5%) for the dispersed organic phase being carried down with the

continuous aqueous phase as it leaves the column stage is also included in the model. Note that major changes in the composition of the organic or aqueous phase may affect the values obtained for H_s and $f_{d,i}$.

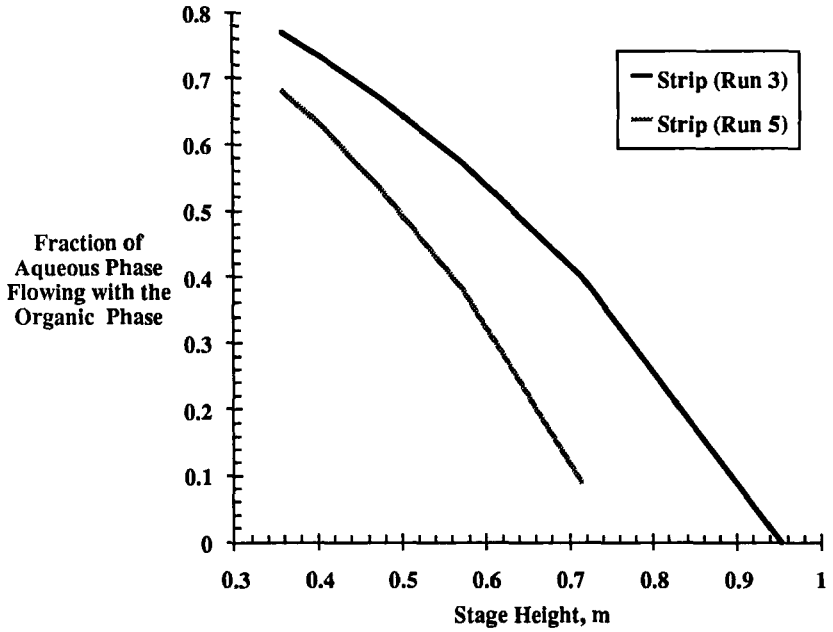

Fig. 5. Locus of Operational Points for Two Stripping Runs

Calculated results from this new backmix model for pulsed columns and two prior methods are given in Table 1. The range for the new backmix model is obtained by setting the backmix fraction at 0.35 (35%) and observing the range of stage heights, H_s, for this level of backmixing. The ranges for HETS and HTU were obtained from Maxey et al. (17) for the same four runs. As can be seen from the table, the range of heights is smallest for the new backmix model. Thus, the use of H_s rather than HETS or HTU gives a better fit of the data. In addition, and most important, the same stage height (and so, the same number of stages in a column) can be used for all components regardless of their D value and O/A flow ratio.

In the model proposed here, it is assumed that a single value for backmixing and for stage height can provide a reasonable model for all components in the column. A first test of this model was quite successful. Further tests are, of course, needed. The ideal test would be a run where several components with a range of D values are in one column, so that, all variables except for the component concentrations and the D values are the same. In addition, work needs to be done comparing the apparent values for

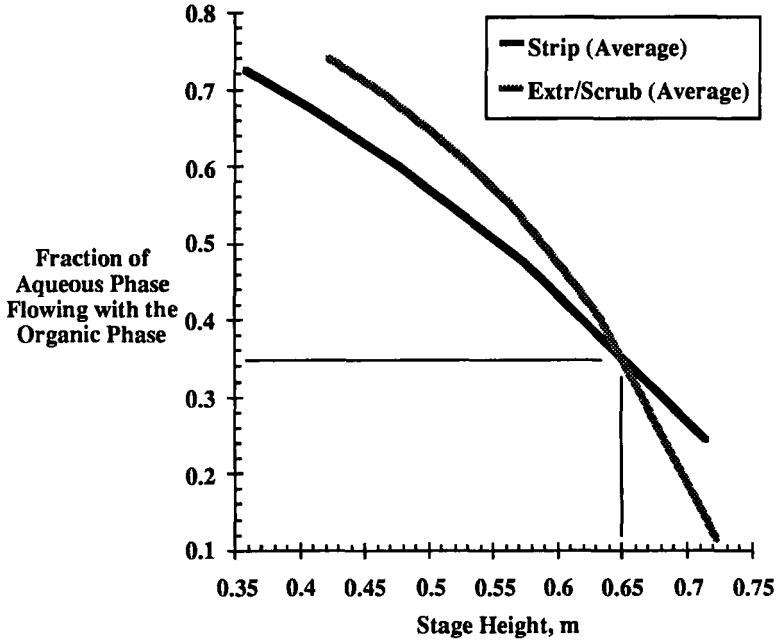

Fig. 6. Intersection of Operational Points for Extraction and Stripping Runs

Table 1. Stage Height Calculated by Three Different Models for the Same Four Pulsed Column Runs

Model	Stage Height for Extraction and Stripping, m
Height Equivalent Theoretical Stage (HETS)	0.73 - 1.50
Height Transfer Unit (HTU)	0.50 - 0.79 (0.50 - 4.9 with scrub included)
Stage Height (H_S) with 35% of the continuous phase leaving with the dispersed phase	0.59 - 0.75 (0.65 is best value)

backmixing obtained from this model with actual values observed in a column. If a correlation can be established between these two ways of measuring backmixing, then earlier work on backmixing could be incorporated into this new model.

