DATE ISSUED MAY 22 1979

ORNL-5471

7P0831

ORNL
MASTER COPY

SEPHIS-MOD4: A User's Manual to a Revised Model of the Purex Solvent Extraction System

A. D. Mitchell

[redacted]

Per David Hamm

OAK RIDGE NATIONAL LABORATORY
OPERATED BY UNION CARBIDE CORPORATION · FOR THE DEPARTMENT OF ENERGY

Printed in the United States of America. Available from
the Department of Energy,
Technical Information Center
P.O. Box 62, Oak Ridge, Tennessee 37830
Price: Printed Copy $6.00; Microfiche $3.00

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, contractors, subcontractors, or their employees, makes any warranty, express or implied, nor assumes any legal liability or responsibility for any third party's use or the results of such use of any information, apparatus, product or process disclosed in this report, nor represents that its use by such third party would not infringe privately owned rights.

ORNL-5471
Dist. Category UC-79c

Contract No. W-7405-eng-26

CONSOLIDATED FUEL REPROCESSING PROGRAM

SEPHIS-MOD4: A USER'S MANUAL TO A REVISED MODEL OF THE PUREX SOLVENT EXTRACTION SYSTEM

A. D. Mitchell 03

Chemical Technology Division

Date Published: May 1979

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
UNION CARBIDE CORPORATION
for the
DEPARTMENT OF ENERGY

CONTENTS

Page

ABSTRACT 1

1. THE CONCEPTUAL AND MATHEMATICAL BASIS FOR SEPHIS-MOD4 . . 1

2. THE MECHANICS OF SEPHIS-MOD4 10

3. APPROXIMATIONS AND ASSUMPTIONS USED BY SEPHIS-MOD4 . . . 15

4. RESULTS TO BE EXPECTED FROM SEPHIS-MOD4 19

5. INPUT CARDS FOR SEPHIS-MOD4 25

6. CHOOSING CONDITIONS FOR SEPHIS-MOD4 31

6.1 Steady-State Cases 31
6.2 Transient Cases. 32

7. EXAMPLES OF SEPHIS-MOD4 CALCULATIONS 35

7.1 Example 1 - A Steady-State Calculation for a Six-Stage Contactor 35

7.2 Example 2 - Steady-State Calculation for a Batch Extraction Process 39

7.3 Example 3 - Transient Calculation for Two Pulse Columns. 43

8. REFERENCES 45

APPENDIX A. Program Listing 53

APPENDIX B. Table of Nomenclature 73

SEPHIS-MOD4: A USER'S MANUAL TO A REVISED MODEL OF THE PUREX SOLVENT EXTRACTION SYSTEM

A. D. Mitchell

ABSTRACT

The SEPHIS computer program is a tool for simulating the operation of mixer-settlers in the solvent extraction portions of the Purex process. SEPHIS-MOD4 is a new and significantly improved version of the SEPHIS program. This report gives a detailed description of how the solvent extraction system is being simulated so that the user can more fully understand the results of the program. Although it is not necessary to run the program, an explanation of the program's mechanics is given to help remove the mystery which usually surrounds computer codes. Due to the finite nature of computers, several approximations and assumptions were made to simplify the system so that a computer can easily handle the process. A description of these approximations is given to help the user of the program understand why differences are found between the predicted and experimental concentrations in a system. In order to run the program, a description of the input cards and some examples are given. SEPHIS-MOD4 is more flexible than the previous versions of SEPHIS; thus, familiarity with some of the variables is helpful in limiting the output to only the desired results. A listing of the computer code is given in the appendices.

1. THE CONCEPTUAL AND MATHEMATICAL BASIS FOR SEPHIS-MOD4

SEPHIS-MOD4 is an improved simulation of the Purex process based on an idealized model for mixer-settlers.[1] The components considered by SEPHIS-MOD4 are nitric acid, uranium, plutonium(IV), plutonium(III), a plutonium reductant, and inextractable nitrate salts. Differential equations are used to describe the flow of the solutes through the model. Empirical correlations determine how each solute is distributed between the aqueous and organic phases. Because a computer is a finite machine, various methods must be used to break the problem into segments which can be handled conveniently by a computer.

The idealized model for mixer-settlers that is used by SEPHIS-MOD4 is depicted in Fig. 1. Definitions of the variables used are listed in Appendix B. Solutes enter each mixer via aqueous and organic feed streams, the aqueous stream from the preceding stage and the organic stream from the succeeding stage. These streams are mixed with the contents

ORNL DWG 78-371

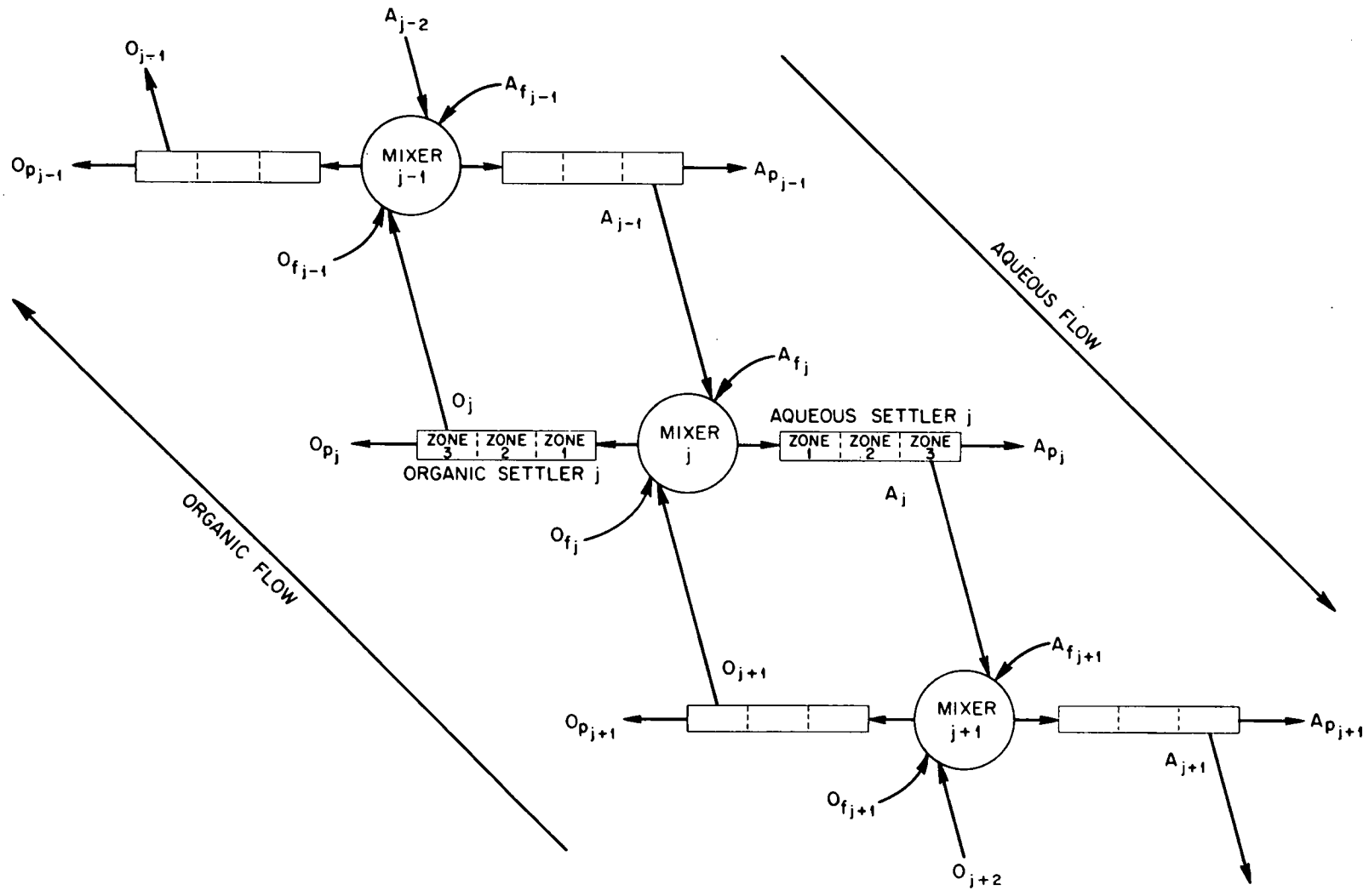

Fig. 1. The idealized model for mixer-settlers which is used by SEPHIS-MOD4.

of the mixer so that the solutes achieve an equilibrium distribution between the phases. Two streams leave each mixer and enter the first of three aqueous or organic settler zones. Each zone is homogeneously mixed and overflows into the next zone. After leaving the third settler zone, the stream may either exit the system as a product stream or proceed to the next mixer as an interstage flow.

Feed and product streams may be specified for either phase in any stage. The volume of the aqueous and organic phases may be specified individually for both the mixers and settlers. The time interval used in the integration may be set to any value within the limits of stability for the equations used by the program. The period between successive printings of the concentration profile may be varied so that only the desired output will be printed. Almost all of the variables may be given new values at any time during the computation in order to more accurately simulate transient changes in conditions.

To simulate the flow of solutes through the apparatus, the differential equations describing the mixers and settlers must be formulated in terms which the computer can evaluate. The equations start with an unsteady-state mass balance around a mixer. The streams that flow into the mixer are the aqueous stream from the settler of the preceding stage (A_{j-1}), the organic stream from the settler of the succeeding stage (O_{j+1}), and any feed streams to the stage (A_{fj}, O_{fj}). The streams that flow out of the mixer are the aqueous ($A_j + A_{pj}$) and organic ($O_j + O_{pj}$) streams to the settlers. Any changes in the amount of a particular component i in stage j must be equal to the difference between the amount that flows into and the amount that leaves the mixer. Thus,

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

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

In order to simplify this equation, the volumes and flow rates are assumed to be constant, and the solutes in the mixer are assumed to be at an equilibrium distribution between the phases; hence,

$$y_{i,j} = D_i x_{i,j} \quad . \qquad (2)$$

Applying these assumptions to Eq. (1),

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

$$- [A_j + A_{pj} + D_i(O_j + O_{pj})]x_{i,j}\}/(V_{maj} + D_iV_{moj}) \ . \qquad (3)$$

Since each of the concentrations (except the feed 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 particular interval of time, so the remaining variables are $x_{i,j}$, D_i, $x_{i,j-1}$, and $y_{i,j+1}$. The value of $x_{i,j}$ is determined by the Runge-Kutta integration scheme. 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 the concentration at the start of the time interval and the concentration at the end. Thus,

$$x_{i,j-1} = (x_{i,j-1,t} + x_{i,j-1,t+\Delta t})/2 \qquad (4)$$

and

$$y_{i,j+1} = (y_{i,j+1,t} + y_{i,j+1,t+\Delta t})/2 \ . \qquad (5)$$

All the variables have now been specified, so the differential can be evaluated by an iterative procedure.

The iterative procedure that the program employs may be pictured as a grid of points in Cartesian coordinates, 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 represents a time when the concentration in that stage needs to be calculated. The circled points in the figure indicate that the concentrations have already been determined for that stage at that time. In this figure, the concentrations have been calculated up to stage j at time $t + \Delta t$. All the variables that are required to compute $x_{i,j,t+\Delta t}$ have previously calculated values except for $y_{i,j+1,t+\Delta t}$. The simplest solution to this problem is to say that

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

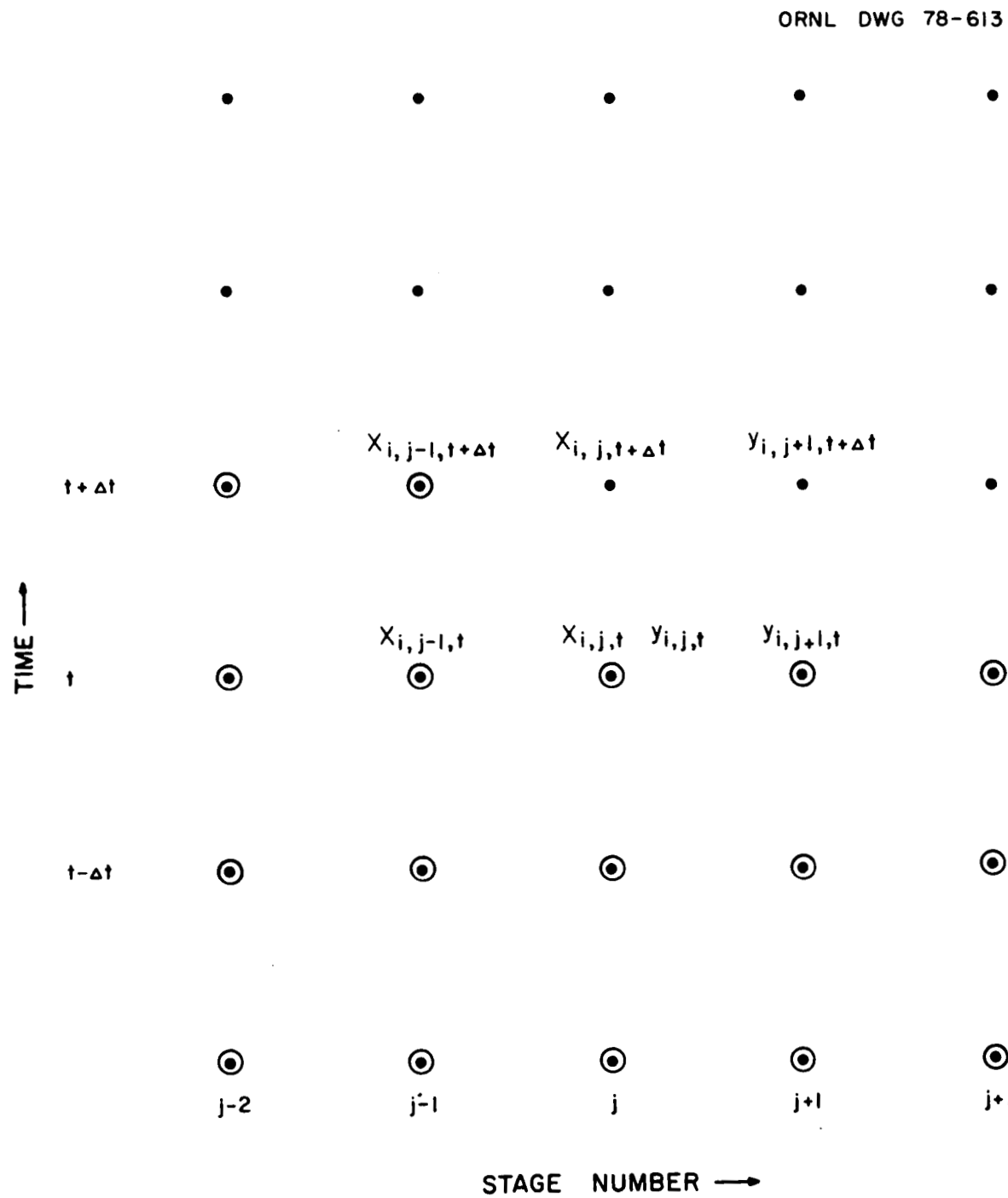

Fig. 2. A representation of the iterative procedure used by SEPHIS-MOD4.

The differential can now be evaluated and integrated by the Runge-Kutta integration scheme used by the program. The result of the integration is a new concentration ($x_{i,j,t+\Delta t}$) for the point in question. The iterative procedure then moves on to the next stage where the procedure is repeated. After all of the stages have values for the concentrations, the next row of points can be considered. In the next row of points, the stages are computed in the opposite direction. Changing the order of computation should help to offset any bias resulting from the approximation in Eq. (6). While moving in the opposite direction, the corresponding approximation that is used is:

$$x_{i,j-1,t+\Delta t} = x_{i,j-1,t} \quad . \tag{7}$$

The iterative procedure continues to scan the column in this manner until all the desired time intervals have been completed. However, between the mixers 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 changes phase in the settler in the model, this calculation essentially propagates the concentration changes through the settler. In this way, a time delay is added between when a solute exits a mixer and when it enters the next mixer.

The settler equations are formulated in the same manner as those of the mixers. Each settler is subdivided into three equal-volume, perfectly mixed zones. The only stream entering a settler is the phase flow out of the mixer. This stream passes through the settler and either leaves as a product stream or continues to the next stage. The mass balance for component i in zone k of stage j is then

$$\frac{V_{saj}}{3}\left(\frac{dx_{i,j,k}}{dt}\right) = A_{sj}x_{i,j,k-1} - A_{sj}x_{i,j,k} \quad . \tag{8}$$

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

$$\frac{V_{saj}}{3}\left(\frac{x_{i,j,k,t+\Delta t} - x_{i,j,k,t}}{\Delta t}\right) = A_{sj}\left(\frac{x_{i,j,k-1,t+\Delta t} + x_{i,j,k-1,t}}{2} - \frac{x_{i,j,k,t+\Delta t} + x_{i,j,k,t}}{2}\right) . \tag{9}$$

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

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

With these equations, the concentrations in the mixer are computed and then propagated through the settler zones. Thus, all the unknown concentrations are calculated before the next stage is considered. After all the stages have been completed, time is incremented and the next point in time is evaluated. This procedure is continued until the user specifies that it should stop.

The Runge-Kutta integration appears to be a very accurate method when used to calculate the concentrations and very stable with the equations which are used. Unfortunately, it takes more time to obtain the desired results. To bypass this problem, a second integration method was added to the program. The equation for the mixer starts with Eq. (3). The differential is substituted with a finite difference form. The concentration variables are evaluated in the same manner as in Eqs. (4) and (5). The only unknown remaining in the equation is $x_{i,j,t+\Delta t}$. Rearranging the equation gives, in final form,

$$x_{i,j,t+\Delta t} = \{V_{maj}x_{i,j,t} + V_{moj}y_{i,j,t} + \Delta t[A_{j-1}x_{i,j-1} + O_{j+1}y_{i,j+1}$$

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

$$[V_{maj} + D_iV_{moj} + \frac{\Delta t}{2}(A_j + A_{pj} + D_i(O_j + O_{pj}))] . \quad (11)$$

Calculations in the settlers and the iterative procedure are not affected. This integration method is twice as fast as the Runge-Kutta method. This fast technique is recommended for use when only steady-state results are desired, or when the concentrations are changing slowly.

The distribution coefficients, which appear in the mixer equations [Eqs. (3) and (11)], are calculated using a set of correlations based on the aqueous concentrations.[2] The solutes in the organic phase are considered to have reacted with the tributylphosphate (TBP) in reactions such as

$$UO_2^{2+} + 2NO_3^- + 2TBP \rightleftarrows UO_2(NO_3)_2 \cdot 2TBP \ .$$

A pseudo mass-action equilibrium constant is defined for each reaction according to:

$$K_u' = \frac{[UO_2(NO_3)_2 \cdot 2TBP]}{[UO_2^{2+}][NO_3^-]^2[TBP]^2} \ . \tag{12}$$

The correlations are the result of a mathematical fit of experimental data to the form:

$$K_u = \frac{[UO_2(NO_3)_2 \cdot 2TBP]}{[UO_2^{2+}][TBP]^2} = K_u'[NO_3^-]^2 \ . \tag{13}$$

Similar reactions and equations are written for the nitric acid and plutonium in the organic phase. Correction factors for other temperatures and TBP concentrations are also included.

Chemical reactions between the components are handled in special subroutines in the program. Ordinarily, a chemical reaction would appear as a generation or depletion term in Eq. (1). This was not advisable for SEPHIS-MOD4. Such a term could require that the time increment for a calculation be limited by the reaction rate rather than by the residence time for a stage,which is generally more important. Thus, chemical reactions are considered to be essentially independent of the unsteady-state mass balance equations.

Chemical reactions occurring in the mixer are considered to take place only at the aqueous-phase composition. The solute in the organic phase acts to buffer the aqueous concentration by an approximation that the distribution coefficients change only slightly due to the reaction. To determine the extent of reaction, the aqueous concentrations are put into an integrated rate equation. The extent of reaction is factored into the amount of solute in the mixer according to the specified stoichiometry of the reaction. The distribution of the resulting solutes between the phases is adjusted to account for the altered concentrations.

Chemical reactions occurring in the settlers are much less complicated. No interphase approximations are necessary. The concentrations in the zones determine the extent of reaction. The extent of reaction is factored directly into the concentrations.

Three reaction mechanisms are presently available. The simplest mechanism is for instantaneous reduction of plutonium. The assumed reaction is:

$$Pu^{4+} + \text{reductant} \rightarrow Pu^{3+} \quad .$$

The second mechanism is for reduction of plutonium by uranium(IV).[3] The reaction is shown as follows:

$$2Pu^{4+} + U^{4+} + 2H_2O \rightarrow 2Pu^{3+} + UO_2^{2+} + 4H^+ \quad ,$$

with an empirical rate equation,

$$-\frac{d[Pu(IV)]}{dt} = 170 \frac{M}{min} \frac{[U(IV)][Pu(IV)]}{[HNO_3]^2} \quad . \tag{14}$$

The integrated rate equation assumes that the nitric acid concentration is constant.

The third mechanism is for reduction of plutonium by hydroxylamine.[4] The reaction is assumed to be:

$$2NH_3OH^+ + 2Pu^{4+} \rightarrow 2Pu^{3+} + N_2 + 2H_2O + 4H^+ \quad ,$$

since, in practice, the hydroxylamine concentration is usually larger than the plutonium(IV) concentration. The rate equation is:

$$-\frac{d[Pu(IV)]}{dt} = k' \frac{[Pu(IV)]^2[NH_3OH^+]^2}{[Pu(III)]^2[H^+]^4(K_d + [NO_3^-])^2} \quad . \tag{15}$$

The rate constant (k') at a temperature of 30°C is equal to 0.029 $\underline{M}^5$/sec, with an activation energy of 31 kcal/mole. The dissociation constant for $PuNO_3^{3+}$ (K_d) is 0.33 $\underline{M}$. This rate equation is integrated by assuming constant acidity and nitrate concentrations. The proper root of the resulting equation is then localized by a binary search.

The operation of a stage is separated into a series of discrete steps by SEPHIS-MOD4. The contents of the mixer and all the streams flowing into that mixer are combined and reacted. The resulting solutions are mixed again to account for the change in the distribution coefficients due to the reaction. A portion of the mixer contents is separated and mixed into the first settler zone. The first zone overflows into the second, and the second zone overflows into the third. The overflow from the third zone is removed as a product stream or directed to the next mixer.

