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A Comparison Between SEPHIS-MOD4 and Previous Models of the Purex Solvent Extraction System

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A COMPARISON BETWEEN SEPHIS-MOD4 AND PREVIOUS MODELS OF THE PUREX SOLVENT EXTRACTION SYSTEM

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CONTENTS

PAGE

ABSTRACT 1

1. INTRODUCTION 1

2. CALCULATIONAL FEATURES OF SEPHIS-MOD4 AND PREVIOUS MODELS OF THE PUREX SYSTEM 1

2.1 SEPHIS-MOD4 2
2.2 SEPHIS-MOD1 8
2.3 SEPHIS-MOD2 9
2.4 SEPHIS-MOD3 10
2.5 SOLVEX. 10

3. RESULTS OF THE SEPHIS MODIFICATIONS 12

3.1 Steady-State Predictions 12
3.2 Transient Behavior 14
3.3 Integration Technique 15
3.4 Representation of Mixer-Settlers 15
3.5 Computer Time Consumption 18

4. CONCLUSIONS 19

5. APPENDIX 21

6. REFERENCES 23

A COMPARISON BETWEEN SEPHIS-MOD4 AND PREVIOUS MODELS OF THE PUREX SOLVENT EXTRACTION SYSTEM

A. D. Mitchell

ABSTRACT

SEPHIS-MOD4 is a revised computer model of the Purex solvent extraction system. To demonstrate that this version of the SEPHIS program is a significant improvement over the previous versions, the methods and results of SEPHIS-MOD4 are compared with earlier computer models of the Purex process. This comparison indicates that SEPHIS-MOD4 is better able to calculate transient and steady-state solute concentrations in solvent extraction equipment.

1. INTRODUCTION

The SEPHIS computer program is a tool used for simulating the solvent extraction portions of the Purex process. The program was developed to calculate (or predict) transient and steady-state concentrations in countercurrent contactors. Although the previous versions of the program did produce satisfactory results for the purposes of the users, several improvements have been made which have significantly affected both the transient and steady-state concentrations predicted by the program. To differentiate this most recent version of the program from preceding versions, the improved SEPHIS code has been redesignated SEPHIS-MOD4.

2. CALCULATIONAL FEATURES OF SEPHIS-MOD4 AND PREVIOUS MODELS OF THE PUREX SYSTEM

To provide a firm basis of comparison for the various computer models involved, an explanation of their relevant features is in order. The conceptual model of a mixer-settler stage is the foundation of the mathematics in all the programs. The equations that are used to describe the conceptual model have a large impact on the final results. In each of the programs, a specific criterion is used to test for the convergence to a steady state. An explanation of how the distribution coefficients are computed is given even though no change has been made from "SEPHIS-MOD3" to SEPHIS-MOD4.

SEPHIS-MOD4 is the latest in a series of attempts to mimic the Purex process.[1] The original program, which will be referred to as "SEPHIS-MOD1," was written by W. S. Groenier to predict the time-dependent behavior of the solvent extraction process.[2] "SEPHIS-MOD2" contains revisions made by G. L. Richardson to improve the correlations used to calculate the distribution coefficients.[3,4] R. H. Rainey and S. B. Watson modified the program further to include the effects of additional nitrate salts ("SEPHIS-MOD3").[5] Another solvent extraction program (SOLVEX), written by W. C. Scotten, improves the mathematical simulation of the process equipment but requires the user to provide distribution coefficients.[6] SEPHIS-MOD4 has its foundation in these previous works and has built and improved upon all of them.

2.1 SEPHIS-MOD4

SEPHIS-MOD4 has borrowed and refined many ideas from the previous models of the Purex solvent extraction process. The conceptual model of a mixer-settler bank is slightly changed from that of the SOLVEX program. The equations that define the model have been changed to a greater degree. The criterion for determining when steady state is achieved has been improved.

The conceptual model of a mixer-settler bank which is used by SEPHIS-MOD4 is shown in Fig. 1. All of the symbols are defined in the Appendix (Table of Nomenclature). The streams from the preceding and succeeding stages (A_{j-1}, O_{j+1}) enter the mixer of stage j with any feed streams (A_{fj}, O_{fj}) to the stage. After combining with the contents of the mixer, the phases are separated and directed to the settlers. In SEPHIS-MOD4, the settlers are subdivided into three consecutive, well-mixed zones. After leaving the third zone, the streams can proceed to the next stage (A_j, O_j) or leave the system as a product stream (A_{pj}, O_{pj}).

The equations used to describe this conceptual model are derived from the basic mass balance for the mixer:

$$\frac{d(V_{maj}x_{i,j} + V_{moj}y_{i,j})}{dt} = A_{j-1}x_{i,j-1} + O_{j+1}y_{i,j+1} + A_{fj}x_{fi,j}$$