SEPARATING ZONE MODEL

Another problem encountered in the design of solvent extraction columns is the size of the separating (disengaging) zone. This zone, which occurs at either the top or the bottom of the column, is the space where the dispersed phase droplets coalesce to form a continuous phase that exits the column. Based on the work of Leonard et al. (18), the dispersion number, N_{Di}, is fairly constant for a given solvent pair if the continuous phase is known. For solvents which use normal dodecane or similar normal paraffin hydrocarbons as the diluent, N_{Di} is about 8×10^{-4} if the organic phase is the continuous phase, and about twice that if the aqueous phase is the continuous phase. For batch tests, N_{Di} is given by

$$N_{Di} = (\Delta z)^{0.5}/(g^{0.5}t_B) \tag{24}$$

where g is gravitational acceleration, t_B is the time for the dispersion to break, and Δz is the initial thickness of the dispersion. For continuous flow tests in gravity systems, N_{Di} is given by

$$N_{Di} = (\Delta z)^{0.5}/(g^{0.5}t_R) \tag{25}$$

where t_R is the residence time in the dispersion band and Δz is the thickness of the dispersion during steady-state operations.

The N_{Di} can be applied to the design of the separating zone in a solvent extraction column would proceed as follows. The N_{Di} for the solvent pair is measured on the benchtop by dispersing the two phases in a 100-mL graduated cylinder and then using the results in Eq. 24. The residence time in the solvent extraction column is calculated using

$$t_R = A_{sx}\Delta z/q_T \tag{26}$$

where A_{sx} is the cross-sectional area of the separating (disengaging) zone, q_T is the total flow rate of the two phases, and Δz is the thickness of the dispersion in the separating zone. Combining Eqs. 25 and 26 and solving for Δz give

$$\Delta z = [q_T/(A_{sx}N_{Di})]^2/g \tag{27}$$

Equation 27 allows one to balance the values for A_{sx} and Δz to obtain an appropriate size for the separating zone. In applying this equation, use a conservative value for N_{Di}, about 50% of the normal N_{Di} value is recommended because N_{Di} is based on less than 1% other-phase carryover. With this lower N_{Di} value, other-phase carryover would typically be closer to 0.1%. In addition, the appropriate flow rate to use is a value that is between that for the dispersed phase and q_T. The use of q_T is a conservative choice and is appropriate when experimental data are not available.

OTHER MODEL TOPICS

For the above calculations, concentrations are in molar (M) units with volumetric flow rates in L/min. If it is desired to work in molal (m) units instead, the same equations apply; however, one must give the flow rates in kilograms of solvent/minute and the D values in molal units. Also, the O/A flow ratios will have units of kilograms of solvent/minute for each phase. In the aqueous phase, the solvent is water. In the organic phase, the solvent is the extractant dissolved in the diluent or diluents.

In the above discussion, the backmixing term, $f_{d,i}$, is taken to be a single variable associated with the flow of the dispersed phase, but it is expected that, in general, $f_{d,i}$ will be more complicated. In particular, it is expected that $f_{d,i}$ will have two parts. The one part will be continuous-phase liquid carried along by the dispersed-phase droplets as they move through the continuous phase. The other part will be continuous-phase liquid which is carried in the direction of dispersed-phase flow by its own turbulence. This second part of $f_{d,i}$ will come to the fore when the flow of the dispersed phase is much less than that for the continuous phase. It would be important at very high or very low O/A flow ratios.

This paper only lays out the model and shows how it was successfully applied to the data from one type of solvent extraction column. More testing of the model is necessary to validate it, especially under conditions where several components are followed for a particular set of column operating conditions. Also, it would be helpful to know how $f_{d,i}$ and H_s vary as plate geometry, plate spacing, pulse amplitude, and pulse frequency change. Along these lines, the intensity of the turbulence in the column may be useful in developing a more general correlation for backmixing and stage height.

CONCLUSIONS

A new backmix model for pulsed columns was tested and found to work well. This model is a key step for including pulsed columns in the Generic TRUEX Model. It is important to the GTM because a single stage height, and hence a fixed number of stages, can be used for all components in the pulsed column. This characteristic, a fixed number of stages for all components, should prove useful for modeling many solvent extraction systems. In addition, the new model is implemented in such a way that (1) there can be a different D value at each stage for every component, (2) an aqueous feed or an organic feed or both can be introduced at any stage, (3) an aqueous effluent or an organic effluent or both can be taken from any stage, and (4) the model can be set up on a computer spreadsheet in a way that is both fast and easy to use.

ACKNOWLEDGMENTS

This work was supported by the U.S. Department of Energy under Contract W-31-109-Eng-38.

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