2. THE MECHANICS OF SEPHIS-MOD4

Although the computer code tells the complete story of how the program works, it is often helpful for the user to understand what happens during the computer run. SEPHIS-MOD4 is comprised of the main program and eight subroutines. The function of each routine is very specific. The main program directs the operation of SEPHIS-MOD4 and acts as an administrator. STARTS handles most of the input to the program. CONVRT converts the units of the input data to the units used during the calculations. MOLAL provides the conversion factors between molar and molal units. Once all the input data have been read in by the program, STAGES performs the stagewise calculations which predict the changes in concentrations. UCOR computes values for the distribution coefficients. MCHEM and SCHEM perform any required chemical reactions in the mixers and settlers. PRTOUT reconverts the units and prints the concentration profiles. This organization adds considerably to the complexity of the program but simplifies any further modifications.

The organization of the program was influenced by two modes of organization. The program is primarily divided into segments which perform general functions. STARTS does most of the input, STAGES calculates the changes in concentration, and the main program does most of the output. The secondary mode of organization separates the portions of the program dealing exclusively with solvent extraction from those which limit the program to the Purex process. The main program, STARTS, and STAGES are very general routines and could be used in many different solvent extraction processes. The remaining subroutines perform various functions or provide the needed correlations which limit the program to the Purex process. When only the Purex process is being simulated, the additional mode of organization is unnecessary. However, to change the program in order to work with another system, only the relatively short subroutines (CONVRT, MOLAL, UCOR, MCHEM, SCHEM, and PRTOUT) need to be replaced.

Each computer run is divided into one or more cases. A solvent extraction case is defined by the general mode of operation of the contactor. The number of stages, the TBP content of the organic phase, any special piping, and a chemical reaction mechanism characterize the

general mode of operation. Each case is subdivided into a number of separate time periods. A time period is described by the input-stream flow rates and concentrations, the product-stream flow rates, the volumes in the system, and an initial concentration profile. The time interval Δt, the time between profile printings, and the convergence tolerance may be changed as desired within any time period. The calculations for a time period may be terminated at any point so that the flow rates, volumes, feed concentrations, or profile may be changed. Similarly, any case may be ended at any time so that the number of stages, the TBP content, or the special piping may be altered. The program allows for a very flexible choice of operating conditions and changes in operating conditions. It is important to note that any specified change in the operating conditions will be made regardless of whether such a change can be realistically made in process equipment. For example, an increase in volumes from one time period to the next is allowed by the program. The result is an instantaneous increase in the inventory of the various components; thus, mass has been "created" by the volume changes. Such results were not corrected since the primary concern was to follow changes in concentration. The user should be aware that any specified change will be made.

The computer run begins in the main program. The title of the new case is read along with the number of stages, the TBP content, and the special piping. All the initializations required for the case are performed so that nothing from a previous case will interfere. A control card is read to start the next time period. This card contains the time increment and several variables which indicate the information that is to be read before the calculations begin. If new feed-stream flow rates or concentrations, product-stream flow rates, volumes, or an initial profile are to be given, the main program calls in the subroutine STARTS. This subroutine processes all the new information and eliminates any old values of the same type. When new feed streams are to be given, all the old feed-stream flow rates and concentrations are set to zero. The information is read from the feed-stream cards until no cards remain. The specified streams are listed in order. The flow rates and concentrations are converted to molal units, which are ready for computation.

The product streams are treated in a similar manner.

If an initial profile is to be read in, all the concentrations in all the mixers must be given. The program assumes that the initial profile values also apply to the settlers. The concentrations are converted to a molal basis before the calculations begin. The actual conversions are done with the aid of the CONVRT and MOLAL subroutines. CONVRT prints the input stream data. The uranium and plutonium concentrations in the input stream data and the initial concentration profile are converted from grams per liter to moles per liter. These molar concentrations are passed to the MOLAL subroutine, which calculates a conversion factor to change the units from a molar to a molal basis.

Since the input and output streams have been specified, the flow through each stage and the interstage flows can be calculated for the entire solvent extraction system by the subroutine STARTS. If a product stream was specified to be larger than the total phase flow into the stage, the interstage flow from the settler is set to zero and the product stream flow is set to the total phase flow into the stage. This is simply imposing a condition that no more of a particular phase can flow out of a stage than that which flowed into the stage. Thus, the hydraulics of the system are set.

The volumes are given last. This program makes a clear distinction between the mixer and the settler for each phase; hence, four volumes are required for each stage. These volumes may be specified in a number of ways. For the mixers, the aqueous volume and the organic volume may be specified independently. If the phase split in the mixers is assumed to be proportional to the phase flow through the mixer, only the total mixer volume needs to be given. The phase volumes will be set by:

$$V_{maj} = V_{mj} \frac{A_{mj}}{A_{mj} + O_{mj}} \quad . \tag{16}$$

When the volumes are not important to the problem (or when only steady-state results are desired), the mixer volumes can be set equal to the phase flows.

The volumes do not need to be given for every stage. If the volumes for a particular stage are not given, the program will assume that the required volume is the same as that in the previous stage. For example,

if the total mixer volume is to be given and none is specified for a stage, the total mixer volume will be set equal to that of the previous stage. Also, in this case, the phase ratio will be adjusted to reflect any changes in the flows. If no volumes are given for the first stage, the phase flows will be used.

The volumes in the settlers are given in the same manner as those in the mixers. Once all the volume cards have been read in, the STARTS subroutine checks to be sure that each of the four required volumes in every stage has a value.

If an initial concentration profile is to be used, a check is made to ensure that the phases are in equilibrium. If the solute concentrations do not conform to the calculated distribution coefficients, the solutes will be redistributed between the phases until an equilibrium composition is found.

This completes all the information required for a single time period. The current values for the flow rates, volumes, and concentrations are listed. This listing gives all the information pertaining to the time period so that the calculation may be repeated or identified easily. This listing should also be used to check the input information. After this printing has been completed, control returns to the main program.

The main program only directs the iterative procedure. It determines the elapsed time, the time when a profile should be printed, and whether the calculation is to be continued. The bulk of the computation is done in the STAGES subroutine. The STAGES subroutine is called once for each time increment. After the new concentrations and temperatures have been determined, control returns to the main program.

The subroutine STAGES works through the solvent extraction system by computing the concentrations and temperatures for each stage before moving to the next stage. The temperatures are evaluated by simple heat balances, and the mixer concentrations are evaluated by one of two integration techniques. The slower but more accurate approach is to integrate the unsteady-state mass balance with a fourth-order Runge-Kutta integration. The faster technique is a finite difference method derived from the mass balance. During either form of integration, STAGES calls the UCOR subroutine to calculate distribution coefficients for the various components. These distribution coefficients are used to calculate the changes in concentrations. However, since the values of the coefficients are also

dependent on the concentrations, checks are made every time the concentrations change to help ensure that the concentrations and distribution coefficients match. The subroutine STAGES calls in the UCOR subroutine a minimum of five times for each stage during any time interval with the Runge-Kutta integration. With the fast integration, the UCOR subroutine might be called only once for each stage. The distribution coefficients for the transferring components are calculated using a type of mass action equation. The coefficients for the nontransferring components [plutonium(III), the plutonium reductant, and the inextractable nitrates] are always set to zero.

After the solutes have been divided between the phases, MCHEM is called to compute the results of any chemical reaction that might be taking place in the mixer. These reactions are assumed to occur only in the aqueous phase, so the aqueous concentration is used to compute the extent of reaction. The chemical reaction is considered to be a change in the solute inventory for each component involved in the reaction. Since the change in solute inventory will result in a change in the distribution coefficients, the solutes are redistributed between the phases.

After calculations for the mixer have been completed, STAGES evaluates the concentrations and temperatures in the settler zones. A finite difference method is used in these calculations. SCHEM is called to determine the concentrations resulting from any chemical reaction that occurs in the settlers. This is done in a manner similar to that of MCHEM. This completes the work required for one stage; the next stage is then considered. Once the calculation is finished in all the stages, the program control returns to the main program.

The management chores are handled in the main program. Time is incremented, and a check is made to determine whether the calculation has converged to the desired tolerance. The tolerance is compared with the maximum change in the mixer inventory of every solute in each stage. The change in mixer inventory and the tolerance are expressed as percent per minute. If either the calculation has converged, the time period has ended, or results are desired at this time, a concentration profile for the system is printed. Before printing, the program will convert the concentrations and

flow rates from the molal form used in the calculations to the more standard units used on the printout. Because the conversions and printing are specifically tailored to the Purex process, a separate subroutine (PRTOUT) is used. PRTOUT performs the conversions with the aid of MOLAL and prints the profile. These conversions are also required for the punched card output, but the actual punching is done in the main program.

If the time period has not ended, the program will continue to calculate results for the next point in time. When the time period ends, several more checks are made. The final profile of the time period may be punched on cards for use in future runs. A card is read to determine what will be done next. This card can be used to either continue the calculation with a new time increment and tolerance or start a new time period with different feed streams. This card may also start a new case with a different solvent extraction system. If all the desired calculations have been completed, this card will also end the execution of the program.

3. APPROXIMATIONS AND ASSUMPTIONS USED BY SEPHIS-MOD4

Several assumptions and approximations are made by SEPHIS-MOD4. None of the assumptions are necessary, but they result in a significant simplification of the system being studied and a large savings in computation time. The approximations can be grouped in five major areas:

1. Concentrations in the contactor change relatively slowly.
2. The volumes and flow rates remain constant until changed by the user.
3. The mechanical operation of the contactor conforms with the idealities of the model.
4. Certain chemical effects or conditions are assumed to exist or not exist.
5. Many heat effects are neglected.

The approximations necessarily lead to differences between the calculated concentrations and experimental results, but these differences can generally be localized to specific portions of a contactor.

The approximations that were made in order to numerically integrate the differential equations become more exact if the concentrations in the contactor change relatively slowly. This does not imply that the predictions are worthless or invalid when the concentrations are changing rapidly. The correct implication is that the largest integration errors will occur just after a step change has been made in the contactor conditions, particularly when the contactor start-up procedure is being simulated. Figure 3 displays the integration errors in the uranium concentration which were found in the feed stage during the start-up procedure. The initial peak (the first half minute) amounts to a total error of 0.3 g/liter in the feed stage. After 1 min, the total error in concentration is $\sim$0.23 g/liter. For comparison, the concentration in the stage increased from 0.0 to 52 g of uranium per liter during the first minute. Thus, the integration errors are relatively small, and the approximation of slowly changing concentrations does not lead to serious problems.

The solvent extraction system being studied has many solution nonidealities which cause the flow rates and volumes in the system to vary with changes in concentration. However, in deriving the differential equations, the flow rates and volumes in the system were assumed to be constant. These approximations are not strictly applied to the system. The calculations with the flow rates and concentrations are performed in molal units in order to bypass this problem. The volumes are also converted to molal units before the calculations are made. The molal concentrations and flow rates do not change due to the nature of molal units, but the volumes do change since the "real" volume in liters is assumed to be constant. These changes in the molal volume lead to accumulation terms in the differential equations since

$$\frac{d(Vx)}{dt} = V\frac{dx}{dt} + x\frac{dV}{dt} . \tag{17}$$

To justify the use of the assumption, a comparison was made between these accumulation terms for a number of situations. Generally, $V(dx/dt)$ (the term kept by the program) was 100 times larger than $x(dV/dt)$ (the term neglected by the program). The neglected term assumed importance only when the concentration of one component was held constant while the other concentrations were changing. Even in the most extreme case tried, the neglected term accounted for <10% of the total accumulation term. Thus,

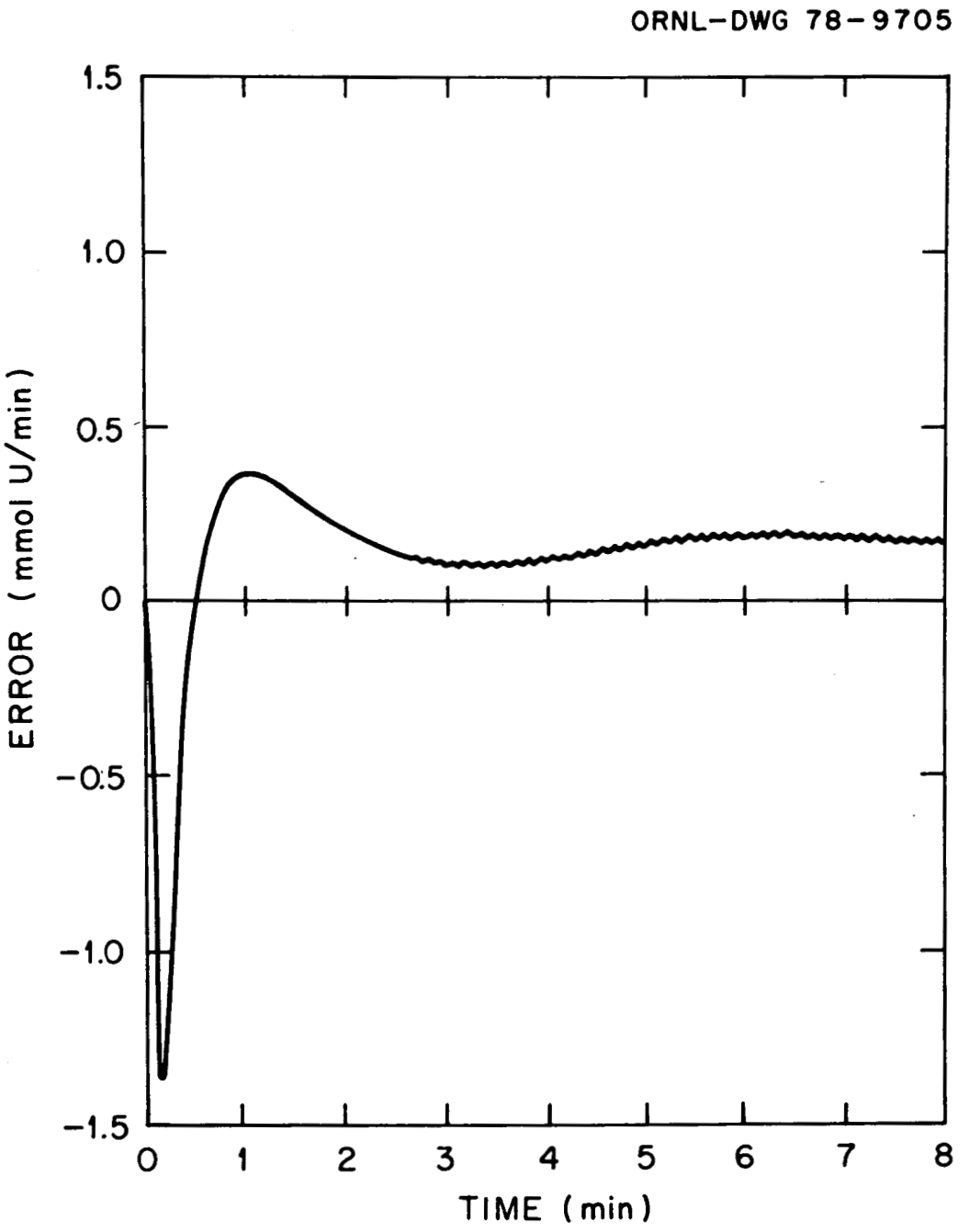

Fig. 3. Integration errors produced by SEPHIS-MOD4.

neglecting these solution nonidealities should not lead to problems with the predicted concentrations.

The mechanical operation of the contactor is assumed to be ideal in many ways. Any change in the feed-stream flow rates or stage volumes is assumed to occur instantaneously. This assumption is necessary in order to limit the simulation to changes in concentration rather than fluid dynamics-type changes. Attempting to accurately describe the fluid flow characteristics would essentially allow calculations to be performed for only one mixer-settlers design.

Perfect mixing is assumed to occur in the mixers and in each zone of the settlers. Without this approximation, the program would have to follow the concentration of discrete packets of fluid as they moved through the contactor. That approach to the problem is unwarranted for the usual uses of the program.

Entrainment is not considered by SEPHIS-MOD4. After leaving the mixer, the phases are separated absolutely and put into the settlers where no phase transfer is allowed. The approximation was made to simplify the system. Entrainment could have been simulated by the program by directing small streams of both phases in the wrong direction.

The chemistry of the Purex system is very complex, and the effects of many components in the system are not fully known. Other approximations dealing with the chemistry were made to simplify the process. Since equilibrium is desired in the stages so that the experimental results can be compared with results using ideal conditions, the components in the mixers are always assumed to be at an equilibrium distribution between the phases. Nonequilibrium conditions could have been simulated by the insertion of an efficiency in the distribution relation between the aqueous and organic concentrations [Eq. (2)].

Plutonium(III), the reductant, and the inextractable nitrate salts are assumed to remain in the aqueous phase ($D_i = 0.0$). Because its distribution coefficient is so low, plutonium is reduced to plutonium(III) to remove it from the organic phase. The reductant is assumed to be inextractable to simplify the process. Inextractable nitrates are generally added to the system to improve the extraction of uranium and plutonium. If the inextractable nitrates entered the organic phase in significant amounts, the extraction of uranium and plutonium would be

hindered, and the nitrates would not have been added. One could perform data fitting to describe the distribution of these components, if desired.

No solvent degradation products are simulated. HDBP or H_2MBP are formed by radiolysis and by reactions of TBP with nitric acid. These products tend to hold the uranium and plutonium in the organic phase. One could simulate these products knowing their formation rate and behavior as extractants. However, if the solvent degradation products were an important factor in a particular system, the process would probably be too poor to use in practice, and attempts to experimentally demonstrate the feasibility of the process would fail.

All nonideal heat effects are neglected. Temperature profiles are calculated using approximate heat capacities for the phases. A "mixing cup" temperature is used. No heats of mixing, contributions due to radiation, or gains or losses to the surroundings are considered. These effects can be simulated by inserting very small pseudo streams with very high or very low temperatures. Such streams could be used to heat or cool the contactor without changing the phase ratios.

In addition to these assumptions and approximations, other more implicit assumptions may be found in the program. Any approximation that is made will lead to differences between the calculated and experimental results. Most of these differences are of minor importance for the uses of the program and are usually confined to specific areas in the contactor, as described in the next section.

4. RESULTS TO BE EXPECTED FROM SEPHIS-MOD4

Computer simulations are made to approximate results that would occur under actual conditions. Sometimes these simulations are quite accurate, and the results can be used with some confidence. At other times, the simulation should be viewed with more skepticism. The SEPHIS-MOD4 user should be aware of this situation when interpreting the results for any given case.

In actual situations, changes in the feed-stream flow rates or concentrations will lead to transient conditions in the contactor. Solutes will pass through the contactor as discrete waves. It is important to know what the maximum concentration is likely to be and where it will

occur. SEPHIS-MOD4 was designed to produce such results. Figures 4 and 5 show the uranium and nitric acid response curves, respectively, computed by SEPHIS-MOD4 along with the experimental data points. The agreement is very good, especially after considering the sparsity of flow-rate data points. The important observation to make from these figures is that SEPHIS-MOD4 is able to predict the time when the wave of solute will appear and the approximate peak concentration.

Experimental steady-state data demonstrate the ability of the program to predict concentrations in various sections of a contactor. Steady-state concentrations are influenced primarily by the flow rates and the distribution coefficients. Mixer efficiencies are a major factor in the extraction and strip sections. Figures 6 and 7 show the effects of these factors on the aqueous and organic uranium profile concentrations, respectively. Experimental data points and the SEPHIS-MOD4 prediction are depicted.

The strip section (stages 1-16) shows the cumulative impact of mixer efficiencies and uncertain distribution coefficients. In most of the strip section (stages 5-16), the difference between the experimental and predicted concentrations is minor. In the region of low concentration (stages 1-5), the differences become large. Observation of the contactor indicated that much of this difference could be due to entrainment. However, the discrepancy between the experimental and predicted concentrations could also be attributed to uncertainties in the calculated distribution coefficients. The concentration of uranium in stage 16 is determined by a mass balance around the entire system. The concentration in stage 15 is relatively certain because it is only one stage away from stage 16. However, the concentration in stage 1 is influenced by all the distribution coefficients in the strip section. Each of these calculated coefficients has a degree of uncertainty, so the predicted concentration in stage 1 is the most uncertain value in this section of the contactor.

The concentrations in the scrub section (stages 17-24) are determined primarily by a mass balance around the entire system. This is because the same amount of uranium must leave stage 17 in the organic phase as that which entered stage 25 in the aqueous feed stream under the conditions used. The concentration profile in the scrub section also tends to be flat; hence, it is little surprise that the experimental and predicted concentrations in the scrub section are so close.

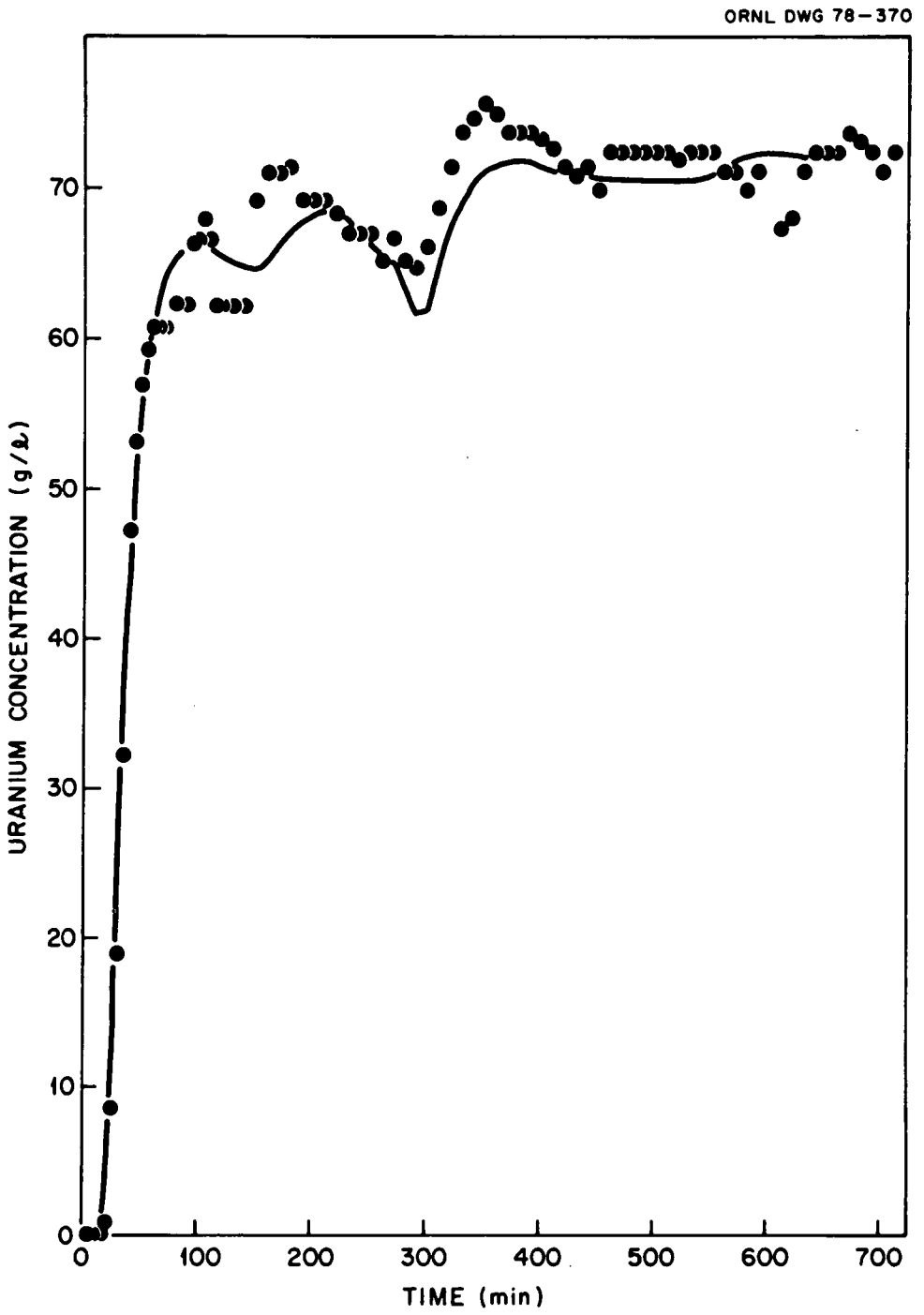

Fig. 4. A comparison of the uranium response curve data points with the curve calculated by SEPHIS-MOD4.