$$+ O_{fj}y_{fi,j} - (A_j + A_{pj})x_{i,j} - (O_j + O_{pj})y_{i,j}. \qquad (1)$$

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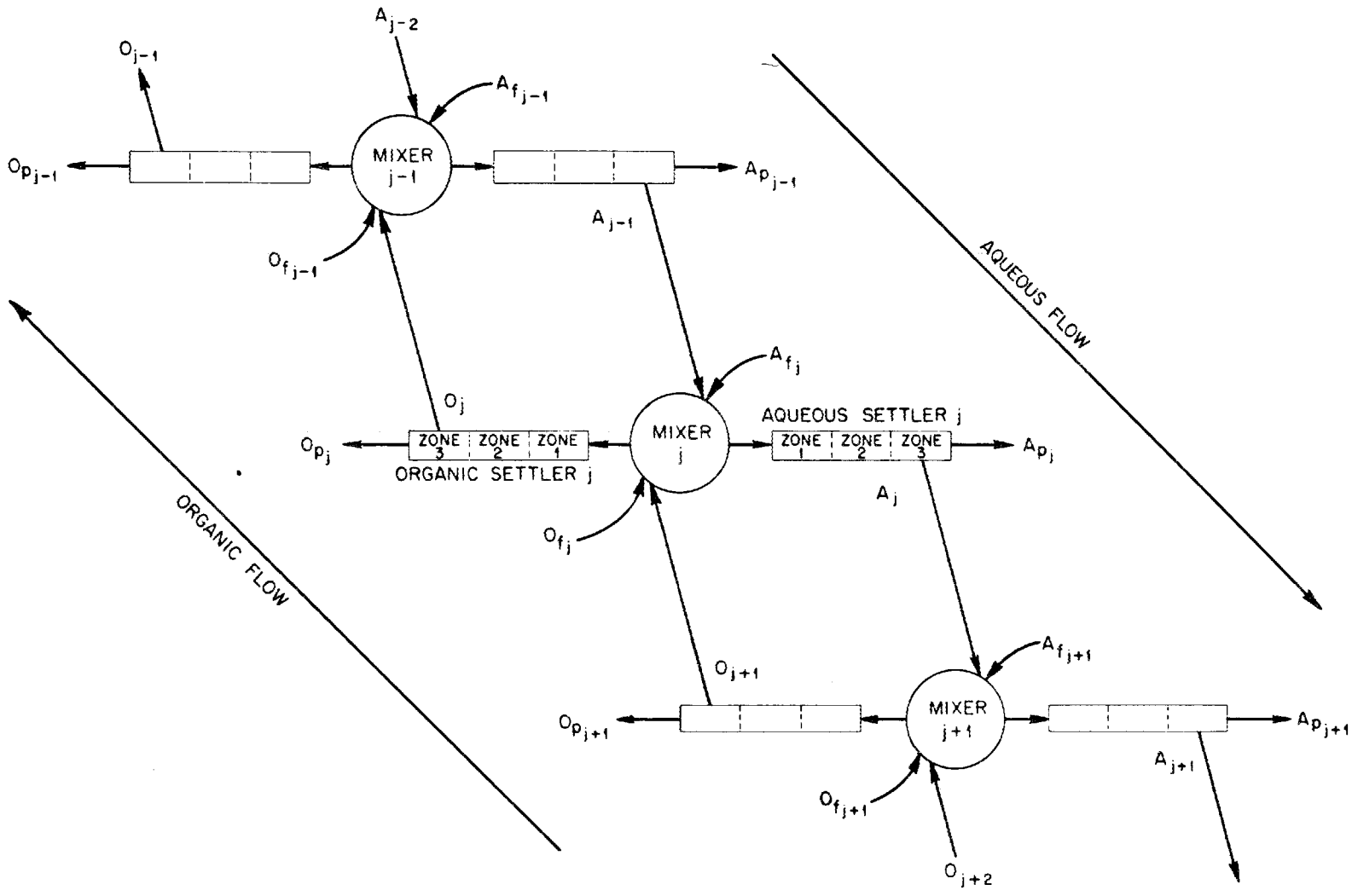

Fig. 1. The conceptual model of mixer-settler stages as used by SEPHIS-MOD4.

An approximation is made that the flow rates and volumes in the system are constant during a given time interval. This assumption simplifies the mass balance to:

$$V_{maj} \frac{dx_{i,j}}{dt} + V_{moj} \frac{dy_{i,j}}{dt} = A_{j-1}x_{i,j-1} + O_{j+1}y_{i,j+1} + A_{fj}x_{fi,j}$$

$$+ O_{fj}y_{fi,j} - (A_j + A_{pj})x_{i,j} - (O_j + O_{pj})y_{i,j}. \qquad (2)$$

The mixers are assumed to have an equilibrium distribution of the solutes between the phases, so the efficiency of the mixers is not considered. Thus, the unknown organic concentration in the mixers is defined by

$$y_{i,j} = D_i x_{i,j}. \qquad (3)$$

Substitution of Eq. (3) into Eq. (2) yields:

$$\frac{dx_{i,j}}{dt} = \Big\{A_{j-1}x_{i,j-1} + O_{j+1}y_{i,j+1} + A_{fj}x_{fi,j} + O_{fj}y_{fi,j}$$

$$- [A_j + A_{pj} + D_i(O_j + O_{pj})]\, x_{i,j}\Big\} \Big/ (V_{maj} + D_i V_{moj}). \qquad (4)$$

Since each of the concentrations (except the input stream concentrations) can vary during any time interval, a reasonable method of evaluating these concentrations must be chosen. All the flow rates, volumes, and feed streams are considered to be constant over a given interval of time. Thus, the remaining variables are $x_{i,j}$, D_i, $x_{i,j-1}$, and $y_{i,j+1}$. The evaluation of $x_{i,j}$ is determined by the Runge-Kutta integration scheme in SEPHIS-MOD4. The value of D_i is calculated once $x_{i,j}$ is known. Assuming that $x_{i,j-1}$ and $y_{i,j+1}$ will vary by only small amounts during the time interval, a reasonable choice for these values is an average of their starting concentrations and the final concentrations over the time interval. Thus,

$$x_{i,j-1} = (x_{i,j-1,t} + x_{i,j-1,t+\Delta t})/2 \quad , \qquad (5)$$

and

$$y_{i,j+1} = (y_{i,j+1,t} + y_{i,j+1,t+\Delta t})/2 \quad . \qquad (6)$$

All the variables have now been specified, so the differential in Eq. (4) can be evaluated.

The iterative procedure which the program employs may be pictured as a grid of points, as shown in Fig. 2. The horizontal axis determines the stage number, while the vertical axis indicates the progression of time. Each point in the grid indicates a time when the concentration in that stage needs to be calculated. Circles are drawn around the points in the figure to indicate that the concentrations have already been determined for that point.