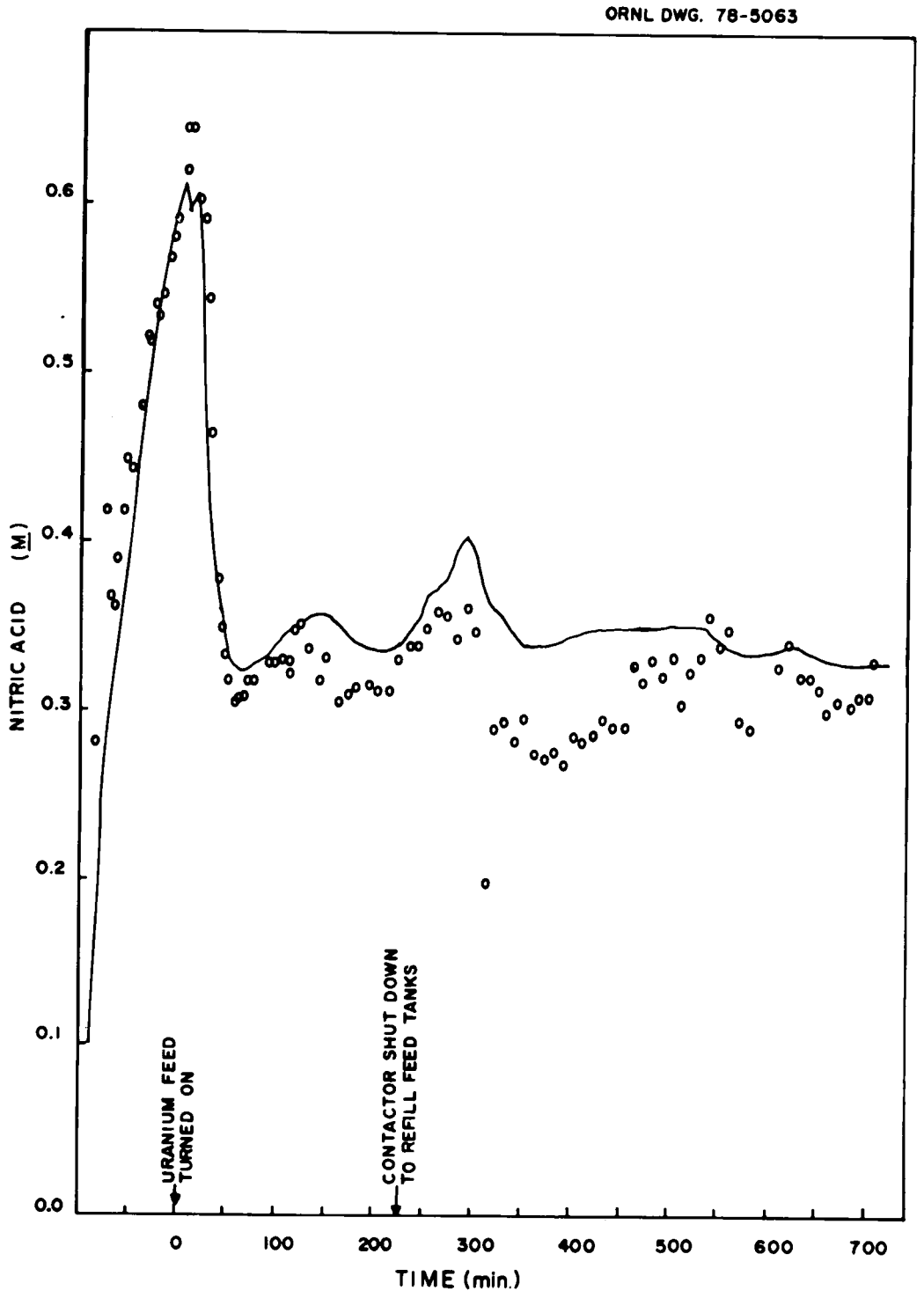

Fig. 5. A comparison of the nitric acid response curve data points with the curve calculated by SEPHIS-MOD4.

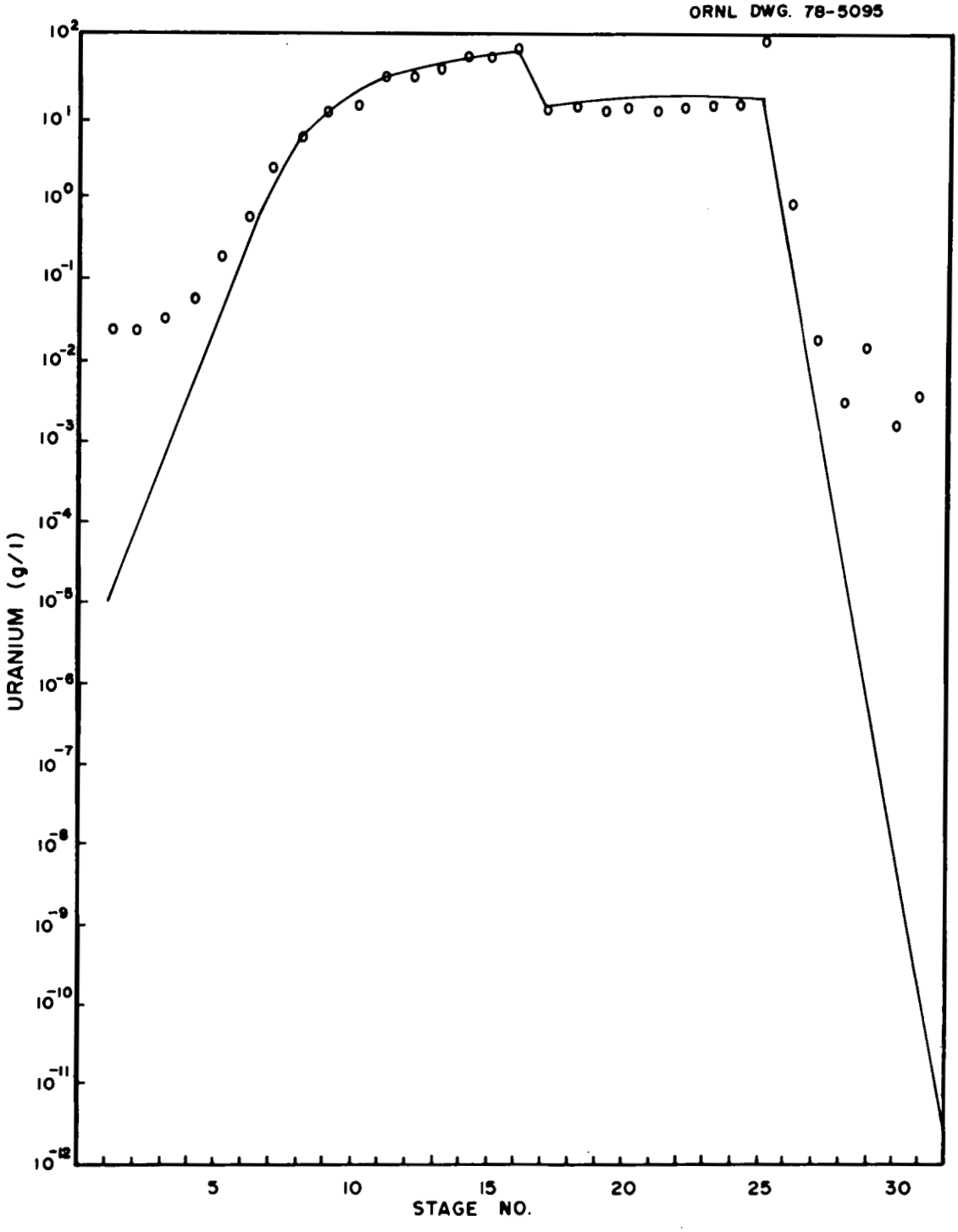

Fig. 6. A comparison of the experimental uranium concentration profile in the aqueous phase with the profile calculated by SEPHIS-MOD4.

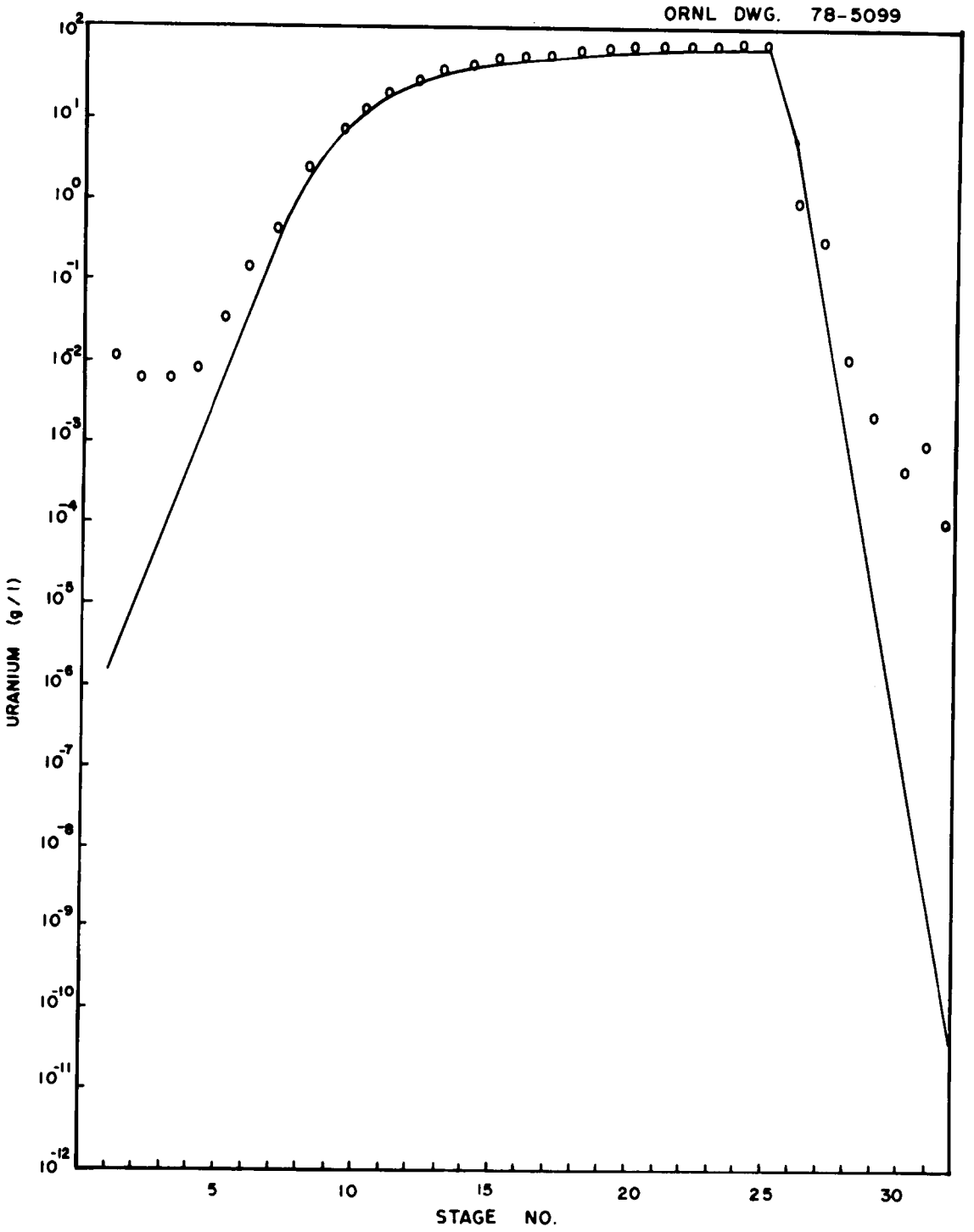

Fig. 7. A comparison of the experimental uranium concentration profile in the organic phase with the profile calculated by SEPHIS-MOD4.

The feed stage (stage 25) shows the effects of incomplete mixing. There is a very small difference between the experimental organic concentration and the predicted value. This is due to the overall mass balance for the same reason as in the scrub section. However, the experimental aqueous concentration is much higher than the predicted value. This is due to incomplete mixing of the 300-kg U/m^3 feed stream with the contents of the mixer. Such nonidealities are not simulated by the program.

The extraction section (stages 25-32) is similar to the strip section. In regions of low concentration, the predicted concentrations give a poor indication of the actual results. This is due to entrainment, mixer inefficiencies, and the uncertainty in the calculated distribution coefficients.

SEPHIS-MOD4 is intended to predict both transient and steady-state concentrations in solvent extraction contactors. Experimental transient results demonstrate the ability of the program to predict the timing of waves of solutes passing through the contactor. Steady-state results indicate which sections of the contactor are satisfactorily simulated by the program. With this information, the user should be able to judge when to trust and when to disregard the results of SEPHIS-MOD4.

5. INPUT CARDS FOR SEPHIS-MOD4

Any computer run with the program is comprised of one or more cases. Each case is defined by a title, the number of stages, the TBP content of the organic phase, and any special piping. The case is subdivided into one or more time periods. A time period is characterized by the feed-stream flow rates and concentrations, the stage volumes, the initial profile, and the product-stream flow rates. The time increment, the time between profile printings, and the convergence tolerance may be changed at any time within a given time period. The input deck is as follows:

Card No.	Card columns	Variable description
Start of the next case		
1		FORMAT (2I2, 2F8.0, 4I2)
	1-2	NTTL = number of title cards (up to ten).
	3-4	NTOST = number of stages (up to 100).
	5-12	CTBP = volume fraction of TBP in the organic phase.
	13-20	TEMPI = initial and default temperature.
	21-22	NSTR = special piping indicator. = 1 for special routing indicated by by ISTR and JSTR. = 0 otherwise.
	23-24	ISTR = stage number.
	25-26	JSTR = stage number. When special piping is used, the organic stream from stage ISTR is fed to stage JSTR.
	27-28	IRXN = indication of reaction rate equation being used. = 0 for no reaction. = 1 for instantaneous reduction of Pu(IV). = 2 for reduction of Pu(IV) by U(IV). = 3 for reduction of Pu(IV) by hydroxylamine.
2		FORMAT (10A8)
	1-80	Case title to be printed. Up to ten cards which describe the case.

After the title cards have been read, the new case is begun. All volumes, flows, and concentrations are set to zero.

Card No.	Card columns	Variable description
3		FORMAT (4F8.0, 7I2)
	1-8	DTHETA = time increment (min).
	9-16	DPRINT = time between successive printings of the concentration profile.

Card No.	Card columns	Variable description
	17-24	TSTOP = time when the calculations will stop and a new card No. 3 will be read to start a new time period or case.
	25-32	TOL = tolerance (percent per minute). When the tolerance is met in every stage, a new card No. 3 will be read to start a new time period or case.
	34	NEWIN = 1, if new feed streams are to be specified. = 0, if the present feed streams are to be continued.
	36	NEWOUT = 1, if new product streams are to be specified. = 0, if the present product streams are to be continued.
	38	IVOLM specifies how mixer volumes will be given. = 0, if the present mixer volumes will be continued. = 1, if the new volumes are to be given by phase. = 2, if the new volumes are to be given as a total volume, with the phase split according to the flow ratio. = 3, if the new volumes are to be given by the phase flow multiplied by a unit time.
	40	IVOLS specifies how the settler volumes will be given. The indicators are identical to those for IVOLM.
	42	IPRO = 0, if the present concentration profile is to be continued. = 1, if a new initial profile is to be read in.

Card No.	Card column	Variable description
	44	IFAST = 0, if the Runge-Kutta integration is to be used. = 1, if the faster, but less accurate, integration is desired.
	46	IPNCH = 0, if cards are not wanted. = 1, if concentration profile cards are to be punched when TSTOP or TOL is reached.
4		FORMAT (2I2, 8F8.0, I2) Feed stream cards which will be read only if NEWIN = 1.
	1-2	I = stage number where this feed will enter.
	4	JHAS = 0 for organic feed streams. = 1 for aqueous feed streams.
	5-12	FDRT = flow rate (liters/min).
	13-20	CON1 = nitric acid concentration (M).
	21-28	CON2 = uranium concentration (g/liter).
	29-36	CON3 = plutonium(IV) concentration (g/liter).
	37-44	CON4 = plutonium(III) concentration (g/liter).
	45-52	CON5 = plutonium reductant concentration (M).
	53-60	CON6 = inextractable nitrate ion concentration (M).
	61-68	TEMP = feed temperature (°C). If TEMP = 0.0, the default temperature (TEMPI) is used.
	70	INDEX = 0, if this is the last feed-stream card. = 1, if more feed-stream cards follow.
5		FORMAT (2I2, F8.0, I2). Product stream cards which will be read only if NEWOUT = 1.

Card No.	Card column	Variable description
	1-2	I = stage number where the stream will leave.
	4	JHAS = 0 for an organic product stream. = 1 for an aqueous product stream.
	5-12	OTRT = flow rate of product stream. If OTRT is larger than the appropriate flow through stage I, the exiting rate will be set so that the entire phase, but no more, is removed.
	14	INDEX = 0, if no more product-stream cards follow. = 1, if more product-stream cards follow.
6		FORMAT (7F10.0) Initial profile cards which will be read only if IPRO = 1. An aqueous card No. 6 followed by an organic card No. 7 is required for every stage.
	1-10	CON1 = nitric acid concentration (M).
	11-20	CON2 = uranium concentration (g/liter).
	21-30	CON3 = plutonium(IV) concentration (g/liter).
	31-40	CON4 = plutonium(III) concentration (g/liter).
	41-50	CON5 = plutonium reductant concentration (M).
	51-60	CON6 = inextractable nitrate concentration (M).
	61-70	TPROF = stage temperature (°C).
7		FORMAT (7F10.0) Organic profile card.
	1-10	CON1 = nitric acid concentration (M).
	11-20	CON2 = uranium concentration (g/liter).
	21-30	CON3 = plutonium(IV) concentration (g/liter).
	31-40	CON4 = plutonium(III) concentration (M).
	41-50	CON5 = plutonium reductant concentration (M).
	51-60	CON6 = inextractable nitrate concentration (M).

Card No.	Card column	Variable description
	61-70	EQCKDG = This variable is a check on how the profile cards were created. The user should not put anything in this field. When the profile cards are punched by the program, a 1.0 is put here to signify that the phases are in approximate chemical equilibrium.
8		FORMAT (2I2, 2F8.0, I2). Volumes for mixers and settlers. These cards are needed only if IVOLM or IVOLS equals 1 or 2.
	2	ISEC = 1 for mixer volumes. = 2 for settler volumes.
	3-4	I = stage number.
	5-12	VOLA If IVOLM = 1 and ISEC = 1, or if IVOLS = 1 and ISEC = 2, VOLA = aqueous volume. However, if IVOLM = 2 and ISEC = 1, or if IVOLS = 2 and ISEC = 2, VOLA = total volume.
	13-20	VOLO = organic volume if IVOLM = 1 and ISEC = 1, or IVOLS = 1 and ISEC = 2.
	22	INDX = 0 for the last volume card. = 1, if more volume cards follow.

After the last volume card has been read in, the program begins calculating concentrations. When the elapsed time is equal to TSTOP or the tolerance is met, a new card No. 3 is read. If this card is merely giving new DTHETA, DPRINT, TSTOP, TOL, IFAST, or IPNCH values, the calculation continues as before but with the new values. If this card requests that new feed streams, product streams, concentration profiles, or volumes be used, the desired information will be read in and the calculation restarted for the new time period. At the start of a new time period, the elapsed time will be set to 0.0.

To signal that calculations are to be done on a new case, the card No. 3 must have DTHETA = 0.0 and DPRINT = 1.0. When such a card is used, the new case is begun, and a card No. 1 is read in.

When all calculations have been completed, the card No. 3 should have DTHETA = 0.0 and DPRINT = 0.0 or just a blank card. This will stop the execution of the program.

6. CHOOSING CONDITIONS FOR SEPHIS-MOD4

Choosing conditions for SEPHIS-MOD4 is a relatively easy task. Certain conventions are used to arrange the stages and streams for the program. For steady-state cases, only the feed-stream flow rates and concentrations are important in determining the final concentration profile. The remaining variables, however, are still important to the program and should be chosen correctly. Cases involving transient periods tend to be more complex, but experience with the program is helpful in choosing values for the more important variables.

The stages in a contactor are arranged so that the aqueous streams flow toward higher numbered stages and the organic streams flow toward lower numbered stages. One exception to this rule is allowed. The organic stream from one stage can be directed to any other stage through the use of NSTR, ISTR, and JSTR on card No. 1. This arrangement of the stages allows many combinations of contactors to be simulated. Simple examples of this are given in the next section.

6.1 Steady-State Cases

Steady-state calculations are used primarily for flow sheet testing and depend mainly on the number of stages and the input streams. Since only the final results are important, certain variables (stage volumes, the initial concentration profile, and the method of integration) may be neglected. These variables have only a small impact on the calculated final concentrations. However, if appropriate values are given to these variables, the calculational procedure is smoother, faster, and easier.

Assuming that the stage arrangement and flow rates have been determined, the first variable to be set on card No. 3 is DTHETA. This is the time increment. DTHETA should always be set in relation to the residence time for a stage, as defined by:

$$\tau = \frac{\text{volume}}{\text{flow rate through the volume}} \tag{18}$$

For steady-state calculations, a reasonable choice is to let DTHETA equal the residence time for a mixer, or half of the residence time. Larger values may produce instabilities in the equations, while smaller values consume computer time unnecessarily.

DPRINT and TSTOP are the next values to be determined. TSTOP sets the time when the calculations will stop if the tolerance has not been met. Since steady-state values are desired, TSTOP should be set to a high value (such as 1000.0) so that the calculations will most likely be stopped by the steady-state tolerance. DPRINT determines the time interval between successive printings of the concentration profile. If only the steady-state values are to be printed, DPRINT can be set equal to TSTOP. A smaller value for DPRINT can be used to check the progress toward steady state.

TOL sets the steady-state tolerance used to stop the calculations. When the inventories of all the solutes in all the stages are changing by less than TOL (percent per minute), a steady state is declared and the profile is printed. A low value should be chosen for TOL; a value of 0.01 is usually sufficient.

IVOLM and IVOLS indicate how the volumes will be determined. The easiest method for steady-state calculations is to set IVOLM and IVOLS equal to 3 so that no volume cards need to be punched.

IPRO can be set as desired since the initial profile has little effect on the final profile. The calculations may take more (or less) time if the initial profile is read from cards.

6.2 Transient Cases

It is relatively simple to select conditions for steady-state calculations because fewer variables need to be specified for an accurate prediction of steady-state concentrations for a contactor. Transient cases are more complex since more variables are important. The initial

state of the contactor should be specified more closely; likewise, the stage volumes and the choice of DTHETA are more important.

The initial state of the contactor is important simply because it is the starting point for the calculations. The concentration profile should be given; otherwise, the program will assume that the contactor contains only water and the solvent. The initial state can be specified by a set of profile cards (cards 6 and 7) or by the results of a preceding calculation.

The volumes in the contactor may be specified by any desired method which gives an accurate representation of the contactor in question. The volumes are crucial in determining the time lag associated with the changes and rates of changes in concentration. Thus, good predictions of transient periods require reasonably good values for the volumes in a contactor.

DTHETA has an important impact on the errors associated with the integration methods used by SEPHIS-MOD4. The desire for small errors must be balanced against the concomitant requirement of longer computing times. Table 1 indicates the effect of DTHETA. The results apply to a simple perfect mixer case. The analytical solution was found by an exact integration of the differential equation which defines a perfect mixer. The results from SEPHIS-MOD4 apply to a nontransferring component which should exactly follow the analytical solution. For the Runge-Kutta integration scheme, all values of DTHETA that were less than one-fourth of the residence time were in good agreement with the analytical solution. Larger values for DTHETA show a gradual increase in the integration errors; that is, the size of the error increased as DTHETA increased. The faster trapezoidal integration produced errors even with much lower DTHETA values. It should be noted that this table only indicates how well the program integrates differential equations. A comparison with actual conditions is given in an earlier section. For accurate predictions of transient periods with the Runge-Kutta integration method, DTHETA should be, at most, equal to one-quarter of the residence time. Even lower values are suggested if the concentrations are changing rapidly. The trapezoidal method should not be used for transient predictions unless the concentrations are changing slowly.

Table 1. The effect of DTHETA on integration accuracy

Time	Analytical solution	Runge-Kutta integration DTHETA/τ =			Trapezoidal integration DTHETA/τ =		
		1/4	1/2	1	1/4	1/2	1
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.25	0.2212	0.2212			0.2222		
0.5	0.3935	0.3935	0.3932		0.3951	0.4000	
0.75	0.5276	0.5276			0.5295		
1.0	0.6321	0.6321	0.6318	0.6250	0.6340	0.6400	0.6667
1.25	0.7135	0.7135			0.7154		
1.5	0.7769	0.7769	0.7766		0.7786	0.7840	
1.75	0.8262	0.8262			0.8278		
2.0	0.8647	0.8647	0.8645	0.8594	0.8661	0.8704	0.8889
2.25	0.8946	0.8946			0.8958		
2.5	0.9179	0.9179	0.9178		0.9190	0.9222	
2.75	0.9361	0.9361			0.9370		
3.0	0.9502	0.9502	0.9501	0.9473	0.9510	0.9533	0.9630

These generalizations concerning the ranges of values for the variables are intended to indicate some of the ways the program may be run. Different priorities, however, will lead to the choice of different values for the variables, and the user should rely on his experience with the program to determine which values will suit his requirements.

7. EXAMPLES OF SEPHIS-MOD4 CALCULATIONS

7.1 Example 1 - A Steady-State Calculation for a Six-Stage Contactor

This is a simple example calculation for a six-stage uranium-stripping contactor as shown in Fig. 8. Only steady-state results are desired, so only the final concentration profile will be printed. No volume or initial profile cards are necessary, since they have a negligible impact on the steady-state concentrations. For this type of calculation, only the feed streams (and product streams if present) need to be specified. The results that are printed list all the information required to repeat the calculation. The final concentration profile indicates what concentrations may be expected in the contactor and in the end streams. This calculation took 2.1 sec of execution time on the ORNL IBM 360/91.

The cards that were used to produce the following results are:

```
 2 6 0.3    30.0     0 0 0 0
EXAMPLE 1
THIS IS A SIMPLE TEST OF A SIX STAGE URANIUM STRIPPING COLUMN.
1.0     1000.0  1000.0  0.01     1 0 3 3 0 1 0
 1 1 15.0   0.15    0.0     0.0     0.0     0.0     0.0     25.0     1
 6 0 10.0   0.25    50.0    0.0     0.0     0.0     0.0     55.0     0
0.0     0.0
```

ORNL DWG 78-4911

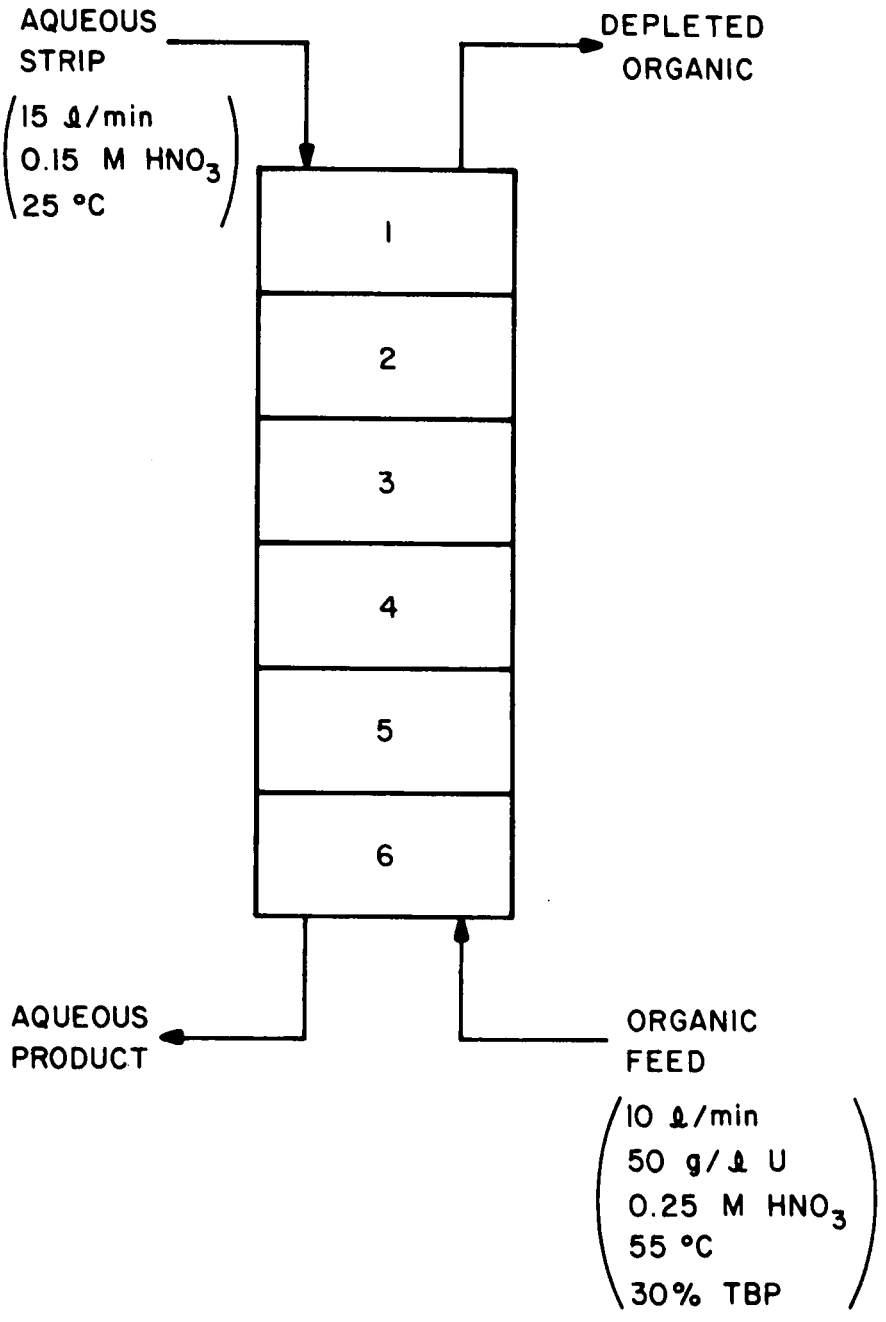

Fig. 8. Example 1, a six-stage uranium-stripping contactor.

CALCULATIONS FOR A SOLVENT EXTRACTION PROCESS HAVING INTERACTING SOLUTES

EXAMPLE 1
THIS IS A SIMPLE TEST OF A SIX STAGE URANIUM STRIPPING COLUMN.

DTEFTA = 1.000 MINUTES PER TIME INCREMENT
DPRINT = 1000.000 MINUTES BETWEEN PRINTING OF PROFILES
IFAST = 1 THE FAST INTEGRATION TECHNIQUE WILL BE USED
THIS TIME PERIOD WILL END WHEN TIME = TSTOP = 1000.000 MINUTES, OR A TOLERANCE OF TOL = 0.0100 % PER MINUTE IS REACHED
NUMBER OF STAGES = 6
NEWIN = 1 NEW INPUT FLOWS WILL BE GIVEN
NEWOUT = 0 OUTPUT STREAMS WILL BE UNCHANGED
IVOLM = 3 MIXER VOLUMES DETERMINED BY PHASE FLOW
IVOLS = 3 SETTLER VOLUMES GIVEN BY PHASE FLOW
IPRO = 0 A NEW INITIAL PROFILE WILL NOT BE READ
IPUNCH = 0 NO PUNCHED CARD OUTPUT
NSTR = 0 NO UNUSUAL ROUTING PATTERN
TEMPI = 3.000E 01 INITIAL & DEFAULT TEMPERATURE
IRXN = 0 NO REACTIONS WILL BE CONSIDERED

FEED & PRODUCT STREAM DATA	STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	FLOW RATE (L/MIN)	TEMP (C)
AQUEOUS	1	1.500E-01	0.0	0.0	0.0	0.0	0.0	1.500E 01	25.0
30.0 % TBP	6	2.500E-01	5.000E 01	0.0	0.0	0.0	0.0	1.000E 01	55.0

STAGE NO.	MIXER VOLUME BY PHASE		SETTLER VOLUME BY PHASE		MIXER FLOW RATE		INTERSTAGE FLOW RATE	
	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC
1	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00
2	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00
3	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00
4	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00
5	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00
6	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00	1.493E 01	9.655E 00

TRANSIENT BEHAVIOR RESULTS MIXER CONCENTRATION GIVEN

TIME = 0.0 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	0.0	0.0	0.0	0.0	0.0	0.0	9.971E-01	1.493E 01	3.000E 01
2	0.0	0.0	0.0	0.0	0.0	0.0	9.971E-01	1.493E 01	3.000E 01
3	0.0	0.0	0.0	0.0	0.0	0.0	9.971E-01	1.493E 01	3.000E 01
4	0.0	0.0	0.0	0.0	0.0	0.0	9.971E-01	1.493E 01	3.000E 01
5	0.0	0.0	0.0	0.0	0.0	0.0	9.971E-01	1.493E 01	3.000E 01
6	0.0	0.0	0.0	0.0	0.0	0.0	9.971E-01	1.493E 01	3.000E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	0.0	0.0	0.0	0.0	0.0	0.0	8.171E-01	9.738E 00	2.000E 02
2	0.0	0.0	0.0	0.0	0.0	0.0	8.171E-01	9.738E 00	2.000E 02
3	0.0	0.0	0.0	0.0	0.0	0.0	8.171E-01	9.738E 00	2.000E 02
4	0.0	0.0	0.0	0.0	0.0	0.0	8.171E-01	9.738E 00	2.000E 02
5	0.0	0.0	0.0	0.0	0.0	0.0	8.171E-01	9.738E 00	2.000E 02
6	0.0	0.0	0.0	0.0	0.0	0.0	8.171E-01	9.738E 00	2.000E 02

TIME = 191.00 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	1.508E-01	1.710E 00	0.0	0.0	0.0	0.0	1.004E 00	1.501E 01	2.500E 01
2	1.515E-01	5.571E 00	0.0	0.0	0.0	0.0	1.010E 00	1.503E 01	2.502E 01
3	1.518E-01	1.161E 01	0.0	0.0	0.0	0.0	1.018E 00	1.505E 01	2.507E 01
4	1.522E-01	1.906E 01	0.0	0.0	0.0	0.0	1.028E 00	1.509E 01	2.533E 01
5	1.617E-01	2.738E 01	0.0	0.0	0.0	0.0	1.040E 00	1.513E 01	2.649E 01
6	2.054E-01	3.230E 01	0.0	0.0	0.0	0.0	1.052E 00	1.522E 01	3.168E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	1.028E-02	8.298E-01	0.0	3.152E-01	0.0	4.426E-02	8.185E-01	9.746E 00	9.236E-03
2	1.161E-02	3.460E 00	0.0	4.032E-01	0.0	4.974E-02	8.221E-01	9.755E 00	8.526E-03
3	1.301E-02	9.394E 00	0.0	5.253E-01	0.0	5.565E-02	8.301E-01	9.776E 00	6.149E-03
4	1.385E-02	1.866E 01	0.0	6.363E-01	0.0	5.915E-02	8.426E-01	9.807E 00	3.952E-03
5	1.495E-02	3.004E 01	0.0	7.139E-01	0.0	6.015E-02	8.581E-01	9.846E 00	2.166E-03
6	2.957E-02	4.271E 01	0.0	8.592E-01	0.0	6.377E-02	8.759E-01	9.893E 00	1.074E-03

7.2 Example 2 - Steady-State Calculation for a Batch Extraction Process

This is an example of how a batch extraction process can be simulated with the SEPHIS program. This process is rather simple to describe but difficult to imagine as a continuous operation which SEPHIS can handle. One volume of aqueous is to be contacted with two portions of pure solvent. A phase ratio (organic to aqueous) of 2:1 is to be used in each of the two contacts. The two resulting organic solutions are to be combined and stripped. Five strip contacts are to be made with 0.4 M nitric acid. This phase ratio (2:1) is also to be used in the stripping operations.

The batch operation can be modeled by the SEPHIS program as a series of crosscurrent contacts, as shown in Fig. 9. The strip contacts are in stages 1-5, and the extraction contacts are in stages 6 and 7. The following cards were used to perform the calculations.

```
 2 7 0.3    25.0     1 7 5 0
EXAMPLE 2
THIS IS A BATCH EXTRACTION PROCESS MODELED AS CROSS CURRENT CONTACTS.
1.0      1000.0  1000.0  0.01      1 1 3 3 1 1 0
 1 1 2.0    0.4      0.0      0.0      0.0      0.0      0.0      25.0     1
 2 1 2.0    0.4      0.0      0.0      0.0      0.0      0.0      25.0     1
 3 1 2.0    0.4      0.0      0.0      0.0      0.0      0.0      25.0     1
 4 1 2.0    0.4      0.0      0.0      0.0      0.0      0.0      25.0     1
 5 1 2.0    0.4      0.0      0.0      0.0      0.0      0.0      25.0     1
 6 1 1.0    2.0      300.0    3.0      0.0      0.0      0.0      25.0     1
 6 0 2.0    0.0      0.0      0.0      0.0      0.0      0.0      25.0     1
 7 0 2.0    0.0      0.0      0.0      0.0      0.0      0.0      25.0     0
 1 1 3.0     1
 2 1 3.0     1
 3 1 3.0     1
 4 1 3.0     1
 5 1 3.0     0
2.0        300.0     3.0       0.0       0.0       0.0       25.0
0.0        0.0       0.0       0.0       0.0       0.0
2.0        300.0     3.0       0.0       0.0       0.0       25.0
0.0        0.0       0.0       0.0       0.0       0.0
2.0        300.0     3.0       0.0       0.0       0.0       25.0
0.0        0.0       0.0       0.0       0.0       0.0
2.0        300.0     3.0       0.0       0.0       0.0       25.0
0.0        0.0       0.0       0.0       0.0       0.0
2.0        300.0     3.0       0.0       0.0       0.0       25.0
0.0        0.0       0.0       0.0       0.0       0.0
2.0        300.0     3.0       0.0       0.0       0.0       25.0
0.0        0.0       0.0       0.0       0.0       0.0
2.0        300.0     3.0       0.0       0.0       0.0       25.0
0.0        0.0       0.0       0.0       0.0       0.0
0.0      0.0
```

The crosscurrent process has many more input and exit streams; hence, more cards are required to describe the process. An initial profile is also used in this example. In some calculations, the use of this profile speeds the convergence to a steady-state result.

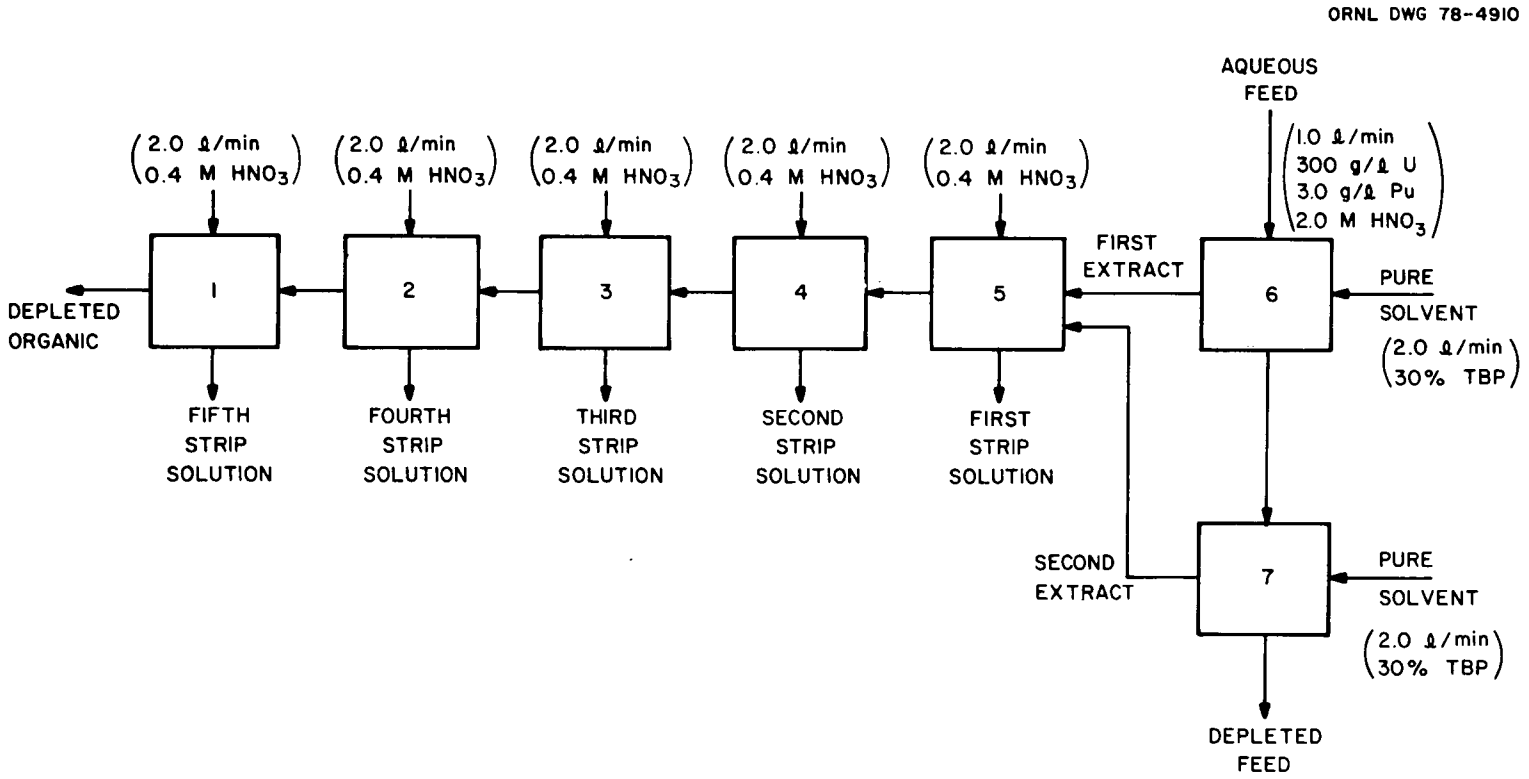

Fig. 9. Example 2, a batch operation simulated by crosscurrent contacts.

EXAMPLE 2
THIS IS A BATCH EXTRACTION PROCESS MODELED AS CROSS CURRENT CONTACTS.