In this figure, the concentrations have been calculated up to stage j at time $t + \Delta t$. Of the variables required by the equations to calculate $x_{i,j,t+\Delta t}$, only $y_{i,j+1,t+\Delta t}$ does not have a previously calculated value. An approximation that

$$y_{i,j+1,t+\Delta t} = y_{i,j+1,t} \tag{7}$$

is used to bypass this problem. The differential can then be evaluated by the Runge-Kutta integration, giving the values for $x_{i,j,t+\Delta t}$ and $y_{i,j,t+\Delta t}$. The iterative procedure then moves horizontally from one stage to the next until all the stages in that row have been evaluated. In the next row of points, the stages are computed in the other direction. This reversal of order should help offset any bias which the approximation in Eq. (7) might have on the results. While moving from left to right, a value for $y_{i,j+1,t+\Delta t}$ had to be assumed. When the calculation proceeds from right to left, the corresponding assumption is

$$x_{i,j-1,t+\Delta t} = x_{i,j-1,t}. \tag{8}$$

The iterative procedure continues to scan the column in this manner until all the specified time intervals have been completed. However, between each mixer is a settler which must also be considered. After the concentrations have been calculated for a mixer, the settler of the stage is evaluated. Since no mass transfer occurs in the settler in this model, this calculation provides a time delay between when a solute exits a mixer and when it enters the next mixer.

The equations for the settler split the computation into separate, but identical, equations for the aqueous and organic phases. Each phase

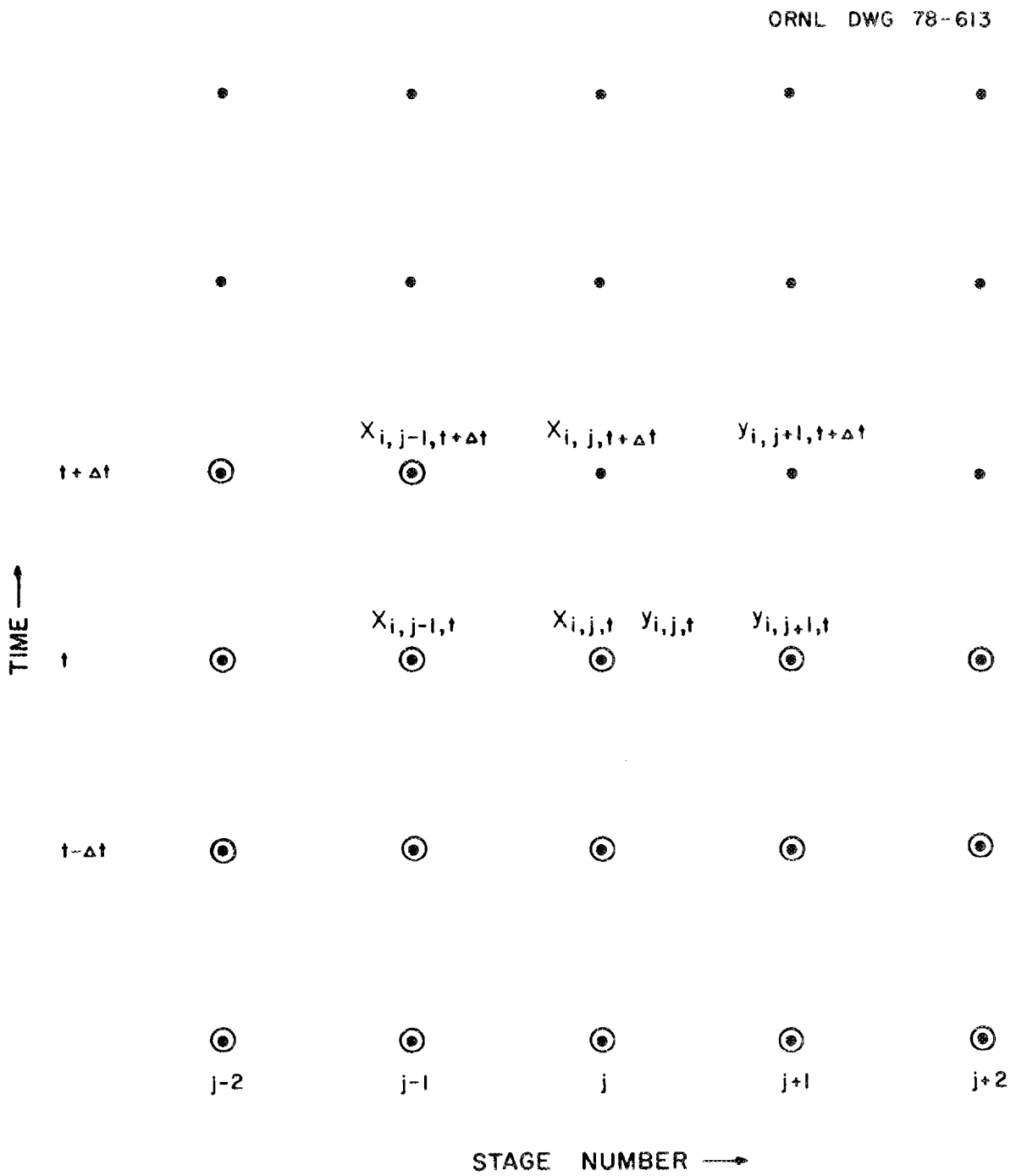

Fig. 2. An idealized view of the iterative procedure used by SEPHIS-MOD4.

in the settler is divided into three equal-volume, perfectly mixed zones. The only stream entering or exiting is the phase flow through the settler. The mass balance for component i in zone k of stage j is then:

$$\frac{V_{saj}}{3} \frac{dx_{i,j,k}}{dt} = A_{sj}x_{i,j,k-1} - A_{sj}x_{i,j,k}. \tag{9}$$

The differential equation is put into a simple finite difference form, and the concentrations are evaluated in the same manner as in the mixers to give:

$$\frac{V_{saj}}{3} \frac{x_{i,j,k,t+\Delta t} - x_{i,j,k,t}}{\Delta t} = A_{sj} \left(\frac{x_{i,j,k-1,t+\Delta t} + x_{i,j,k-1,t}}{2}\right) - A_{sj} \left(\frac{x_{i,j,k,t+\Delta t} + x_{i,j,k,t}}{2}\right). \tag{10}$$

The only unknown value is $x_{i,j,k,t+\Delta t}$, so solving the equation gives:

$$x_{i,j,k,t+\Delta t} = \frac{2V_{saj}x_{i,j,k,t} + 3A_{sj}\,\Delta t(x_{i,j,k-1,t+\Delta t} + x_{i,j,k-1,t} - x_{i,j,k,t})}{2B_{saj} + 3A_{sj}\Delta t}. \tag{11}$$

The criterion for the steady-state determination in SEPHIS-MOD4 is based on a mass balance. This mass balance is applied to each stage. When the inventory of every component in every stage is changing by less than a user-defined tolerance, a steady state is declared and the computation is discontinued.