DTHETA = 1.000 MINUTES PER TIME INCREMENT
DPRINT = 1000.000 MINUTES BETWEEN PRINTING OF PROFILES
IFAST = 1 THE FAST INTEGRATION TECHNIQUE WILL BE USED
THIS TIME PERIOD WILL END WHEN TIME = TSTOP = 1000.000 MINUTES, OR A TOLERANCE OF TOL = 0.0100 % PER MINUTE IS REACHED
NUMBER OF STAGES = 7
NEWIN = 1 NEW INPUT FLOWS WILL BE GIVEN
NEWOUT = 1 NEW OUTPUT FLOWS WILL BE GIVEN
IVOLM = 3 MIXER VOLUMES DETERMINED BY PHASE FLOW
IVOLS = 3 SETTLER VOLUMES GIVEN BY PHASE FLOW
IPRO = 1 A NEW INITIAL PROFILE WILL BE READ
IPNCH = 0 NO PUNCHED CARD OUTPUT
NSTR = 1 ROUTING PATTERN OTHER THAN NORMAL
ORGANIC STREAM EXITING AT STAGE 7 FEEDS STAGE 5
TEMPI = 2.500E 01 INITIAL & DEFAULT TEMPERATURE
IRXN = 0 NO REACTIONS WILL BE CONSIDERED

FEED & PRODUCT STREAM DATA	STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	FLOW RATE (L/MIN)	TEMP (C)
AQUEOUS	1	4.000E-01	0.0	0.0	0.0	0.0	0.0	2.000E 00	25.0
AQUEOUS	2	4.000E-01	0.0	0.0	0.0	0.0	0.0	2.000E 00	25.0
AQUEOUS	3	4.000E-01	0.0	0.0	0.0	0.0	0.0	2.000E 00	25.0
AQUEOUS	4	4.000E-01	0.0	0.0	0.0	0.0	0.0	2.000E 00	25.0
AQUEOUS	5	4.000E-01	0.0	0.0	0.0	0.0	0.0	2.000E 00	25.0
AQUEOUS	6	2.000E 00	3.000E 02	3.000E 00	0.0	0.0	0.0	1.000E 00	25.0
30.0 % TBP	6	0.0	0.0	0.0	0.0	0.0	0.0	2.000E 00	25.0
30.0 % TBP	7	0.0	0.0	0.0	0.0	0.0	0.0	2.000E 00	25.0
AQUEOUS	1	PRODUCT STREAM REMOVED (FLOW RATE IN MOLAL UNITS)						3.000E 00	
AQUEOUS	2	PRODUCT STREAM REMOVED (FLOW RATE IN MOLAL UNITS)						3.000E 00	
AQUEOUS	3	PRODUCT STREAM REMOVED (FLOW RATE IN MOLAL UNITS)						3.000E 00	
AQUEOUS	4	PRODUCT STREAM REMOVED (FLOW RATE IN MOLAL UNITS)						3.000E 00	
AQUEOUS	5	PRODUCT STREAM REMOVED (FLOW RATE IN MOLAL UNITS)						3.000E 00	

STAGE NO.	MIXER VOLUME BY PHASE		SETTLER VOLUME BY PHASE		MIXER FLOW RATE		INTERSTAGE FLOW RATE	
	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC
1	1.975E 00	3.966E 00	1.975E 00	3.966E 00	1.975E 00	3.966E 00	0.0	3.966E 00
2	1.975E 00	3.966E 00	1.975E 00	3.966E 00	1.975E 00	3.966E 00	0.0	3.966E 00
3	1.975E 00	3.966E 00	1.975E 00	3.966E 00	1.975E 00	3.966E 00	0.0	3.966E 00
4	1.975E 00	3.966E 00	1.975E 00	3.966E 00	1.975E 00	3.966E 00	0.0	3.966E 00
5	1.975E 00	3.966E 00	1.975E 00	3.966E 00	1.975E 00	3.966E 00	0.0	3.966E 00
6	8.453E-01	1.983E 00	8.453E-01	1.983E 00	8.453E-01	1.983E 00	8.453E-01	1.983E 00
7	8.453E-01	1.983E 00	8.453E-01	1.983E 00	8.453E-01	1.983E 00	8.453E-01	1.983E 00

TRANSIENT BEHAVIOR RESULTS MIXER CONCENTRATION GIVEN

TIME = 0.0 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	2.014E 00	1.300E 02	1.977E 00	0.0	0.0	0.0	1.269E 00	2.202E 00	2.500E 01
1	PRODUCT STREAM							2.202E 00	
2	2.014E 00	1.300E 02	1.977E 00	0.0	0.0	0.0	1.269E 00	2.202E 00	2.500E 01
2	PRODUCT STREAM							2.202E 00	
3	2.014E 00	1.300E 02	1.977E 00	0.0	0.0	0.0	1.269E 00	2.202E 00	2.500E 01
3	PRODUCT STREAM							2.202E 00	
4	2.014E 00	1.300E 02	1.977E 00	0.0	0.0	0.0	1.269E 00	2.202E 00	2.500E 01
4	PRODUCT STREAM							2.202E 00	
5	2.014E 00	1.300E 02	1.977E 00	0.0	0.0	0.0	1.269E 00	2.202E 00	2.500E 01
5	PRODUCT STREAM							2.202E 00	
6	2.002E 00	1.108E 02	1.801E 00	0.0	0.0	0.0	1.237E 00	9.356E-01	2.500E 01
7	2.002E 00	1.108E 02	1.801E 00	0.0	0.0	0.0	1.237E 00	9.356E-01	2.500E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	5.753E-02	9.992E 01	6.402E-01	1.450E 00	6.107E-01	5.387E-02	9.583E-01	4.152E 00	2.000E 02
2	5.753E-02	9.992E 01	6.402E-01	1.450E 00	6.107E-01	5.387E-02	9.583E-01	4.152E 00	2.000E 02
3	5.753E-02	9.992E 01	6.402E-01	1.450E 00	6.107E-01	5.387E-02	9.583E-01	4.152E 00	2.000E 02
4	5.753E-02	9.992E 01	6.402E-01	1.450E 00	6.107E-01	5.387E-02	9.583E-01	4.152E 00	2.000E 02
5	5.753E-02	9.992E 01	6.402E-01	1.450E 00	6.107E-01	5.387E-02	9.583E-01	4.152E 00	2.000E 02
6	6.133E-02	9.475E 01	6.342E-01	1.895E 00	7.799E-01	6.787E-02	9.510E-01	2.073E 00	2.000E 02
7	6.133E-02	9.475E 01	6.342E-01	1.895E 00	7.799E-01	6.787E-02	9.510E-01	2.073E 00	2.000E 02

TIME = 24.00 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	3.952E-01	1.192E 01	5.464E-02	0.0	0.0	0.0	1.026E 00	2.007E 00	2.500E 01
1	PRODUCT STREAM							2.007E 00	
2	3.946E-01	1.540E 01	1.020E-01	0.0	0.0	0.0	1.031E 00	2.009E 00	2.500E 01
2	PRODUCT STREAM							2.009E 00	
3	3.980E-01	2.005E 01	1.927E-01	0.0	0.0	0.0	1.038E 00	2.013E 00	2.500E 01
3	PRODUCT STREAM							2.013E 00	
4	4.252E-01	2.589E 01	3.622E-01	0.0	0.0	0.0	1.047E 00	2.018E 00	2.500E 01
4	PRODUCT STREAM							2.018E 00	
5	5.966E-01	2.971E 01	6.026E-01	0.0	0.0	0.0	1.059E 00	2.032E 00	2.500E 01
5	PRODUCT STREAM							2.032E 00	
6	1.983E 00	8.507E 01	1.551E 00	0.0	0.0	0.0	1.196E 00	9.269E-01	2.500E 01
7	1.523E 00	4.950E 00	2.382E-01	0.0	0.0	0.0	1.056E 00	8.886E-01	2.500E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	4.690E-02	2.178E 01	3.228E-02	3.668E 00	1.188E 00	2.387E-01	8.478E-01	4.037E 00	9.436E-03
2	4.512E-02	2.761E 01	5.932E-02	3.610E 00	1.171E 00	2.302E-01	8.558E-01	4.045E 00	4.457E-04
3	4.325E-02	3.517E 01	1.097E-01	3.535E 00	1.147E 00	2.190E-01	8.661E-01	4.056E 00	0.0
4	4.332E-02	4.496E 01	2.046E-01	3.502E 00	1.139E 00	2.055E-01	8.797E-01	4.070E 00	7.833E-05
5	5.731E-02	5.751E 01	3.824E-01	3.897E 00	1.277E 00	1.934E-01	8.979E-01	4.090E 00	5.925E-05
6	7.799E-02	1.062E 02	7.502E-01	2.805E 00	1.087E 00	8.838E-02	9.682E-01	2.083E 00	0.0
7	2.368E-01	3.641E 01	5.996E-01	1.693E 01	5.792E 00	3.577E-01	8.746E-01	2.045E 00	0.0

The results of the calculations indicate the concentrations which may be expected in all the batch contacts. A simple mass balance around any stage demonstrates that the continuous crosscurrent process is acceptable as a model of the batch process (as expected). Thus, the SEPHIS program may be used for many processes other than continuous countercurrent mixer-settlers. The calculation required only 0.6 sec of computing time on the ORNL IBM 360/91.

7.3 Example 3 - Transient Calculation for Two Pulse Columns

Transient calculations usually require more information if a good prediction is to be made. In this case, two pulse columns are modeled as shown in Fig. 10. It should be noted that SEPHIS-MOD4 is tailored to simulate the actions of mixer-settlers rather than pulse columns. Each mixer-settler stage modeled by SEPHIS-MOD4 is a theoretical stage. However, columns are commonly characterized by their HETS (height equivalent to a theoretical stage), so the changes in column concentration may also be simulated by the program. The simulation is relatively crude, but it should still provide a useful representation of the changes in concentration which would occur in a column.

Since an accurate representation of the column is desired, the volumes for the mixing and settling portions must be specified. These volumes are crucial in determining the time delays associated with the columns. In the interior section of the columns, the stage volume is determined by the HETS. The split by phases is equal to the flow ratio, and the split between the mixers and settlers is arbitrary. At the ends of each column are phase disengaging sections and additional piping. These volumes are simply added to the appropriate settler.

Thus, the volumes for column A are:

stage volume = HETS x column cross section

$$= 10 \text{ cm} \times \pi \times (4.5 \text{ cm})^2 = 0.64 \text{ liter.}$$

aqueous volumes = [A/(A + O)] x stage volume = 0.14.

aqueous mixer volume = 0.25 x aqueous volume = 0.036 liter.

aqueous settler volume = 0.11 liter.

Similarly, for the organic phase,

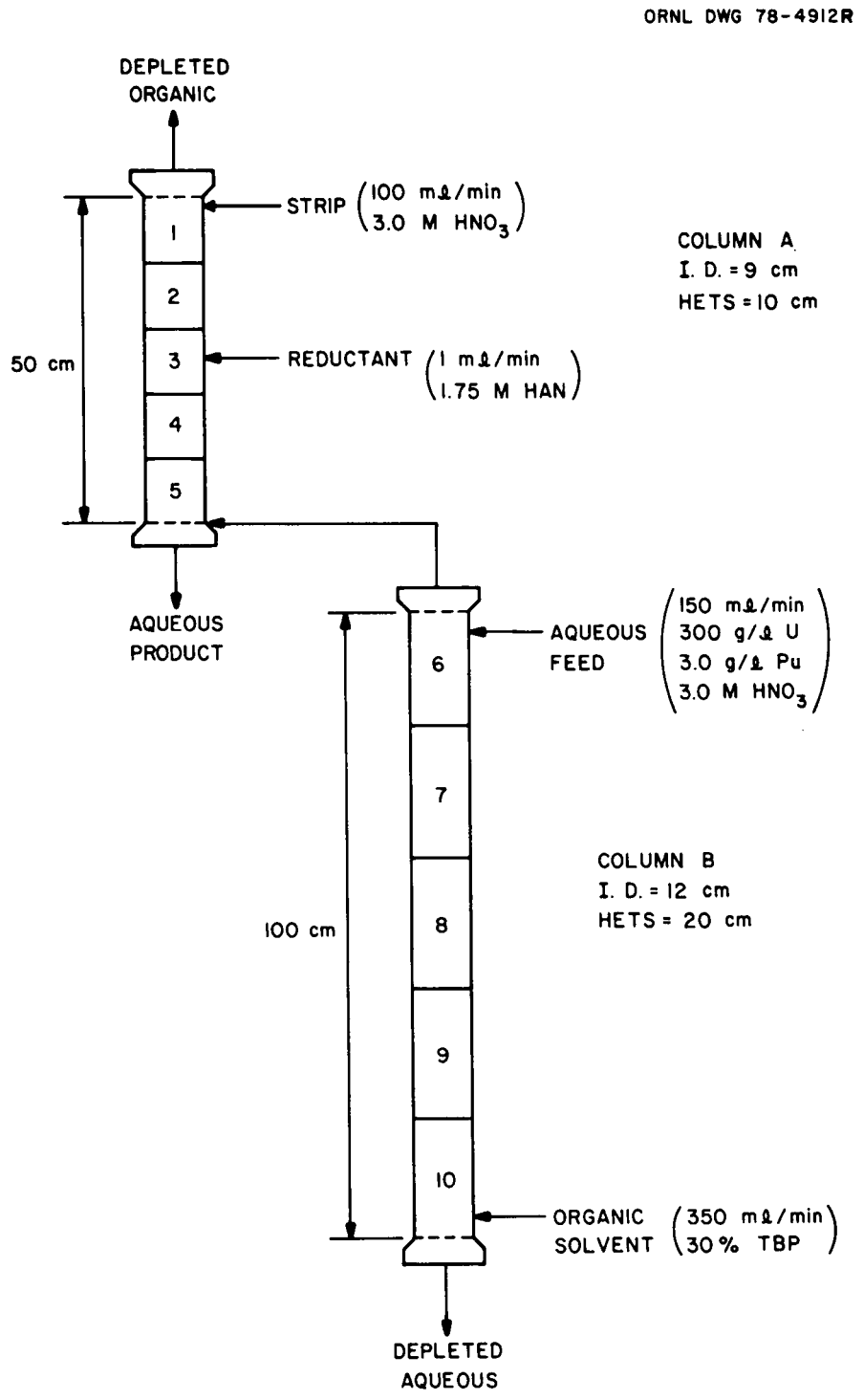

Fig. 10. Example 3, an extraction and partial partitioning column.

organic mixer volume = 0.12 liter,

organic settler volume = 0.38 liter.

For stage 1, there is an additional 0.2 liter in the organic settler, and in stage 5 the 0.2 liter is added to the aqueous settler. These additional volumes are due to the disengaging sections.

The volumes for column B are determined in the same manner:

aqueous mixer volume = 0.17 liter,

aqueous settler volume = 0.51 liter,

organic mixer volume = 0.40 liter,

organic settler volume = 1.18 liters,

stage 6 organic settler volume = 1.70 liters,

stage 10 aqueous settler volume = 0.70 liter.

The situation being simulated is the complete loss of the small reductant stream for 30 min. The input cards and results show how the problem can be handled. The starting point is a steady-state profile that was produced by an earlier computer run. Since this is a transient case, the time increment is set to a value somewhat lower than the shortest residence time in the columns. This helps the integration routine follow the changes in concentration more accurately. After the 30 min have elapsed, the reductant stream is reinserted and the calculation is continued for another 30 min. This calculation required 27 sec on the ORNL IBM 360/91.

8. REFERENCES

1. A. D. Mitchell, A Comparison Between SEPHIS-MOD4 and Previous Models of the Purex Solvent Extraction System, ORNL/TM-6565 (in preparation).
2. S. B. Watson and R. H. Rainey, Modifications of the SEPHIS Computer Code for Calculating the Purex Solvent Extraction System, ORNL/TM-5123 (December 1975).
3. W. Baxter and A. Naylor, "Uranium(IV) as a Process Reductant for Plutonium(IV)," p. 117 in Solvent Extraction Chemistry of Metals, H. A. C. McKay, et al., Eds., Macmillan, London, 1965.
4. G. S. Barney, "A Kinetic Study of the Reaction of Plutonium(IV) with Hydroxylamine," J. Inorg. Nucl. Chem. 38, 1677 (1976).

```
 710 0.3    40.0     0 0 0 1
EXAMPLE 3
THIS IS A TRANSIENT CASE FOR TWO COLUMNS.  EACH COLUMN HAS FIVE STAGES
WITH THE STAGE VOLUMES DETERMINED BY THE COLUMN DIMENSIONS.  AN INITIAL PROFILE
HAS BEEN PREVIOUSLY CALCULATED, AND IS USED AS A STARTING POINT FOR THIS
RUN.  THE SITUATION BEING MODELED IS THE COMPLETE LOSS OF THE REDUCTANT
STREAM IN STAGE 3.  AFTER THIRTY MINUTES WITH NO REDUCTANT, THE STREAM IS
TURNED ON AND THE CONCENTRATION FOLOWED FOR ANOTHER THIRTY MINUTES.
0.125   10.0    30.0    0.01     1 1 1 1 1 0 0
 1 1 0.1    3.0      0.0      0.0      0.0      0.0      0.0      40.0     1
 6 1 0.15   3.0      300.0    3.0      0.0      0.0      0.0      40.0     1
10 0 0.35   0.0      0.0      0.0      0.0      0.0      0.0      40.0     0
 5 1 10.0    0
 2.838E 00 2.770E 01 0.0        0.0        0.0        0.0        4.000E 01
 2.046E-01 8.746E 01 0.0        0.0        0.0        0.0        1.000E 00
 2.746E 00 4.282E 01 0.0        0.0        0.0        0.0        4.000E 01
 1.628E-01 9.500E 01 0.0        0.0        0.0        0.0        1.000E 00
 2.642E 00 5.564E 01 0.0        0.0        1.720E-02 1.720E-02 4.000E 01
 1.389E-01 9.914E 01 0.0        0.0        0.0        0.0        1.000E 00
 2.550E 00 7.190E 01 0.0        4.469E-02 1.697E-02 1.716E-02 4.000E 01
 1.187E-01 1.028E 02 0.0        0.0        0.0        0.0        1.000E 00
 2.413E 00 1.000E 02 1.747E-02 4.081E 00 0.0        1.707E-02 4.000E 01
 9.479E-02 1.073E 02 1.230E-02 0.0        0.0        0.0        1.000E 00
 3.000E 00 3.001E 02 2.873E 00 0.0        0.0        0.0        4.000E 01
 5.958E-02 1.151E 02 1.131E 00 0.0        0.0        0.0        1.000E 00
 3.004E 00 2.998E 02 2.737E 00 0.0        0.0        0.0        4.000E 01
 5.969E-02 1.151E 02 1.079E 00 0.0        0.0        0.0        1.000E 00
 3.051E 00 2.942E 02 2.552E 00 0.0        0.0        0.0        4.000E 01
 6.117E-02 1.150E 02 1.023E 00 0.0        0.0        0.0        1.000E 00
 3.484E 00 2.235E 02 1.908E 00 0.0        0.0        0.0        4.000E 01
 8.005E-02 1.127E 02 9.470E-01 0.0        0.0        0.0        1.000E 00
 3.142E 00 2.144E 01 2.674E-01 0.0        0.0        0.0        4.000E 01
 2.439E-01 8.306E 01 6.777E-01 0.0        0.0        0.0        1.000E 00
 1 1 0.036  0.12     1
 1 6 0.17   0.4      1
 2 1 0.11   0.58     1
 2 2 0.11   0.38     1
 2 5 0.31   0.38     1
 2 6 0.51   1.70     1
 2 7 0.51   1.18     1
 210 0.70   1.18     0
0.125   10.0    30.0    0.01     1 1 0 0 0 0 0
 1 1 0.1    3.0      0.0      0.0      0.0      0.0      0.0      40.0     1
 3 1 0.001  0.0      0.0      0.0      0.0      1.75     1.75     40.0     1
 6 1 0.15   3.0      300.0    3.0      0.0      0.0      0.0      40.0     1
10 0 0.35   0.0      0.0      0.0      0.0      0.0      0.0      40.0     0
 5 1 10.0    0
0.0     0.0
```

CALCULATIONS FOR A SOLVENT EXTRACTION PROCESS HAVING INTERACTING SOLUTES

EXAMPLE 3
THIS IS A TRANSIENT CASE FOR TWO COLUMNS. EACH COLUMN HAS FIVE STAGES WITH THE STAGE VOLUMES DETERMINED BY THE COLUMN DIMENSIONS. AN INITIAL PROFILE HAS BEEN PREVIOUSLY CALCULATED, AND IS USED AS A STARTING POINT FOR THIS RUN. THE SITUATION BEING MODELED IS THE COMPLETE LOSS OF THE REDUCTANT STREAM IN STAGE 3. AFTER THIRTY MINUTES WITH NO REDUCTANT, THE STREAM IS TURNED ON AND THE CONCENTRATION FOLLOWED FOR ANOTHER THIRTY MINUTES.

DTETA = 0.125 MINUTES PER TIME INCREMENT
DPRINT = 10.000 MINUTES BETWEEN PRINTING OF PROFILES
IRAST = 0 THE RUNGE-KUTTA INTEGRATION WILL BE USED
THIS TIME PERIOD WILL END WHEN TIME = TSTOP = 30.000 MINUTES, OR A TOLERANCE OF TOL = 0.0100 % PER MINUTE IS REACHED
NUMBER OF STAGES = 10
NEWIN = 1 NEW INPUT FLOWS WILL BE GIVEN
NEWOUT = 1 NEW OUTPUT FLOWS WILL BE GIVEN
IVCLM = 1 AQUEOUS AND ORGANIC MIXER VOLUMES GIVEN
IVCLS = 1 AQUEOUS AND ORGANIC SETTLER VOLUMES GIVEN
IERO = 1 A NEW INITIAL PROFILE WILL BE READ
IPNCH = 0 NO PUNCHED CARD OUTPUT
NSTR = 0 NO UNUSUAL ROUTING PATTERN
TEMPI = 4.000E 01 INITIAL & DEFAULT TEMPERATURE
IRXN = 1 INSTANTANEOUS REDUCTION OF PLUTONIUM

FEED & PRODUCT STREAM DATA	STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	FLOW RATE (L/MIN)	TEMP (C)
AQUEOUS	1	3.000E 00	0.0	0.0	0.0	0.0	0.0	1.000E-01	40.0
AQUEOUS	6	3.000E 00	3.000E 02	3.000E 00	0.0	0.0	0.0	1.500E-01	40.0
30.0 % TBP	10	0.0	0.0	0.0	0.0	0.0	0.0	3.500E-01	40.0
AQUEOUS	5	PRODUCT STREAM REMOVED (FLOW RATE IN MOLAL UNITS)						1.000E 01	

STAGE NO.	MIXER VOLUME BY PHASE AQUEOUS	MIXER VOLUME BY PHASE ORGANIC	SETTLER VOLUME BY PHASE AQUEOUS	SETTLER VOLUME BY PHASE ORGANIC	MIXER FLOW RATE AQUEOUS	MIXER FLOW RATE ORGANIC	INTERSTAGE FLOW RATE AQUEOUS	INTERSTAGE FLOW RATE ORGANIC
1	3.600E-02	1.200E-01	1.100E-01	5.800E-01	9.073E-02	3.472E-01	9.073E-02	3.472E-01
2	3.600E-02	1.200E-01	1.100E-01	3.800E-01	9.073E-02	3.472E-01	9.073E-02	3.472E-01
3	3.600E-02	1.200E-01	1.100E-01	3.800E-01	9.073E-02	3.472E-01	9.073E-02	3.472E-01
4	3.600E-02	1.200E-01	1.100E-01	3.800E-01	9.073E-02	3.472E-01	9.073E-02	3.472E-01
5	3.600E-02	1.200E-01	3.100E-01	3.800E-01	9.073E-02	3.472E-01	0.0	3.472E-01
6	1.700E-01	4.000E-01	5.100E-01	1.700E 00	1.222E-01	3.472E-01	1.222E-01	3.472E-01
7	1.700E-01	4.000E-01	5.100E-01	1.180E 00	1.222E-01	3.472E-01	1.222E-01	3.472E-01
8	1.700E-01	4.000E-01	5.100E-01	1.180E 00	1.222E-01	3.472E-01	1.222E-01	3.472E-01
9	1.700E-01	4.000E-01	5.100E-01	1.180E 00	1.222E-01	3.472E-01	1.222E-01	3.472E-01
10	1.700E-01	4.000E-01	7.000E-01	1.180E 00	1.222E-01	3.472E-01	1.222E-01	3.472E-01

TRANSIENT BEHAVIOR RESULTS MIXER CONCENTRATION GIVEN

TIME = 0.0 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	2.838E 00	2.770E 01	0.0	0.0	0.0	0.0	1.140E 00	1.004E-01	4.000E 01
2	2.746E 00	4.282E 01	0.0	0.0	0.0	0.0	1.159E 00	1.006E-01	4.000E 01
3	2.642E 00	5.564E 01	0.0	0.0	1.720E-02	1.720E-02	1.178E 00	1.007E-01	4.000E 01
4	2.550E 00	7.190E 01	0.0	4.469E-02	1.697E-02	1.716E-02	1.200E 00	1.009E-01	4.000E 01
5	2.413E 00	1.000E 02	1.747E-02	4.081E 00	0.0	1.707E-02	1.246E 00	1.014E-01	4.000E 01
5	PRODUCT STREAM							1.014E-01	
6	3.000E 00	3.001E 02	2.873E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
7	3.004E 00	2.998E 02	2.737E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
8	3.051E 00	2.942E 02	2.552E 00	0.0	0.0	0.0	1.611E 00	1.499E-01	4.000E 01
9	3.484E 00	2.235E 02	1.908E 00	0.0	0.0	0.0	1.504E 00	1.484E-01	4.000E 01
10	3.142E 00	2.144E 01	2.674E-01	0.0	0.0	0.0	1.143E 00	1.363E-01	4.000E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	2.046E-01	8.746E 01	0.0	1.144E 01	0.0	2.613E-01	9.444E-01	3.639E-01	2.000E 02
2	1.628E-01	9.500E 01	0.0	8.035E 00	0.0	2.147E-01	9.537E-01	3.642E-01	2.000E 02
3	1.389E-01	9.914E 01	0.0	6.447E 00	0.0	1.902E-01	9.589E-01	3.644E-01	2.000E 02
4	1.187E-01	1.028E 02	0.0	5.164E 00	0.0	1.681E-01	9.634E-01	3.646E-01	2.000E 02
5	5.479E-02	1.073E 02	1.230E-02	3.860E 00	1.079E-02	1.413E-01	9.691E-01	3.649E-01	2.000E 02
6	5.958E-02	1.151E 02	1.131E 00	9.348E-01	9.595E-01	4.841E-02	9.811E-01	3.656E-01	2.000E 02
7	5.969E-02	1.151E 02	1.079E 00	9.358E-01	9.609E-01	4.843E-02	9.810E-01	3.656E-01	2.000E 02
8	6.117E-02	1.150E 02	1.023E 00	9.532E-01	9.775E-01	4.889E-02	9.808E-01	3.656E-01	2.000E 02
9	8.005E-02	1.127E 02	9.470E-01	1.242E 00	1.223E 00	5.660E-02	9.780E-01	3.655E-01	2.000E 02
10	2.439E-01	8.305E 01	6.777E-01	1.034E 01	6.768E 00	2.073E-01	9.406E-01	3.640E-01	2.000E 02

TIME = 10.00 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	2.838E 00	2.757E 01	1.545E-01	0.0	0.0	0.0	1.140E 00	1.004E-01	4.000E 01
2	2.749E 00	4.251E 01	3.493E-01	0.0	0.0	0.0	1.160E 00	1.006E-01	4.000E 01
3	2.670E 00	5.548E 01	5.955E-01	2.887E-12	0.0	1.208E-14	1.177E 00	1.008E-01	4.000E 01
4	2.575E 00	7.175E 01	9.118E-01	1.089E-07	0.0	4.557E-10	1.199E 00	1.010E-01	4.000E 01
5	2.435E 00	1.026E 02	1.426E 00	4.927E-05	0.0	2.061E-07	1.243E 00	1.016E-01	4.000E 01
5	PRODUCT STREAM							1.016E-01	
6	3.000E 00	3.001E 02	2.873E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
7	3.004E 00	2.998E 02	2.737E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
8	3.051E 00	2.942E 02	2.552E 00	0.0	0.0	0.0	1.611E 00	1.499E-01	4.000E 01
9	3.484E 00	2.234E 02	1.908E 00	0.0	0.0	0.0	1.504E 00	1.484E-01	4.000E 01
10	3.141E 00	2.144E 01	2.674E-01	0.0	0.0	0.0	1.143E 00	1.363E-01	4.000E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	2.047E-01	8.713E 01	3.071E-01	1.186E 01	7.205E 00	2.614E-01	9.444E-01	3.639E-01	2.877E 01
2	1.631E-01	9.449E 01	4.913E-01	8.049E 00	5.093E 00	2.148E-01	9.539E-01	3.643E-01	1.634E 01
3	1.399E-01	9.847E 01	6.722E-01	6.419E 00	4.083E 00	1.894E-01	9.591E-01	3.645E-01	8.642E 00
4	1.193E-01	1.020E 02	8.304E-01	5.131E 00	3.288E 00	1.672E-01	9.637E-01	3.647E-01	3.942E 00
5	9.437E-02	1.065E 02	9.683E-01	3.730E 00	2.439E 00	1.391E-01	9.696E-01	3.649E-01	1.331E 00
6	5.958E-02	1.151E 02	1.131E 00	9.348E-01	9.596E-01	4.840E-02	9.811E-01	3.656E-01	1.582E-03
7	5.970E-02	1.151E 02	1.079E 00	9.361E-01	9.609E-01	4.844E-02	9.811E-01	3.656E-01	5.381E-04
8	6.117E-02	1.150E 02	1.023E 00	9.532E-01	9.778E-01	4.889E-02	9.808E-01	3.656E-01	1.232E-03
9	8.005E-02	1.127E 02	9.470E-01	1.242E 00	1.223E 00	5.660E-02	9.780E-01	3.655E-01	6.649E-04
10	2.439E-01	8.306E 01	6.776E-01	1.035E 01	6.768E 00	2.073E-01	9.406E-01	3.640E-01	2.107E-03

TIME = 20.00 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MCL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	2.837E 00	2.746E 01	3.489E-01	0.0	0.0	0.0	1.140E 00	1.004E-01	4.000E 01
2	2.747E 00	4.251E 01	5.698E-01	0.0	0.0	0.0	1.160E 00	1.006E-01	4.000E 01
3	2.668E 00	5.571E 01	7.732E-01	0.0	0.0	0.0	1.177E 00	1.008E-01	4.000E 01
4	2.573E 00	7.220E 01	1.027E 00	0.0	0.0	0.0	1.200E 00	1.010E-01	4.000E 01
5	2.434E 00	1.031E 02	1.483E 00	2.023E-15	0.0	8.465E-18	1.244E 00	1.016E-01	4.000E 01
5	PRODUCT STREAM							1.016E-01	
6	3.000E 00	3.001E 02	2.873E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
7	3.004E 00	2.998E 02	2.737E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
8	3.051E 00	2.942E 02	2.552E 00	0.0	0.0	0.0	1.611E 00	1.499E-01	4.000E 01
9	3.485E 00	2.234E 02	1.908E 00	0.0	0.0	0.0	1.504E 00	1.484E-01	4.000E 01
10	3.141E 00	2.143E 01	2.673E-01	0.0	0.0	0.0	1.143E 00	1.363E-01	4.000E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MCL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	2.046E-01	8.676E 01	6.931E-01	1.145E 01	7.202E 00	2.614E-01	9.446E-01	3.639E-01	1.041E 00
2	1.627E-01	9.424E 01	7.992E-01	8.027E 00	5.079E 00	2.145E-01	9.540E-01	3.643E-01	7.096E-01
3	1.393E-01	9.836E 01	8.685E-01	6.385E 00	4.062E 00	1.889E-01	9.593E-01	3.645E-01	4.072E-01
4	1.187E-01	1.020E 02	9.300E-01	5.099E 00	3.268E 00	1.666E-01	9.639E-01	3.647E-01	1.961E-01
5	9.405E-02	1.066E 02	1.003E 00	3.711E 00	2.428E 00	1.387E-01	9.697E-01	3.649E-01	7.040E-02
6	5.958E-02	1.151E 02	1.131E 00	9.348E-01	9.596E-01	4.840E-02	9.811E-01	3.656E-01	6.751E-04
7	5.970E-02	1.151E 02	1.079E 00	9.360E-01	9.609E-01	4.843E-02	9.811E-01	3.656E-01	6.319E-04
8	6.118E-02	1.150E 02	1.023E 00	9.531E-01	9.778E-01	4.889E-02	9.808E-01	3.656E-01	5.027E-04
9	8.006E-02	1.127E 02	9.470E-01	1.243E 00	1.223E 00	5.661E-02	9.780E-01	3.655E-01	8.357E-04
10	2.439E-01	8.305E 01	6.776E-01	1.035E 01	6.769E 00	2.074E-01	9.406E-01	3.640E-01	6.994E-04

TIME = 30.00 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MCL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	2.837E 00	2.749E 01	3.622E-01	0.0	0.0	0.0	1.140E 00	1.004E-01	4.000E 01
2	2.747E 00	4.259E 01	5.845E-01	0.0	0.0	0.0	1.160E 00	1.006E-01	4.000E 01
3	2.668E 00	5.582E 01	7.849E-01	0.0	0.0	0.0	1.178E 00	1.008E-01	4.000E 01
4	2.572E 00	7.234E 01	1.035E 00	0.0	0.0	0.0	1.200E 00	1.010E-01	4.000E 01
5	2.434E 00	1.032E 02	1.488E 00	0.0	0.0	0.0	1.244E 00	1.016E-01	4.000E 01
5	PRODUCT STREAM							1.016E-01	
6	3.000E 00	3.001E 02	2.873E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
7	3.004E 00	2.998E 02	2.737E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
8	3.051E 00	2.942E 02	2.552E 00	0.0	0.0	0.0	1.611E 00	1.499E-01	4.000E 01
9	3.485E 00	2.234E 02	1.908E 00	0.0	0.0	0.0	1.504E 00	1.484E-01	4.000E 01
10	3.142E 00	2.143E 01	2.673E-01	0.0	0.0	0.0	1.143E 00	1.363E-01	4.000E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MCL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	2.044E-01	8.676E 01	7.188E-01	1.144E 01	7.194E 00	2.612E-01	9.446E-01	3.639E-01	6.120E-02
2	1.625E-01	9.425E 01	8.185E-01	8.014E 00	5.071E 00	2.143E-01	9.541E-01	3.643E-01	4.286E-02
3	1.392E-01	9.838E 01	8.801E-01	6.373E 00	4.055E 00	1.887E-01	9.593E-01	3.645E-01	2.747E-02
4	1.186E-01	1.020E 02	9.357E-01	5.090E 00	3.263E 00	1.664E-01	9.639E-01	3.647E-01	1.442E-02
5	9.397E-02	1.066E 02	1.005E 00	3.706E 00	2.426E 00	1.386E-01	9.698E-01	3.649E-01	6.955E-03
6	5.958E-02	1.151E 02	1.131E 00	9.348E-01	9.596E-01	4.840E-02	9.811E-01	3.656E-01	8.273E-04
7	5.970E-02	1.151E 02	1.079E 00	9.360E-01	9.609E-01	4.843E-02	9.811E-01	3.656E-01	5.138E-04
8	6.118E-02	1.150E 02	1.023E 00	9.531E-01	9.778E-01	4.889E-02	9.808E-01	3.656E-01	0.0
9	8.006E-02	1.127E 02	9.471E-01	1.243E 00	1.223E 00	5.661E-02	9.780E-01	3.655E-01	3.697E-04
10	2.439E-01	8.305E 01	6.776E-01	1.035E 01	6.770E 00	2.074E-01	9.406E-01	3.640E-01	7.995E-04

CALCULATIONS FOR A SOLVENT EXTRACTION PROCESS HAVING INTERACTING SOLUTES

EXAMPLE 3
THIS IS A TRANSIENT CASE FOR TWO COLUMNS. EACH COLUMN HAS FIVE STAGES
WITH THE STAGE VOLUMES DETERMINED BY THE COLUMN DIMENSIONS. AN INITIAL PROFILE
HAS BEEN PREVIOUSLY CALCULATED, AND IS USED AS A STARTING POINT FOR THIS
RUN. THE SITUATION BEING MODELED IS THE COMPLETE LOSS OF THE REDUCTANT
STREAM IN STAGE 3. AFTER THIRTY MINUTES WITH NO REDUCTANT, THE STREAM IS
TURNED ON AND THE CONCENTRATION FOLLOWED FOR ANOTHER THIRTY MINUTES.

DTHETA = 0.125 MINUTES PER TIME INCREMENT
DPRINT = 10.000 MINUTES BETWEEN PRINTING OF PROFILES
IFAST = 0 THE RUNGE-KUTTA INTEGRATION WILL BE USED
THIS TIME PERIOD WILL END WHEN TIME = TSTOP = 30.000 MINUTES, OR A TOLERANCE OF TOL = 0.0100 % PER MINUTE IS REACHED
NUMBER OF STAGES = 10
NEWIN = 1 NEW INPUT FLOWS WILL BE GIVEN
NEWOUT = 1 NEW OUTPUT FLOWS WILL BE GIVEN
IVCIM = 0 MIXER VOLUMES WILL BE UNCHANGED
IVCIS = 0 SETTLER VOLUMES WILL BE UNCHANGED
IENO = 0 A NEW INITIAL PROFILE WILL NOT BE READ
IPUNCH = 0 NO PUNCHED CARD OUTPUT
NSTP = 0 NO UNUSUAL ROUTING PATTERN
TEMPI = 4.000E 01 INITIAL & DEFAULT TEMPERATURE
IPUN = 1 INSTANTANEOUS REDUCTION OF PLUTONIUM

FEED & PRODUCT STREAM DATA		STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	FLOW RATE (L/MIN)	TEMP (C)
	AQUEOUS	1	3.000E 00	0.0	0.0	0.0	0.0	0.0	1.000E-01	40.0
	AQUEOUS	3	0.0	0.0	0.0	0.0	1.750E 00	1.750E 00	1.000E-03	40.0
	AQUEOUS	6	3.000E 00	3.000E 02	3.000E 00	0.0	0.0	0.0	1.500E-01	40.0
	30.0 % TBP	10	0.0	0.0	0.0	0.0	0.0	0.0	3.500E-01	40.0
	AQUEOUS	5	PRODUCT STREAM REMOVED (FLOW RATE IN MOLAL UNITS)						1.000E 01	

STAGE NO.	MIXER VOLUME BY PHASE		SETTLER VOLUME BY PHASE		MIXER FLOW RATE		INTERSTAGE FLOW RATE	
	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC
1	3.600E-02	1.200E-01	1.100E-01	5.800E-01	9.073E-02	3.472E-01	9.073E-02	3.472E-01
2	3.600E-02	1.200E-01	1.100E-01	3.800E-01	9.073E-02	3.472E-01	9.073E-02	3.472E-01
3	3.600E-02	1.200E-01	1.100E-01	3.800E-01	9.168E-02	3.472E-01	9.168E-02	3.472E-01
4	3.600E-02	1.200E-01	1.100E-01	3.800E-01	9.168E-02	3.472E-01	9.168E-02	3.472E-01
5	3.600E-02	1.200E-01	3.100E-01	3.800E-01	9.168E-02	3.472E-01	0.0	3.472E-01
6	1.700E-01	4.000E-01	5.100E-01	1.700E 00	1.222E-01	3.472E-01	1.222E-01	3.472E-01
7	1.700E-01	4.000E-01	5.100E-01	1.180E 00	1.222E-01	3.472E-01	1.222E-01	3.472E-01
8	1.700E-01	4.000E-01	5.100E-01	1.180E 00	1.222E-01	3.472E-01	1.222E-01	3.472E-01
9	1.700E-01	4.000E-01	5.100E-01	1.180E 00	1.222E-01	3.472E-01	1.222E-01	3.472E-01
10	1.700E-01	4.000E-01	7.000E-01	1.180E 00	1.222E-01	3.472E-01	1.222E-01	3.472E-01

TRANSIENT BEHAVIOR RESULTS MIXER CONCENTRATION GIVEN

TIME = 0.0 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	2.837E 00	2.749E 01	3.622E-01	0.0	0.0	0.0	1.140E 00	1.004E-01	4.000E 01
2	2.747E 00	4.259E 01	5.845E-01	0.0	0.0	0.0	1.160E 00	1.006E-01	4.000E 01
3	2.668E 00	5.582E 01	7.849E-01	0.0	0.0	0.0	1.178E 00	1.018E-01	4.000E 01
4	2.572E 00	7.234E 01	1.035E 00	0.0	0.0	0.0	1.200E 00	1.021E-01	4.000E 01
5	2.434E 00	1.032E 02	1.488E 00	0.0	0.0	0.0	1.244E 00	1.027E-01	4.000E 01
5	PRODUCT STREAM							1.027E-01	
6	3.000E 00	3.001E 02	2.873E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
7	3.004E 00	2.998E 02	2.737E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
8	3.051E 00	2.942E 02	2.552E 00	0.0	0.0	0.0	1.611E 00	1.499E-01	4.000E 01
9	3.485E 00	2.234E 02	1.908E 00	0.0	0.0	0.0	1.504E 00	1.484E-01	4.000E 01
10	3.142E 00	2.143E 01	2.673E-01	0.0	0.0	0.0	1.143E 00	1.363E-01	4.000E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	2.044E-01	8.676E 01	7.188E-01	1.144E 01	7.194E 00	2.612E-01	9.446E-01	3.639E-01	6.120E-02
2	1.625E-01	9.425E 01	8.185E-01	8.014E 00	5.071E 00	2.143E-01	9.541E-01	3.643E-01	4.286E-02
3	1.392E-01	9.838E 01	8.801E-01	6.308E 00	4.013E 00	1.867E-01	9.593E-01	3.645E-01	2.747E-02
4	1.186E-01	1.020E 02	9.357E-01	5.038E 00	3.229E 00	1.647E-01	9.639E-01	3.647E-01	1.442E-02
5	9.397E-02	1.066E 02	1.005E 00	3.668E 00	2.401E 00	1.372E-01	9.698E-01	3.649E-01	6.955E-03
6	5.558E-02	1.151E 02	1.131E 00	9.348E-01	9.596E-01	4.840E-02	9.811E-01	3.656E-01	8.273E-04
7	5.970E-02	1.151E 02	1.079E 00	9.360E-01	9.609E-01	4.843E-02	9.811E-01	3.656E-01	5.138E-04
8	6.118E-02	1.150E 02	1.023E 00	9.531E-01	9.778E-01	4.889E-02	9.808E-01	3.656E-01	0.0
9	8.006E-02	1.127E 02	9.471E-01	1.243E 00	1.223E 00	5.661E-02	9.780E-01	3.655E-01	3.697E-04
10	2.439E-01	8.305E 01	6.776E-01	1.035E 01	6.770E 00	2.074E-01	9.406E-01	3.640E-01	7.995E-04

TIME = 10.00 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	2.844E 00	2.681E 01	1.351E-03	0.0	0.0	0.0	1.138E 00	1.004E-01	4.000E 01
2	2.759E 00	4.054E 01	6.899E-04	0.0	0.0	0.0	1.156E 00	1.005E-01	4.000E 01
3	2.653E 00	5.112E 01	0.0	6.015E-01	1.470E-02	1.722E-02	1.173E 00	1.016E-01	4.000E 01
4	2.535E 00	6.348E 01	2.641E-02	4.114E 00	0.0	1.721E-02	1.193E 00	1.017E-01	4.000E 01
5	2.388E 00	9.685E 01	1.187E 00	4.086E 00	0.0	1.710E-02	1.242E 00	1.024E-01	4.000E 01
5	PRODUCT STREAM							1.024E-01	
6	3.000E 00	3.001E 02	2.873E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
7	3.004E 00	2.998E 02	2.737E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
8	3.051E 00	2.942E 02	2.552E 00	0.0	0.0	0.0	1.611E 00	1.499E-01	4.000E 01
9	3.485E 00	2.234E 02	1.908E 00	0.0	0.0	0.0	1.504E 00	1.484E-01	4.000E 01
10	3.142E 00	2.143E 01	2.673E-01	0.0	0.0	0.0	1.143E 00	1.363E-01	4.000E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	2.079E-01	8.686E 01	2.752E-03	1.174E 01	7.382E 00	2.650E-01	9.436E-01	3.638E-01	6.734E 01
2	1.677E-01	9.410E 01	1.012E-03	8.409E 00	5.312E 00	2.202E-01	9.526E-01	3.642E-01	7.864E 01
3	1.453E-01	9.789E 01	0.0	6.864E 00	0.0	1.963E-01	9.573E-01	3.644E-01	5.421E 01
4	1.253E-01	1.013E 02	2.684E-02	5.724E 00	2.325E-02	1.772E-01	9.616E-01	3.645E-01	3.823E 02
5	9.533E-02	1.063E 02	8.489E-01	3.912E 00	5.739E-01	1.423E-01	9.691E-01	3.649E-01	2.625E 00
6	5.558E-02	1.151E 02	1.131E 00	9.348E-01	9.596E-01	4.840E-02	9.811E-01	3.656E-01	0.0
7	5.970E-02	1.151E 02	1.079E 00	9.360E-01	9.609E-01	4.843E-02	9.811E-01	3.656E-01	0.0
8	6.118E-02	1.150E 02	1.023E 00	9.531E-01	9.778E-01	4.889E-02	9.808E-01	3.656E-01	0.0
9	8.006E-02	1.127E 02	9.471E-01	1.243E 00	1.223E 00	5.661E-02	9.780E-01	3.655E-01	0.0
10	2.440E-01	8.305E 01	6.776E-01	1.035E 01	6.771E 00	2.074E-01	9.406E-01	3.640E-01	1.663E-04