Other changes have been made in the mechanics of SEPHIS-MOD4 which extend its abilities. At any time, the iterative procedure can be interrupted so that a new set of conditions can be specified. This ability is particularly useful in mimicking experimental trials where the flow rates may be changing quickly. The program has been separated into sections which deal basically with the general mathematics of solvent extraction and sections which pertain to the Purex process. This was done specifically to aid in the future inclusion of the Thorex process, but the new organization of the program is easily adapted for use with other systems. Similarly, kinetics subroutines have been written for the reduction of plutonium, but they also allow the easy insertion of integrated rate equations for many chemical reactions.

2.2 SEPHIS-MOD1

SEPHIS-MOD1, written by W. S. Groenier, was tailored for use with LMFBR fuels. The basic model and related equations for the process equipment were previously proposed by J. T. Lowe.[7] This model assumes that the volume of the mixing chamber is an insignificant fraction of the stage volume. This assumption is used to set the amount of solute that enters a mixer equal to the amount that exits. By substituting for the unknown organic concentration, $y_{i,j}$, according to Eq. (3), and solving for $x_{i,j}$, the final form of the equation is found. This final equation gives a value for $x_{i,j,t+\Delta t}$ in terms of known quantities:

$$x_{i,j,t+\Delta t} = \frac{A_{j-1}x_{i,j-1,t} + O_{j+1}y_{i,j+1,t} + A_{fj}x_{fi,j} + O_{fj}y_{fi,j}}{A_j + A_{pj} + D_i(O_j + O_{pj})} . \qquad (12)$$

The settlers in SEPHIS-MOD1 are not subdivided into zones as in SEPHIS-MOD4. Plug flow is assumed in the settlers so that the concentrations leaving the mixer at a certain time increment are the same as those entering the next mixer for the next time increment.

Since the holdup for each stage lies totally within the settlers, the mathematics of the program can be described most accurately as simulating the actions of a batch, countercurrent procedure using separatory funnels. All the streams resulting from each contact (time interval) are mixed until equilibrium is achieved. The phases are separated and passed on to the next stage. Additional holdup for a particular stage is simulated by creating a stream from the settler back to the mixer. In this way, the concentration in a stage is affected by the stage concentration during the previous point in time.

The explicit time dependence of the basic mass balance equation was essentially removed when the mixer volume was neglected. As a result, the transient calculations proceed in time intervals equal to the minimum residence time specified for a stage in the bank.

Because of the approximations made concerning the mixer volume and the large time interval employed, this approach gives a relatively crude model of the transient behavior. The steady-state results, however, are not significantly influenced by these factors. The

calculated steady-state concentrations in SEPHIS-MOD1 are most affected by the correlations used to calculate distribution coefficients and by the convergence criterion used to determine when steady state has been achieved.

The SEPHIS-MOD1 program employed the distribution coefficient correlations developed by D. E. Horner.[8] These correlations were based on a fitting of experimental data to the form

$$D_u = K'_u \, [NO_3^-]^2 [TBP]^2, \tag{13}$$

where

$$K'_u = \frac{[UO_2(NO_3)_2 \cdot 2TBP]}{[UO_2^{+2}][NO_3^-]^2[TBP]^2}. \tag{14}$$

Similar equations were used for plutonium and nitric acid. The fitting of K'_u was only valid for 15% TBP and 25°C due to the limited data employed.

The steady-state convergence criterion was based on an overall material balance for the contactor. When the amounts of each solute that flowed out of the contactor equalled the amounts that flowed in (within specified limits), a steady state was declared and the calculation was discontinued. This is a necessary, but insufficient, criterion for the steady-state determination. This criterion can be satisfied even though the solute concentrations in individual stages are still changing.

2.3 SEPHIS-MOD2

G. L. Richardson wrote SEPHIS-MOD2, the second version of the SEPHIS program. SEPHIS-MOD2 retained the basic model of a solvent extraction system and the convergence criterion from SEPHIS-MOD1. A new set of correlations was used to calculate the distribution coefficients. The new correlations were based on K_u, as defined by

$$K_u = \frac{[UO_2(NO_3)_2 \cdot 2TBP]}{[UO_2^{+2}][TBP]^2} = K'_u [NO_3^-]^2, \tag{15}$$

rather than K'_u. The new correlations also allowed the user to specify temperatures other than 25°C and TBP concentrations other than 15%.

2.4 SEPHIS-MOD3

S. B. Watson and R. H. Rainey wrote the third version of SEPHIS (SEPHIS-MOD3). They changed the distribution coefficient correlations again, while retaining the model and steady-state criterion of SEPHIS-MOD1. The salting effects of inextractable nitrate salts were included in the correlations. In addition, provisions for a plutonium reductant were provided by the use of "negative" plutonium concentrations. All calculations were converted to use molal units, which allowed the program to disregard the changes in volume due to changes in concentration. The temperature profile in the contactor can also be calculated by SEPHIS-MOD3.

2.5 SOLVEX

While these changes were being made to the SEPHIS program, the SOLVEX program was being developed by W. C. Scotten. The SOLVEX program is designed to simulate transient and steady-state behavior in a general solvent extraction system. Because the program can be employed for processes other than the Purex system, correlations for distribution coefficients are not included. The user is expected to provide tables of distribution data or equations for the regions of interest.

The conceptual model used by the SOLVEX program is similar to that used by SEPHIS-MOD4, which is shown in Fig. 1. Each settler may be divided into any number of well-mixed zones to provide an adjustment between plug and well-mixed flow in the settlers. Product streams are allowed only in the first and last stages of the contactor. It was assumed that the volumetric phase ratio in the mixers is equal to the flow ratio through the mixer. This assumption is optional in SEPHIS-MOD4.