TIME = 20.00 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	2.842E 00	2.687E 01	1.250E-06	0.0	0.0	0.0	1.139E 00	1.004E-01	4.000E 01
2	2.756E 00	4.089E 01	6.394E-07	0.0	0.0	0.0	1.157E 00	1.005E-01	4.000E 01
3	2.657E 00	5.218E 01	0.0	2.056E-06	1.721E-02	1.721E-02	1.174E 00	1.017E-01	4.000E 01
4	2.559E 00	6.543E 01	0.0	1.252E 00	1.195E-02	1.719E-02	1.192E 00	1.018E-01	4.000E 01
5	2.406E 00	9.261E 01	3.893E-01	4.091E 00	0.0	1.712E-02	1.234E 00	1.022E-01	4.000E 01
5	PRODUCT STREAM							1.022E-01	
6	3.000E 00	3.001E 02	2.873E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
7	3.004E 00	2.998E 02	2.737E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
8	3.051E 00	2.942E 02	2.552E 00	0.0	0.0	0.0	1.611E 00	1.499E-01	4.000E 01
9	3.485E 00	2.234E 02	1.908E 00	0.0	0.0	0.0	1.504E 00	1.484E-01	4.000E 01
10	3.142E 00	2.143E 01	2.673E-01	0.0	0.0	0.0	1.143E 00	1.363E-01	4.000E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	2.077E-01	8.689E 01	2.542E-06	1.172E 01	7.369E 00	2.648E-01	9.437E-01	3.638E-01	1.330E-02
2	1.669E-01	9.424E 01	9.310E-07	8.349E 00	5.274E 00	2.194E-01	9.528E-01	3.642E-01	3.215E-02
3	1.441E-01	9.816E 01	0.0	6.741E 00	0.0	1.943E-01	9.576E-01	3.644E-01	6.125E-02
4	1.247E-01	1.016E 02	0.0	5.558E 00	0.0	1.745E-01	9.619E-01	3.645E-01	1.219E 01
5	9.852E-02	1.062E 02	2.897E-01	4.091E 00	2.308E-01	1.461E-01	9.681E-01	3.648E-01	1.508E 01
6	5.558E-02	1.151E 02	1.131E 00	9.348E-01	9.596E-01	4.840E-02	9.811E-01	3.656E-01	0.0
7	5.970E-02	1.151E 02	1.079E 00	9.360E-01	9.609E-01	4.843E-02	9.811E-01	3.656E-01	0.0
8	6.118E-02	1.150E 02	1.023E 00	9.531E-01	9.778E-01	4.889E-02	9.808E-01	3.656E-01	4.214E-04
9	8.007E-02	1.127E 02	9.471E-01	1.243E 00	1.223E 00	5.661E-02	9.780E-01	3.655E-01	3.594E-04
10	2.440E-01	8.305E 01	6.776E-01	1.035E 01	6.771E 00	2.074E-01	9.406E-01	3.640E-01	0.0

TIME = 30.00 MINUTES

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	DENSITY (G/ML)	MIXER FLOW (L/MIN)	TEMPERATURE (CENTIGRADE)
1	2.841E 00	2.709E 01	1.165E-09	0.0	0.0	0.0	1.139E 00	1.004E-01	4.000E 01
2	2.752E 00	4.148E 01	6.000E-10	0.0	0.0	0.0	1.157E 00	1.006E-01	4.000E 01
3	2.652E 00	5.334E 01	0.0	1.924E-09	1.720E-02	1.720E-02	1.175E 00	1.017E-01	4.000E 01
4	2.562E 00	6.795E 01	0.0	2.548E-01	1.611E-02	1.717E-02	1.195E 00	1.019E-01	4.000E 01
5	2.412E 00	9.238E 01	6.859E-02	4.092E 00	0.0	1.712E-02	1.233E 00	1.022E-01	4.000E 01
5	PRODUCT STREAM							1.022E-01	
6	3.000E 00	3.001E 02	2.873E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
7	3.004E 00	2.998E 02	2.737E 00	0.0	0.0	0.0	1.619E 00	1.500E-01	4.000E 01
8	3.051E 00	2.942E 02	2.552E 00	0.0	0.0	0.0	1.611E 00	1.499E-01	4.000E 01
9	3.485E 00	2.234E 02	1.908E 00	0.0	0.0	0.0	1.504E 00	1.484E-01	4.000E 01
10	3.142E 00	2.143E 01	2.673E-01	0.0	0.0	0.0	1.143E 00	1.363E-01	4.000E 01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU(IV) (G/L)	U EXTRACTION FACTOR	PU EXTRACT FACTOR	HNO3 EXTRACT FACTOR	DENSITY (G/ML)	FLOW RATE (L/MIN)	INVENTORY CHANGE (%)
1	2.068E-01	8.705E 01	2.352E-09	1.165E 01	7.321E 00	2.639E-01	9.439E-01	3.638E-01	2.734E-02
2	1.656E-01	9.448E 01	8.636E-10	8.251E 00	5.213E 00	2.179E-01	9.531E-01	3.642E-01	3.814E-02
3	1.423E-01	9.850E 01	0.0	6.616E 00	0.0	1.922E-01	9.581E-01	3.644E-01	5.403E-02
4	1.226E-01	1.020E 02	0.0	5.372E 00	0.0	1.712E-01	9.625E-01	3.646E-01	1.951E 01
5	9.895E-02	1.063E 02	5.127E-02	4.108E 00	4.398E-02	1.464E-01	9.679E-01	3.648E-01	2.759E 01
6	5.558E-02	1.151E 02	1.131E 00	9.348E-01	9.596E-01	4.840E-02	9.811E-01	3.656E-01	0.0
7	5.970E-02	1.151E 02	1.079E 00	9.360E-01	9.609E-01	4.843E-02	9.811E-01	3.656E-01	3.958E-04
8	6.118E-02	1.150E 02	1.023E 00	9.531E-01	9.778E-01	4.889E-02	9.808E-01	3.656E-01	0.0
9	8.007E-02	1.127E 02	9.471E-01	1.243E 00	1.223E 00	5.661E-02	9.780E-01	3.655E-01	5.121E-04
10	2.440E-01	8.305E 01	6.776E-01	1.035E 01	6.771E 00	2.074E-01	9.406E-01	3.640E-01	2.579E-04