The equations used to simulate the movement of the solutes through the contactor are different from those of SEPHIS-MOD4. Starting with Eq. (2), a finite difference method is used to evaluate the derivatives as

$$\frac{dx_{i,j}}{dt} = \frac{x_{i,j,t+\Delta t} - x_{i,j,t}}{\Delta t} . \qquad (16)$$

The values for $x_{i,j-1}$ and $y_{i,j+1}$ are evaluated at time t. The values for $x_{i,j}$ and $y_{i,j}$ are evaluated by

$$x_{i,j} = \frac{x_{i,j,t+\Delta t} + x_{i,j,t}}{2}. \tag{17}$$

By replacing these in Eq. (6), and substituting for the unknown organic concentration according to

$$y_{i,j} = EDx_{i,j,t+\Delta t} + (1-E)\,\frac{O_{j+1}y_{i,j+1,t} + O_{fj}y_{fi,j}}{O_{j+1} + O_{fj}}, \tag{18}$$

the final form of the SOLVEX mass balance is found:

$$\begin{aligned} x_{i,j,t+\Delta t} = \Big\{ & V_{ma}x_{i,j,t} + V_{mo}y_{i,j,t} - \Big[V_{mo}(1-E) \\ & \frac{(O_{j+1}y_{i,j+1,t} + O_{fj}y_{fi,j})}{O_{j+1} + O_{fj}}\Big] + \Delta t\Big[A_{j-1}x_{i,j-1,t} + A_{fj}x_{fi,j} \\ & + 0.5\,\Big\{- x_{i,j,t}(A_{j-1} + A_{fj}) + (1+E)(O_{j+1}y_{i,j+1,t} \\ & + O_{fj}y_{fi,j}) - y_{i,j,t}(O_{j+1} + O_{fj})\Big\}\Big]\Big\} \Big/ \Big\{ V_{ma} + V_{mo}ED \\ & + \frac{\Delta t}{2}\,[A_{j-1} + A_{fj} + ED(O_{j+1} + O_{fj})]\Big\}. \end{aligned} \tag{19}$$

The concentration for each settler zone, k, is evaluated by the SOLVEX program using the equation:

$$x_{i,j,k,t+\Delta t} = \frac{\frac{\Delta t NA_j}{2V_{sa}}\,(x_{i,j,k-1,t+\Delta t} + x_{i,j,k-1,t} - x_{i,j,k,t}) + x_{i,j,k,t}}{1 + \frac{\Delta t NA_j}{2V_{sa}}}. \tag{20}$$

The steady-state criterion used in the SOLVEX program is similar to that of SEPHIS-MOD1. In addition to checking the overall mass balance for the contactor, the SOLVEX program sets a limit for the rate of change in the total inventory of each solute. In fact, these two criteria are equivalent and show little improvement over SEPHIS-MOD1.

In summary, the SEPHIS program has been modified several times since its inception. The early modifications dealt primarily with the correlations used to calculate the distribution coefficients. The SOLVEX program addressed only the solvent extraction portion of the problem. SEPHIS-MOD4 builds upon all of these programs to achieve a better simulation of the solvent extraction portion of the Purex process. Although the computer program has undergone several changes, the original goal has remained the same.

3. RESULTS OF THE SEPHIS MODIFICATIONS

To determine whether SEPHIS-MOD4 is an improvement over SEPHIS-MOD3, several comparisons were made between the two versions. The ability of the program to model the behavior of solvent extraction systems is the most important comparison. Since SEPHIS is intended to simulate dynamic and steady-state results, both transient and steady-state experimental data were compared with the predicted results. Although accurate results are desired, conservation of computer time (or cost) is also a consideration.

3.1 Steady-State Predictions

Flowsheet testing is one of the primary uses of the SEPHIS program, so accurate prediction of steady-state concentration profiles is very desirable. Because identical distribution coefficient correlations are used by the two versions of SEPHIS, the steady-state results should also be identical. Due to a change in the convergence criterion, however, the computed results differ.

In all previous versions of SEPHIS, the convergence criterion is based on a mass balance around the entire system. The modified version considers that steady state is achieved when the change in the inventory of each mixer is less than a user-defined tolerance. This necessarily includes the mass balance around the entire system.

The difference in these convergence criteria leads to a discrepancy between the predicted steady-state results. Figure 3 shows the two predicted profiles with the experimental data points.

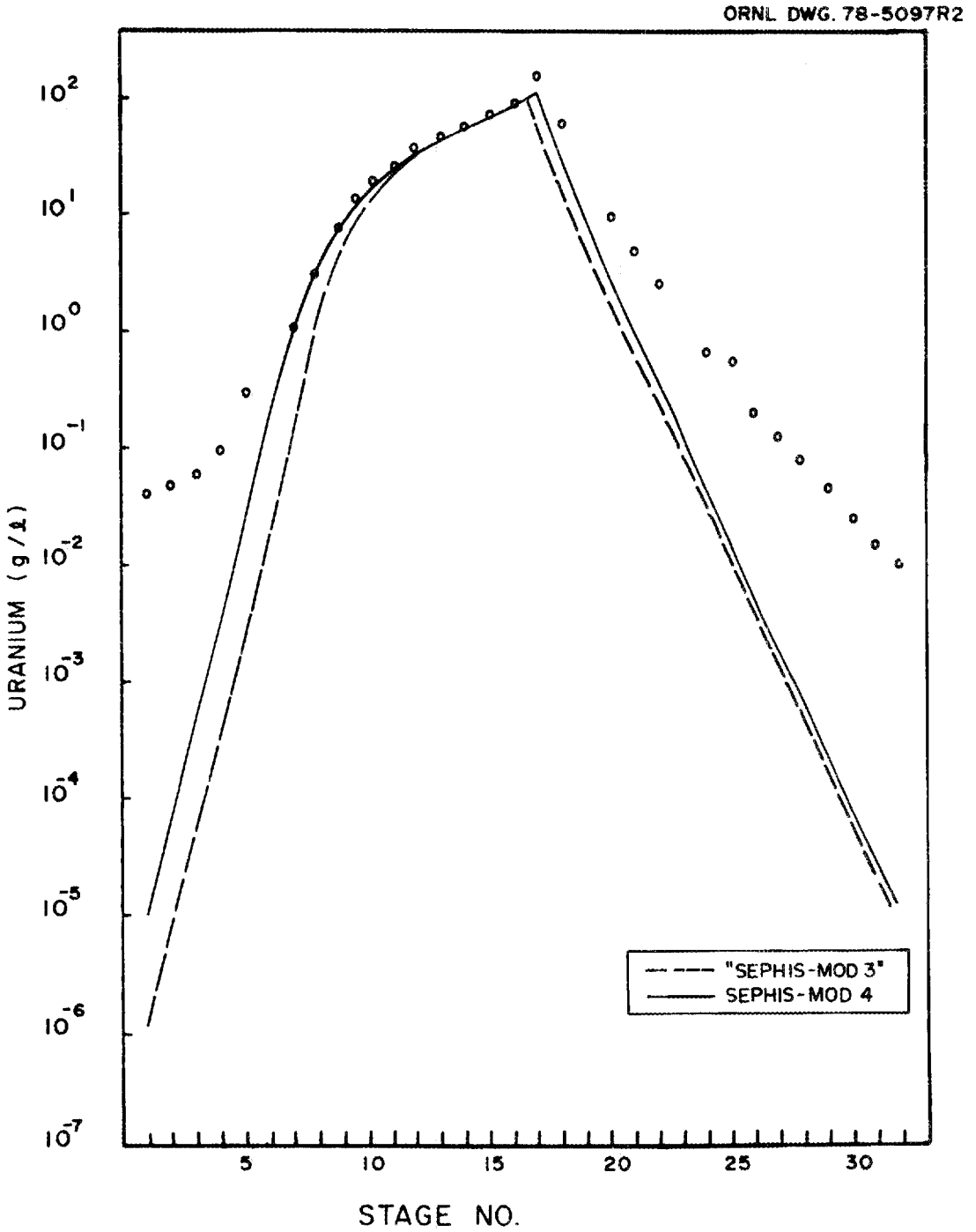

Fig. 3. A comparison of the steady-state concentration profiles predicted by SEPHIS-MOD3 and SEPHIS-MOD4.

While the predictions are very similar in the extraction section (stages 17-32), a factor of ten difference is found in the stripping section (stages 1-16). The convergence criterion for SEPHIS-MOD4 has been improved from a theoretical viewpoint, and the improvement has resulted in significant differences in the predicted profiles. These differences demonstrate the importance of the change.

Figure 3 also illustrates the discrepancy between either form of SEPHIS and the experimental data. Differences between the calculated and experimental concentrations are expected in any simulation model. These differences result from inaccuracies in the experimental data and in the simulation of real contactors by the programs. The data points in the extraction section (stages 17-32) show the same linearity as seen in the predictions; however, the slope is very different. A careful inspection of the data indicates that the problem probably lies in the chemical analysis of the aqueous feed stream acidity. A lower acidity would result in a predicted curve that would be much more comparable with the data. The strip section (stages 1-16) was predicted fairly well, especially in the region of high concentration. The differences between the data and the predicted values may be due to stage inefficiencies, inaccurate flow rate measurements, or inaccurate distribution coefficient correlations. However, the important conclusion remains; that is, the convergence criterion used by SEPHIS-MOD4 is an improvement over that of SEPHIS-MOD3.

3.2 Transient Behavior

The mechanics of the program have been dramatically changed, resulting in superior performance during transient periods. In the experimental mixer-settler used for this comparison, the flow rates of the input streams drifted randomly due to problems with the flow control. These changes produced transient periods in the mixer-settler bank often enough that the system never achieved steady-state operation.

The Watson and Rainey version of SEPHIS calculates strictly from the initial profile until a steady state is achieved. The program simply was not designed to follow experimentally measured changes in flow rates. A transient curve for SEPHIS-MOD3 can show only an asymptotic approach to a final steady-state value.

With SEPHIS-MOD4, one is able to stop the calculation for one set of flow rates at any time and then restart the computation with a different set. Figure 4 depicts a curve predicted by SEPHIS-MOD4 using experimentally measured flow rates, along with the data points for the transient period. This curve exhibits the time delays and curve shapes found in the data. The mechanics of SEPHIS-MOD4 allows the user to more closely mimic experimental data during transient periods.

3.3 Integration Technique

The integration technique used by SEPHIS-MOD4 yields more reasonable results during transient periods. With the methods used by the previous versions of SEPHIS, the calculated results often exhibited paired point behavior. At the start of a transient case, particularly near the feed point, the computed concentrations would show a large increase over one time interval followed by a small increase or decrease during the next time interval. This pattern would be repeated, making the points appear in pairs rather than as the expected smooth curve. An example of this paired point behavior can be found on page 37 of ref. 2. The plutonium concentration of stage 4 in this example is reproduced in Fig. 5. These results are caused by the model used by the program and the integration technique derived from the model. Although this should not affect the steady-state results, the transient results are clearly in error. The model and the integration technique of SEPHIS-MOD4 tend to preclude such errors.

3.4 Representation of Mixer-Settlers

The model of the solvent extraction equipment employed in SEPHIS-MOD4 produces a better representation of mixer-settlers. A study with a TBP-nitric acid system was completed by James E. Halligan and Morton Smutz.[9] This study compared experimental results with mathematical models of a mixer-settler system.

Halligan and Smutz described the model used by the previous versions of SEPHIS as an equilibrium model. This model essentially considers the mixer and settler of a stage to be one chamber. The phases

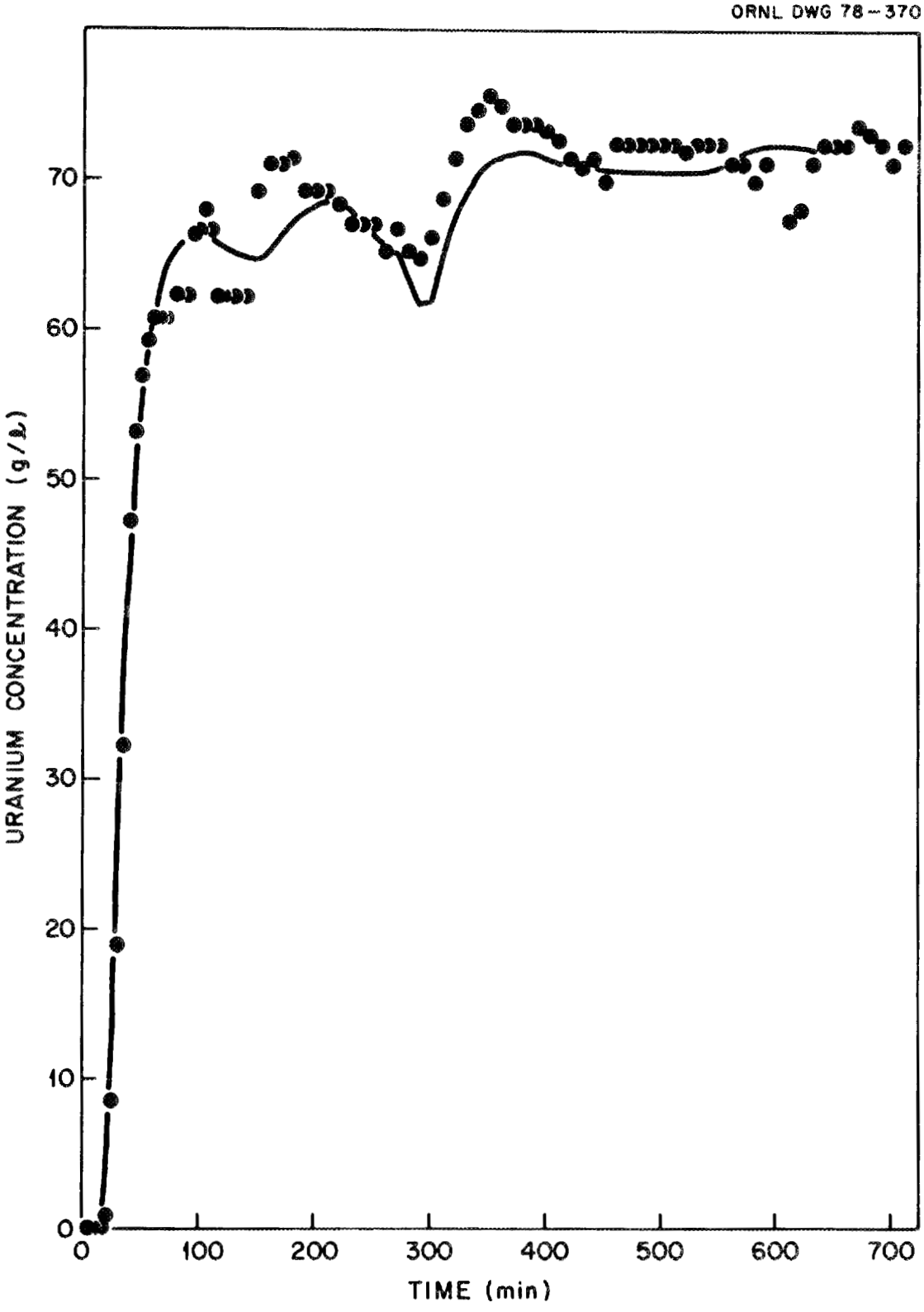

Fig. 4. A comparison of the transient concentration response curve predicted by SEPHIS-MOD4 with experimental data points.

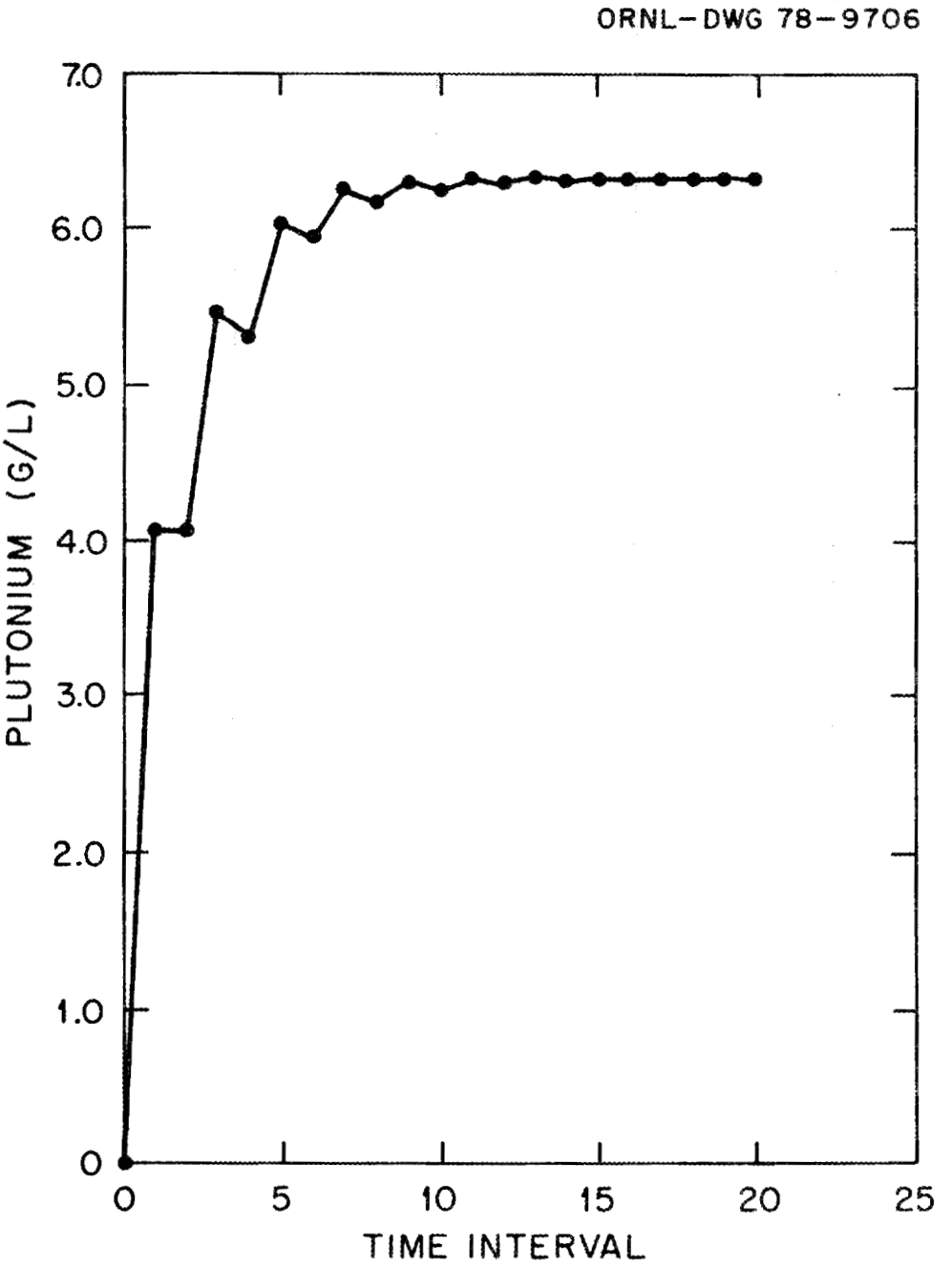

Fig. 5. An example of the paired point behavior found in previous versions of SEPHIS. Source: W. S. Groenier, Calculation of the Transient Behavior of a Dilute-Purex Solvent Extraction Process Having Application to the Reprocessing of LMFBR Fuels, ORNL-4746 (April 1976), p. 37.

are perfectly mixed and are in chemical equilibrium. This model was found to produce good results when only a mixer was studied. However, when both a mixer and a settler were studied, this model produced the poorest results of all the mathematical forms tested for both the aqueous and organic phases.

The model used by SEPHIS-MOD4 is a compromise between what Halligan and Smutz call a plug-flow model and a perfectly mixed model. In both of these models, the mixer is separated from the settler. Perfect mixing is assumed in the mixer. The plug-flow model postulates that the settler has no agitation and the phases experience plug flow through the settler. The perfectly mixed model assumes that each phase is homogeneously mixed in its portion of the settler. Their study found that the aqueous phase was best predicted by the perfectly mixed model, while the organic phase followed a plug-flow response curve. The difference was attributed to the fact that the aqueous phase was the continuous phase in the settler. This is not always the case in mixer-settlers, so the results could easily have been reversed if the organic had been the continuous phase. The compromise made by SEPHIS-MOD4 uses three perfectly mixed zones for the settler. One such zone would be the same as the perfectly mixed model, while an infinite number of these zones would describe the plug-flow model. The use of three zones was chosen arbitrarily in an effort to limit computer core usage. In any case, both the plug-flow model and the perfectly mixed model were significantly better than the equilibrium model. It is reasonable to believe that the compromise employed by SEPHIS-MOD4 will perform at least as well as, and probably better than, either of the idealized models.

3.5 Computer Time Consumption

Considering both transient and steady-state calculations, SEPHIS-MOD4 can more closely mimic experimental data. However, this advantage should be weighed against the concomitant increase in computer costs. The Runge-Kutta integration method takes more computer time since more calculations are performed. Several computer runs were made for a 32-stage contactor. The computer usage was heavily dependent

on the frequency of printing profiles. When profiles were printed once every 20 time intervals, SEPHIS-MOD3 was able to complete 19 time intervals per second of execution time. Under comparable conditions, SEPHIS-MOD4 finished only seven time intervals. When the program was to print every calculated profile, SEPHIS-MOD3 completed six time intervals per second, while SEPHIS-MOD4 finished only two. Thus, one sacrifices some computing speed for the gain in accuracy using SEPHIS-MOD4.

In SEPHIS-MOD4, one may select a faster integration technique. Although slightly slower than SEPHIS-MOD3, this alternative integration scheme is at least twice as fast as the Runge-Kutta method. This faster integration method should certainly be selected when accurate transient results are not required.

It should be noted that SEPHIS-MOD4 will consume additional amounts of time if the reduction of plutonium is used. This is due to the use of the kinetics routines which were not available in the previous versions of SEPHIS.

SEPHIS-MOD3 is able to produce results more quickly. However, the additional time spent by SEPHIS-MOD4 is due to its additional capabilities and accuracy.

4. CONCLUSIONS

SEPHIS-MOD4 is an improved model of the Purex solvent extraction system. When compared with previous models, it provides better steady-state results for flowsheet testing because of a revised convergence criterion. It is also better able to mimic actual run conditions during transient periods because of the mechanics of the program. The integration technique used by SEPHIS-MOD4 produces more reasonable results during transient periods. In addition, the model of the solvent extraction equipment employed in the program better represents the operation of mixer-settlers. Unfortunately, the Runge-Kutta integration used by SEPHIS-MOD4 does increase the amount of computer time required by the program, but this is usually not an important consideration.

5. APPENDIX

Table of Nomenclature

Variables

A	Aqueous flow rate (liters/min)
D	Distribution coefficient
E	Mixer efficiency
K	Pseudo mass equilibrium constant
K'	Pseudo mass equilibrium constant
N	Number of zones in a settler
O	Organic flow rate (liters/min)
t	Time (min)
V	Volume (liters)
x	Aqueous-phase solute concentration
y	Organic-phase solute concentration

Subscripts

a	Aqueous phase
f	Feed stream
i	Solute number
j	Stage number
k	Zone number
m	Mixer
o	Organic phase
p	Product stream
s	Settler
t	Point in time
u	Uranium

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