APPENDIX A. PROGRAM LISTING

```
CCCCCCCCC
C
C  PROGRAM SEPHIS
C     ORNL, MAY, 1978          REVISIONS BY A.D.MITCHELL
C     ORNL REVISION OF THE RAINEY-WATSON MODIFIED VERSION (ORNL-TM-5123)
C     WATSON & RAINEY MODIFIED THE RICHARDSON-WANCE VERSION (HEDL-TME 75-31)
C     ORIGINAL PROGRAM BY W.S.GROENIER (ORNL 4746)
C
C     TRANSIENT STAGE CALCULATIONS FOR PUREX SOLVENT EXTRACTION PROCESS.
C     CALCULATIONS DONE FOR 6 COMPONENTS
C          3 TRANSFERRING COMPONENTS        COMPONENT 1 - NITRIC ACID
C                                           COMPONENT 2 - URANIUM
C                                           COMPONENT 3 - PLUTONIUM (IV)
C          3 NON-TRANSFERRING COMPONENTS    COMPONENT 4 - PLUTONIUM (III)
C                                           COMPONENT 5 - PLUTONIUM REDUCTANT
C                                           COMPONENT 6 - NITRATE ION
C     100 STAGES ALLOWED,   THE 100 ARE GOTTEN BY USING NTOST = 00
C
C
C     DISCRIPTION OF MOST MAJOR VARIABLES
C         AVOL   VOLUME OF AQUEOUS PHASE IN MIXER J
C         OVOL   VOLUME OF ORGANIC PHASE IN MIXER J
C         ASVOL  VOLUME OF AQUEOUS PHASE IN SETTLER J
C         OSVOL  VOLUME OF ORGANIC PHASE IN SETTLER J
C         TPROF  MIXER TEMPERATURE
C         ATS    AQUEOUS TEMPERATURE IN THE SETTLER
C         OTS    ORGANIC TEMPERATURE IN THE SETTLER
C         XFD (I,J)   CONCENTRATION OF COMPONENT I IN AQUEOUS FEED TO STAGE J
C         YFD (I,J)   CONCENTRATION OF COMPONENT I IN ORGANIC FEED TO STAGE J
C         AFDRT   FLOW RATE (LITERS/MIN) OF AQUEOUS FEED TO MIXER J
C         OFDRT   FLOW RATE (LITERS/MIN) OF ORGANIC FEED TO MIXER J
C         AFDTEM  TEMPERATURE OF AQUEOUS FEED TO MIXER J
C         OFDTEM  TEMPERATURE OF ORGANIC FEED TO MIXER J
C         X (I,J,K)  AQUEOUS CONCENTRATION OF COMPONENT I IN MIXER J DURING
C                    A TIME INTERVAL K   K=1  FOR PREVIOUS TIME
C                                        K=2  FOR PRESENT TIME
C         XS (J,L,I,K) AQUEOUS CONC OF COMPONENT I IN SETTLER J, ZONE L, DURING
C                    A TIME INTERVAL K.  EACH SETTLER IS SPLIT INTO THREE
C                    ZONES IN ORDER TO SMOOTH OUT THE CHANGES IN CONCENTRATION
C                    OF ITS MIXER.  THE ZONES CAN BE THOUGHT OF AS WELL
C                    MIXED TANKS FLOWING INTO THE NEXT ZONE OR MIXER.
C         A     AQUEOUS INTERSTAGE FLOW RATE
C         O     ORGANIC INTERSTAGE FLOW RATE
C         AT    AQUEOUS INTRASTAGE FLOW RATE
C         OT    ORGANIC INTRASTAGE FLOW RATE
C         ALVRT FLOW RATE OF AQUEOUS STREAM LEAVING MIXER-SETTLER BANK
C         OLVRT FLOW RATE OF ORGANIC STREAM LEAVING MIXER-SETTLER BANK
C         AOUT, OOUT   INTERSTAGE FLOW RATES IN REAL VOLUME UNITS,
C                      USED ONLY IN PRINT-OUT
C         NSOLU IS THE SUBSCRIPT FOR THE HIGHEST NUMBERED COMPONENT
C               IN THE SYSTEM.  IT IS USED IN THE SAME MANNER AS ISOL.
C         ISOL  INDICATES IF A SOLUTE IS (OR WAS) PRESENT IN THE
C               CONTACTOR.  IT IS USED TO BYPASS USELESS CALCULATIONS
C               OF ZERO CONCENTRATION.
C         SPH   SPECIFIC HEAT OF ORGANIC PHASE  (AQUEOUS ASSUMED TO BE 1)
C         NDIREC DETERMINES THE ORDER OF THE STAGEWISE CALCULATIONS.
C         NDIREC = 1 FOR CALCULATIONS TO START AT THE FIRST STAGE
C                =-1 FOR CALCULATIONS TO START WITH THE LAST STAGE
C         CODUM       LARGEST CHANGE IN SOLUTE INVENTORY OF A COMPONENT
C                     IN THE MIXER
C
C  TITLE IS THE PROBLEM TITLE.
C  NTOST = TOTAL NUMBER OF STAGES, MUST NOT EXCEED 100
C   CTBP = VOLUME FRACTION OF DRY TBP
C  TEMPI = AN INITIAL OR DEFAULT TEMPERATURE
C   NSTR = 0 NO UNUSUAL ROUTING PATTERN DESIRED
C        = 1 ROUTING PATTERN OTHER THAN NORMAL WILL BE USED
C            NSTR, ISTR, JSTR  VARIABLES SPECIFYING THAT THE ORGANIC PHASE
C                              OF STAGE ISTR BE ROUTED TO STAGE JSTR
C   IRXN = INDICATOR OF THE REACTION USED FOR REDUCTION
C DTHETA = TIME INCREMENT (MINUTES)
C DPRINT = ELAPSED TIME BETWEEN THE PRINTING OF PROFILES
C  TSTOP = TIME WHEN THE TIME PERIOD IS TO END
C    TOL = THE TOLERANCE TO BE USED TO TEST FOR CONVERGENCE
C  NEWIN = 0 IF THE PRESENT INPUT STREAMS ARE TO BE CONTINUED
C        = 1 IF NEW INPUT STREAMS ARE TO BE SPECIFIED
C NEWOUT = 0 IF THE PRESENT EXITING STREAMS ARE TO BE CONTINUED
C        = 1 IF NEW EXITING STREAMS ARE TO BE SPECIFIED
C  IVOLM = 1 IF AQUEOUS AND ORGANIC MIXER VOLUMES ARE TO BE GIVEN
C        = 2 IF TOTAL MIXER VOLUME IS GIVEN WITH PHASE VOLUMES DETERMINED
C            BY PHASE FLOW IN THE MIXER
C        = 3 IF ALL MIXER VOLUMES GIVEN BY PHASE FLOW IN THE MIXER*UNIT TIME
C  IVOLS = 1 IF AQUEOUS AND ORGANIC SETTLER VOLUMES ARE TO BE GIVEN
C        = 2 IF TOTAL SETTLER VOLUME IS GIVEN WITH PHASE VOLUMES DETERMINED
C            BY PHASE FLOW IN THE MIXER
C        = 3 IF ALL SETTLER VOLUMES GIVEN BY PHASE FLOW IN THE MIXER*UNIT TIME
C   IPRO = 0 FOR A ZERO INITIAL CONCENTRATION PROFILE
C          1 FOR A NON-ZERO INITIAL PROFILE
C  IFAST = 0  IF THE RUNGE KUTTA INTEGRATION IS TO BE USED
C        = 1  IF THE FASTER INTEGRATION METHOD IS TO BE USED
C  IPNCH = 0 IF NO PUNCHED CARD OUTPUT DESIRED
C          1 FOR FINAL PROFILE OUTPUT ON PUNCHED CARDS
C
CCCCCCCCC
```

```
      COMMON/CONTRL/ NTOST,NSOLU,CTBP,NEWIN,NEWOUT,SPH,IPNCH,IFAST,IRXN,
     .  DTHETA,IVOLM,IVOLS,IPRO,TEMPI,ISOL(6),NSTR,ISTR,JSTR,CODUM(100)
      COMMON/CONCS/ X(6,100,2),Y(6,100,2),XS(100,3,6,2),YS(100,3,6,2)
      COMMON/FLOWS/ A(100),O(100),AT(100),OT(100)
      COMMON/STREAM/ XFD(6,100),YFD(6,100),AFDRT(100),OFDRT(100),
     .   AFDTEM(100),OFDTEM(100),ALVRT(100),OLVRT(100)
      COMMON/TEMPS/ TPROF(100,2),ATS(100,3,2),OTS(100,3,2)
      COMMON/VOLS/ AVOL(100),OVOL(100),ASVOL(100),OSVOL(100)
      REAL*8 TITLE(10,10)
      NDIREC=1
C
C  NEXT CASE IS NEW
C
   10 CONTINUE
      READ 3000,NTTL,NTOST,CTBP,TEMPI,NSTR,ISTR,JSTR,IRXN
      IF(IRXN.LE.0) IRXN=0
      DO 11 J=1,NTTL
      READ 1000,(TITLE(J,N),N=1,10)
   11 CONTINUE
      IF(NTOST.LE.0) NTOST =100
      NSOLU=6
      SPH=0.321+0.078*CTBP
      DO 14 I=1,NSOLU
      ISOL(I)=0
   14 CONTINUE
C
C  ZEROING OF ARRAYS
C
      DO 16 J=1,NTOST
      CODUM(J)=200.
      AVOL(J)=0.0
      OVOL(J)=0.0
      ASVOL(J)=0.0
      OSVOL(J)=0.0
      AFDRT(J) = 0.0
      OFDRT(J) = 0.0
      AFDTEM(J)=TEMPI
      OFDTEM(J)=TEMPI
      A(J) = 0.0
      O(J) = 0.0
      AT(J)=0.0
      OT(J)=0.0
      ALVRT(J) = 0.0
      OLVRT(J) = 0.0
      DO 15 I=1,NSOLU
      X(I,J,1)=0.0
      X(I,J,2)=0.0
      Y(I,J,1)=0.0
      Y(I,J,2)=0.0
      XFD(I,J) = 0.0
      YFD(I,J) = 0.0
   15 CONTINUE
   16 CONTINUE
      DO 20 L=1,2
      DO 19 J=1,NTOST
      TPROF(J,L)=TEMPI
      DO 18 K=1,3
      ATS(J,K,L)=TEMPI
      OTS(J,K,L)=TEMPI
      DO 17 M=1,NSOLU
      XS(J,K,M,L)=0.0
      YS(J,K,M,L)=0.0
   17 CONTINUE
   18 CONTINUE
   19 CONTINUE
   20 CONTINUE
CCCCC
C
C
C  THIS IS THE START OF A NEW TIME PERIOD
C     ANY ONE, OR GROUP OF THESE VARIABLES MAY BE CHANGED FOR THE NEW TIME
C     PERIOD.
C     IF DTHETA=0.0 THE PRESENT CASE IS ENDED AND A NEW ONE BEGUN DEPENDING
C     ON DPRINT.  IF DPRINT=1.0, A NEW CASE IS STARTED AND A NEW TITLE READ
C     IN.  IF DPRINT=0.0, THE PROGRAM STOPS.
C
CCCCC
   21 READ 3001,DTHETA,DPRINT,TSTOP,TOL,NEWIN,NEWOUT,IVOLM,IVOLS,IPRO,
     .       IFAST,IPNCH
      IF(DTHETA.EQ.0.) GO TO 400
      IF(NEWIN+NEWOUT+IVOLM+IVOLS+IPRO.NE.0) GO TO 23
      PRTIME=PRTIME+DPRINT
      PRINT 3201,DTHETA
      PRINT 3202,DPRINT
      IF(IFAST.EQ.1) PRINT 5000
      IF(IFAST.NE.1) PRINT 5001
      PRINT 3203,TSTOP,TOL
      GO TO 140
   23 PRINT 1002
      DO 25 J=1,NTTL
      PRINT 1003,(TITLE(J,I),I=1,10)
   25 CONTINUE
```

```
      PRINT 3201,DTHETA
      PRINT 3202,DPRINT
      IF(IFAST.EQ.1) PRINT 5000
      IF(IFAST.NE.1) PRINT 5001
      PRINT 3203,TSTOP,TOL
      PRINT 2000,NTOST
C
C
C  SCAN INPUT SWITCHES FOR ERRORS
C
      IF(NEWIN.EQ.1) PRINT 3101
      IF(NEWIN.EQ.0) PRINT 3102
      IF(NEWIN.NE.1.AND.NEWIN.NE.0) PRINT 3109,NEWIN
      IF(NEWOUT.EQ.1) PRINT 3103
      IF(NEWOUT.EQ.0) PRINT 3104
      IF(NEWOUT.NE.1.AND.NEWOUT.NE.0) PRINT 3110,NEWOUT
      IF(IVOLM.EQ.0) PRINT 3105
      IF(IVOLM.EQ.1) PRINT 2038
      IF(IVOLM.EQ.2) PRINT 2039
      IF(IVOLM.EQ.3) PRINT 2040
      IF(IVOLM.LT.0.OR.IVOLM.GT.3) PRINT 2041,IVOLM
      IF(IVOLS.EQ.0) PRINT 3106
      IF(IVOLS.EQ.1) PRINT 2042
      IF(IVOLS.EQ.2) PRINT 2043
      IF(IVOLS.EQ.3) PRINT 2044
      IF(IVOLS.LT.0.OR.IVOLS.GT.3) PRINT 2045,IVOLS
      IF(IPRO.EQ.0) PRINT 3107
      IF(IPRO.EQ.1) PRINT 3108
      IF(IPRO.NE.0.AND.IPRO.NE.1) PRINT 2003,IPRO
      IF(IPNCH.EQ.0) PRINT 2026
      IF(IPNCH.EQ.1) PRINT 3111
      IF(IPNCH.NE.0.AND.IPNCH.NE.1) PRINT 2028,IPNCH
      IF(NSTR.EQ.0) PRINT 2034
      IF(NSTR.EQ.1) PRINT 2035
      IF(NSTR.NE.0.AND.NSTR.NE.1) PRINT 2036,NSTR
      IF(NSTR.EQ.1) PRINT 4000,ISTR,JSTR
      PRINT 7000,TEMPI
      IF(IRXN.EQ.0) PRINT 8000
      IF(IRXN.EQ.1) PRINT 8001
      IF(IRXN.EQ.2) PRINT 8002
      IF(IRXN.EQ.3) PRINT 8003
C
C    STARTS DOES ALL THE INPUT REQUIRED BEFORE THE ITERATIONS START
C
      CALL STARTS
C
C
      PRINT 3205
      TOTIME=0.0
      PRTIME=0.0
      DO 50 J=1,NTOST
      DO 50 I=1,NSOLU
      X(I,J,2)=X(I,J,1)
      Y(I,J,2)=Y(I,J,1)
   50 CONTINUE
      GO TO 200
  140 CONTINUE
C
C  STAGES PERFORMS STAGE CALCULATIONS FOR EACH TIME INTERVAL
C
      CALL STAGES (NDIREC)
C
C
      NDIREC=-NDIREC
C
C  MERELY INCREMENTING TIME FOR TEMPS & CONCS
C
      TOTIME=TOTIME+DTHETA
      NSTOP=0
      DO 150 J=1,NTOST
      IF(CODUM(J).GT.TOL) NSTOP=1
      TPROF(J,1)=TPROF(J,2)
      DO 148 KZ=1,3
      ATS(J,KZ,1)=ATS(J,KZ,2)
  148 OTS(J,KZ,1)=OTS(J,KZ,2)
      DO 150 I=1,NSOLU
      IF(ISOL(I).EQ.0) GO TO 150
      X(I,J,1)=X(I,J,2)
      Y(I,J,1)=Y(I,J,2)
      DO 150 KZ=1,3
      XS(J,KZ,I,1)=XS(J,KZ,I,2)
      YS(J,KZ,I,1)=YS(J,KZ,I,2)
  150 CONTINUE
C
C
C  CHECK FOR CONVERGENCE
C
      IF(NSTOP.EQ.0) TSTOP=TOTIME
  200 CONTINUE
      IF(TOTIME.LT.PRTIME.AND.TOTIME.LT.TSTOP) GO TO 140
      PRTIME=PRTIME+DPRINT
```

```
C
C
C  PRINTING CONCENTRATIONS FOR THE TIME INTERVAL
C  SUBROUTINE PRTOUT DOES ALL THE CONVERSIONS AND CALCULATIONS WHICH
C  ARE REQUIRED BEFORE THE PROFILE CAN BE PRINTED OR PUNCHED.  BECAUSE
C  OF THE HEADINGS, THE PRINTING IS DONE IN PRTOUT WHILE THE PUNCHING
C  CAN BE DONE IN THE MAIN PROGRAM.
C
      PRINT 1100,TOTIME
      CALL PRTOUT
C
C
  250 IF(TOTIME.LT.TSTOP) GO TO 140
C
C
C  PUNCHED CARD OUTPUT
C
      IF(IPNCH.EQ.0) GO TO 300
      ONE=1.0
      DO 275 J=1,NTOST
      PUNCH 1202,(X(I,J,2),I=1,6),TPROF(J,2)
      PUNCH 1202,(Y(I,J,2),I=1,6),ONE
  275 CONTINUE
  300 CONTINUE
      PRTIME=PRTIME-DPRINT
      GO TO 21
  400 CONTINUE
      IF(DPRINT.EQ.1.) GO TO 10
      STOP
C
C
 1000 FORMAT(10A8)
 1002 FORMAT('1CALCULATIONS FOR A SOLVENT EXTRACTION PROCESS',
     .  ' HAVING INTERACTING SOLUTES'//)
 1003 FORMAT(' ',10A8)
 1202 FORMAT(1P8E10.3)
 1100 FORMAT ('-  TIME = ',0PF7.2,'  MINUTES')
 2000 FORMAT(' NUMBER OF STAGES = ',I3)
 2003 FORMAT(' IPRO = ',I3,3X,'INVALID VALUE')
 2026 FORMAT(' IPNCH = 0',3X,'NO PUNCHED CARD OUTPUT')
 2028 FORMAT(' IPNCH = ',I3,3X,'INVALID VALUE')
 2034 FORMAT(' NSTR = 0',3X,'NO UNUSUAL ROUTING PATTERN')
 2035 FORMAT(' NSTR = 1',3X,'ROUTING PATTERN OTHER THAN NORMAL')
 2036 FORMAT(' NSTR = ',I3,3X,'INVALID VALUE')
 2038 FORMAT(' IVOLM = 1 AQUEOUS AND ORGANIC MIXER VOLUMES GIVEN')
 2039 FORMAT(' IVOLM = 2 TOTAL MIXER VOLUME GIVEN')
 2040 FORMAT(' IVOLM = 3 MIXER VOLUMES DETERMINED BY PHASE FLOW')
 2041 FORMAT(' IVOLM =',I2,' INVALID VALUE')
 2042 FORMAT(' IVOLS = 1 AQUEOUS AND ORGANIC SETTLER VOLUMES GIVEN')
 2043 FORMAT(' IVOLS = 2 TOTAL SETTLER VOLUME GIVEN')
 2044 FORMAT(' IVOLS = 3 SETTLER VOLUMES GIVEN BY PHASE FLOW')
 2045 FORMAT(' IVOLS =',I2,' INVALID VALUE')
 3000 FORMAT(2I2,2F8.0,4I2)
 3001 FORMAT(4F8.0,8I2)
 3101 FORMAT(' NEWIN = 1 NEW INPUT FLOWS WILL BE GIVEN')
 3102 FORMAT(' NEWIN = 0 INPUT FLOWS WILL BE UNCHANGED')
 3103 FORMAT(' NEWOUT = 1  NEW OUTPUT FLOWS WILL BE GIVEN')
 3104 FORMAT(' NEWOUT = 0  OUTPUT STREAMS WILL BE UNCHANGED')
 3105 FORMAT(' IVOLM = 0  MIXER VOLUMES WILL BE UNCHANGED')
 3106 FORMAT(' IVOLS = 0  SETTLER VOLUMES WILL BE UNCHANGED')
 3107 FORMAT(' IPRO = 0  A NEW INITIAL PROFILE WILL NOT BE READ')
 3108 FORMAT(' IPRO = 1  A NEW INITIAL PROFILE WILL BE READ')
 3109 FORMAT(' NEWIN = ',I2,' INVALID VALUE')
 3110 FORMAT(' NEWOUT = ',I2,' INVALID VALUE')
 3111 FORMAT(' IPNCH = 1  PROFILE CARDS WILL BE PUNCHED AT END OR TIME')
 3201 FORMAT('-DTHETA = ',0PF8.3,' MINUTES PER TIME INCREMENT')
 3202 FORMAT(' DPRINT =',0PF9.3,' MINUTES BETWEEN PRINTING OF PROFILES')
 3203 FORMAT(' THIS TIME PERIOD WILL END WHEN TIME = TSTOP = ',0PF8.3,
     . ' MINUTES, OR A TOLERANCE OF TOL =',0PF8.4,' % PER MINUTE IS REAC
     .HED')
 3205 FORMAT('1TRANSIENT BEHAVIOR RESULTS   MIXER CONCENTRATION GIVEN')
 4000 FORMAT(' ORGANIC STREAM EXITING AT STAGE',I4,' FEEDS STAGE',I4)
 5000 FORMAT(' IFAST = 1  THE FAST INTEGRATION TECHNIQUE WILL BE USED')
 5001 FORMAT(' IFAST = 0  THE RUNGE-KUTTA INTEGRATION WILL BE USED')
 7000 FORMAT(' TEMPI = ',1PE10.3,'  INITIAL & DEFAULT TEMPERATURE')
 8000 FORMAT(' IRXN = 0  NO REACTIONS WILL BE CONSIDERED')
 8001 FORMAT(' IRXN = 1  INSTANTANEOUS REDUCTION OF PLUTONIUM')
 8002 FORMAT(' IRXN = 2  REDUCTION OF PLUTONIUM BY URANIUM (IV)')
 8003 FORMAT(' IRXN = 3  REDUCTION OF PLUTONIUM BY HYDROXYLAMINE ')
      END
```

```
      SUBROUTINE STARTS
C
C
C  SUBROUTINE STARTS DOES GENERAL INPUT FUNCTIONS.  IT READS ALL THE
C  INFORMATION REQUIRED FOR A TIME PERIOD, CONVERTS THE UNITS TO A
C  MOLAL BASIS, AND SETS THE HYDRAULICS FOR THE SYSTEM.
C
      COMMON/CONTRL/ NTOST,NSOLU,CTBP,NEWIN,NEWOUT,SPH,IPNCH,IFAST,IRXN,
     .  DTHETA,IVOLM,IVOLS,IPRO,TEMPI,ISOL(6),NSTR,ISTR,JSTR,CODUM(100)
      COMMON/CONCS/ X(6,100,2),Y(6,100,2),XS(100,3,6,2),YS(100,3,6,2)
      COMMON/DISTRB/ TEMPC,ARY(6),DTRY(6)
      COMMON/FLOWS/ A(100),O(100),AT(100),OT(100)
      COMMON/MOLALC/ AQ(6),OR(6),TEMP,CONVA,CONVO,TCONC
      COMMON/STREAM/ XFD(6,100),YFD(6,100),AFDRT(100),OFDRT(100),
     .   AFDTEM(100),OFDTEM(100),ALVRT(100),OLVRT(100)
      COMMON/TEMPS/ TPROF(100,2),ATS(100,3,2),OTS(100,3,2)
      COMMON/VOLS/ AVOL(100),OVOL(100),ASVOL(100),OSVOL(100)
      DIMENSION CON(6)
C
C
C  EQCKDG IS A CHECK ON THE INITIAL PROFILE.  IF EQCKDG = 1.0 THE PROFILE
C  WAS CREATED BY THE PROGRAM.  OTHERWISE, THE PROFILE CONCENTRATIONS
C  ARE ADJUSTED SO THAT THE PHASES ARE IN EQUILIBRIUM.
C
      EQCKDG=0.0
C
C
C  TCONC IS AN INDICATOR FOR THE MOLAL CONVERSION.  TCONC = -1 SINCE
C  MOLAR CONCENTRATIONS WILL BE PASSED TO THE MOLAL SUBROUTINE.
C
      TCONC=-1.0
C
C
      DO 5 I=1,6
      AQ(I)=0.0
      OR(I)=0.0
    5 CONTINUE
C
C
C  NEWIN DETERMINES IF NEW INPUT STREAMS ARE TO BE SPECIFIED.  NEWIN = 0
C  INDICATES THAT NEW INPUT FLOWS WILL NOT BE GIVEN SO THE APPROPRIATE
C  SECTION OF THE PROGRAM SHOULD BE BYPASSED.
C
      IF(NEWIN.EQ.0) GO TO 40
C
C  THIS SECTION RE-INITIALIZES AND INPUTS ALL THE FEED STREAM INFORMATION.
C
C
      DO 10  J=1,NTOST
      AFDRT(J)=0.0
      OFDRT(J)=0.0
      AFDTEM(J)=TEMPI
      OFDTEM(J)=TEMPI
      DO 10 I=1,NSOLU
      XFD(I,J)=0.0
      YFD(I,J)=0.0
   10 CONTINUE
   15 CONTINUE
      READ (5,1001) J,JHAS,FDRT,(CON(I),I=1,6),TEMP,INDEX
      IF(J.LE.0)  J=100
      IF(JHAS.EQ.1) GO TO 20
      OFDRT(J)=FDRT
      IF(TEMP.NE.0.) OFDTEM(J)=TEMP
      DO 17 I=1,6
      IF(CON(I).NE.0.0) ISOL(I)=1
      YFD(I,J)=CON(I)
   17 CONTINUE
      GO TO 30
   20 CONTINUE
      AFDRT(J)=FDRT
      IF(TEMP.NE.0.) AFDTEM(J)=TEMP
      DO 25 I=1,6
      IF(CON(I).NE.0.0) ISOL(I)=1
      XFD(I,J)=CON(I)
   25 CONTINUE
   30 CONTINUE
      IF(INDEX.EQ.1) GO TO 15
   40 CONTINUE
C
C
C  NEWOUT DETERMINES IF NEW PRODUCT STREAMS ARE TO BE SPECIFIED. NEWOUT = 0
C  INDICATES THAT NO NEW PRODUCT STREAMS WILL BE SPECIFIED, SO THIS SECTION
C  OF THE PROGRAM WILL BE BYPASSED.
C
      IF(NEWOUT.EQ.0) GO TO 60
C
C  THIS SECTION RE-INITIALIZES AND INPUTS ALL THE PRODUCT STREAM INFORMATION.
C
C
      DO 45 J=1,NTOST
      ALVRT(J)=0.0
      OLVRT(J)=0.0
   45 CONTINUE
   50 CONTINUE
```

```
      READ 2001,J,JHAS,OTRT,INDEX
      IF(J.LE.0)  J=100
      IF(JHAS.EQ.1)  ALVRT(J)=OTRT
      IF(JHAS.EQ.0)  OLVRT(J)=OTRT
      IF(INDEX.EQ.1)  GO TO 50
   60 CONTINUE
C
C
C  IPRO DETERMINES IF AN INITIAL PROFILE IS TO BE READ OFF CARDS.  IF NOT
C  (IPRO = 0) THIS SECTION OF THE PROGRAM IS BYPASSED.
C
      IF(IPRO.EQ.0)  GO TO 80
C
C  THIS SECTION RE-INITIALIZES THE CONCENTRATION PROFILES WITH THE VALUES
C  READ OFF OF THE PROFILE CARDS.  SETTLER CONCENTRATIONS ARE ASSUMED TO
C  BE THE SAME AS THE MIXER CONCENTRATIONS FOR A STAGE.
C
C
      DO 70 J=1,NTOST
      READ(5,1002)  (X(I,J,2),I=1,6),TPROF(J,2)
      READ(5,1002)  (Y(I,J,2),I=1,6),EQCKDG
      IF(TPROF(J,2).EQ.0.0)  TPROF(J,2)=TEMPI
      TPROF(J,1)=TPROF(J,2)
      DO 65 I=1,6
      IF(X(I,J,2).NE.0.0)  ISOL(I)=1
      IF(Y(I,J,2).NE.0.0)  ISOL(I)=1
   65 CONTINUE
      DO 70 K=1,3
      DO 70 L=1,2
      ATS(J,K,L)=TPROF(J,1)
      OTS(J,K,L)=TPROF(J,1)
   70 CONTINUE
   80 CONTINUE
C
C
C  NSOLU IS SET TO THE SUBSCRIPT OF THE HIGHEST NUMBERED COMPONENT IN THE
C  SYSTEM.  ISOL INDICATES WHETHER A COMPONENT IS PRESENT.  THIS CHECK
C  SAVES TIME BY BYPASSING CALCULATIONS WHICH WOULD ALWAYS RESULT IN
C  ZERO CONCENTRATION.  THUS IF ONLY NITRIC ACID IS PRESENT, CALCULATIONS
C  FOR THE NON-EXISTANT PLUTONIUM CAN BE SKIPPED IN SOME PLACES.
C
      NSOLU=1
      DO 82 I=1,6
      IF(ISOL(I).EQ.1)  NSOLU=I
   82 CONTINUE
C
C
C  CONVRT PRINTS THE FEED STREAM INFORMATION, AND CONVERTS THE CONCENTRATIONS
C  TO MOLAL UNITS.
C
      IF(NEWIN+IPRO.EQ.0)  GO TO 120
      CALL CONVRT
  120 CONTINUE
C
C
C
      IF(NEWOUT.EQ.0)  GO TO 122
C
C
C  PRINTING THE PRODUCT STREAM FLOWRATES.  THE PRINTED RATES MAY NOT BE
C  THE VALUES USED IN CALCULATIONS DUE TO THE REQUIREMENT THAT NO MORE
C  OF A PHASE MAY FLOW OUT OF A STAGE THAN FLOWED IN.
C
      DO 121 J=1,NTOST
      IF(ALVRT(J).NE.0.0)  PRINT 1007,J,ALVRT(J)
      IF(OLVRT(J).NE.0.0)  PRINT 1008,J,OLVRT(J)
  121 CONTINUE
  122 CONTINUE
      IF(NEWIN+NEWOUT.EQ.0)  GO TO 127
C
C  SET AQUEOUS AND ORGANIC INTERSTAGE FLOW (A AND O)
C
C  A IS AQUEOUS INTERSTAGE FLOW
C  O IS ORGANIC INTERSTAGE FLOW
C  AT IS TOTAL AQUEOUS FLOW WITHIN A STAGE
C  OT IS TOTAL ORGANIC FLOW WITHIN A STAGE
C
C
      IF(ALVRT(1).GT.AFDRT(1))  ALVRT(1)=AFDRT(1)
      A(1)=AFDRT(1)-ALVRT(1)
      AT(1)=AFDRT(1)
      IF(OLVRT(NTOST).GT.OFDRT(NTOST))  OLVRT(NTOST)=OFDRT(NTOST)
      O(NTOST)=OFDRT(NTOST)-OLVRT(NTOST)
      OT(NTOST)=OFDRT(NTOST)
      DO 125 I=2,NTOST
      IF(ALVRT(I).GE.A(I-1)+AFDRT(I))  ALVRT(I)=A(I-1)+AFDRT(I)
      A(I)=A(I-1)+AFDRT(I)-ALVRT(I)
      AT(I)=A(I)+ALVRT(I)
      NST = NTOST+1-I
      IF(OLVRT(NST).GE.O(NST+1)+OFDRT(NST))  OLVRT(NST)=O(NST+1)+
           OFDRT(NST)
      O(NST) = O(NST+1)+OFDRT(NST)-OLVRT(NST)
      IF(NSTR.EQ.1.AND.NST.EQ.ISTR-1)  O(NST)=OFDRT(NST)-OLVRT(NST)
```

```
      IF(NSTR.EQ.1.AND.NST.EQ.JSTR)  O(NST)=O(ISTR)+OFDRT(NST)-OLVRT(NST)
     .  +O(NST+1)
      OT(NST)=O(NST)+OLVRT(NST)
C
C  THE INTERSTAGE FLOWS ARE NOW SET
C
  125 CONTINUE
  127 CONTINUE
C
C
C  IVOLM AND IVOLS ARE NOW CHECKED TO SEE IF ANY VOLUME CARDS ARE TO BE
C  READ, OR IF THE VOLUMES ARE EVEN GOING TO BE CHANGED
C
      IF(IVOLS+IVOLM.EQ.0)  GO TO 310
      DO 128 J=1,NTOST
      IF(IVOLM.NE.0)  AVOL(J)=0.0
      IF(IVOLM.NE.0)  OVOL(J)=0.0
      IF(IVOLS.NE.0)  ASVOL(J)=0.0
      IF(IVOLS.NE.0)  OSVOL(J)=0.0
  128 CONTINUE
      IF(IVOLM.EQ.3.AND.IVOLS.EQ.3)  GO TO 200
      IF(IVOLM.EQ.3.AND.IVOLS.EQ.0)  GO TO 200
      IF(IVOLM.EQ.0.AND.IVOLS.EQ.3)  GO TO 200
C
C  VOLUMES ARE NOW READ IN.  TO MINIMIZE THE INPUT CARDS NEEDED, THE VOLUMES
C        NEED BE SPECIFIED ONLY WHEN THE VOLUME CHANGES FROM THAT OF THE
C        PREVIOUS STAGE.
C
  130 READ(5,2101)  ISEC,I,VOLA,VOLO,INDX
      IF(I.LE.0)  I=100
      IF(ISEC.EQ.1.AND.IVOLM.EQ.0)  GO TO 145
      IF(ISEC.EQ.2.AND.IVOLS.EQ.0)  GO TO 145
      IF(ISEC.EQ.2)  GO TO 140
      AVOL(I)=VOLA
      OVOL(I)=VOLO
      GO TO 145
  140 ASVOL(I)=VOLA
      OSVOL(I)=VOLO
  145 IF(INDX.EQ.1)  GO TO 130
C
C
C  THE VOLUMES ARE NOW PROPAGATED THROUGH OUT THE COLUMN IN THE MANNER CHOSEN
C  ALL VOLUMES AND FLOWS ARE PRINTED IF ANY CHANGES WERE MADE
C
  200 IF(AVOL(1).EQ.0.0)  AVOL(1)=AT(1)
      IF(OVOL(1).EQ.0.0)  OVOL(1)=OT(1)
      IF(ASVOL(1).EQ.0.0)  ASVOL(1)=AT(1)
      IF(OSVOL(1).EQ.0.0)  OSVOL(1)=OT(1)
      DO 300 I=1,NTOST
      J=I-1
      IF(IVOLM.EQ.0)  GO TO 240
      GO TO (210,220,230),IVOLM
  210 IF(AVOL(I).EQ.0.0)  AVOL(I)=AVOL(J)
      IF(OVOL(I).EQ.0.0)  OVOL(I)=OVOL(J)
      GO TO 240
  220 IF(AVOL(I).EQ.0.0)  AVOL(I)=AVOL(J)+OVOL(J)
      OVOL(I)=AVOL(I)*OT(I)/(AT(I)+OT(I))
      AVOL(I)=AVOL(I)-OVOL(I)
      GO TO 240
  230 AVOL(I)=AT(I)
      OVOL(I)=OT(I)
  240 IF(IVOLS.EQ.0)  GO TO 280
      GO TO (250,260,270),IVOLS
  250 IF(ASVOL(I).EQ.0.0)  ASVOL(I)=ASVOL(J)
      IF(OSVOL(I).EQ.0.0)  OSVOL(I)=OSVOL(J)
      GO TO 280
  260 IF(ASVOL(I).EQ.0.0)  ASVOL(I)=ASVOL(J)+OSVOL(J)
      OSVOL(I)=ASVOL(I)*OT(I)/(AT(I)+OT(I))
      ASVOL(I)=ASVOL(I)-OSVOL(I)
      GO TO 280
  270 ASVOL(I)=AT(I)
      OSVOL(I)=OT(I)
  280 IF(AVOL(I).LT.1.0E-4)  AVOL(I)=0.0
      IF(OVOL(I).LT.1.0E-4)  OVOL(I)=0.0
      IF(ASVOL(I).LT.1.0E-4)  ASVOL(I)=0.0
      IF(OSVOL(I).LT.1.0E-4)  OSVOL(I)=0.0
  300 CONTINUE
  310 IF(NEWIN+NEWOUT+IVOLM+IVOLS.EQ.0)  GO TO 400
      PRINT 1106
      PRINT 1107
      PRINT 1108
      DO 320 I=1,NTOST
      PRINT 1101,I,AVOL(I),OVOL(I),ASVOL(I),OSVOL(I),AT(I),OT(I),A(I),
     .  O(I)
  320 CONTINUE
```

```
C
C
C     THIS SECTION INSURES THAT THE PHASES ARE IN CHEMICAL EQUILIBRIUM
C     BEFORE THE ITERATIONS START.  THE CHECK IS DISABLED WHEN THE INITIAL
C     PROFILE WAS CREATED BY THE PROGRAM, OR WHEN THE PROFILE WAS FROM
C     CARDS PUNCHED BY THE PROGRAM.
C
C
      IF(IPRO.EQ.0.OR.EQCKDG.EQ.1.0) GO TO 400
      DO 350 J=1,NTOST
      AV=AVOL(J)+ASVOL(J)
      OV=OVOL(J)+OSVOL(J)
      DO 340 K=1,3
      DO 330 I=1,6
  330 ARY(I)=X(I,J,2)
      ICK=0
      TEMPC=TPROF(J,2)
      CALL UCOR
      DO 335 I=1,NSOLU
      IF(ISOL(I).EQ.0) GO TO 335
      X(I,J,1)=(OV*Y(I,J,2)+AV*X(I,J,2))/(AV+CV*DTRY(I))
      Y(I,J,1)=Y(I,J,2)+(X(I,J,2)-X(I,J,1))*AV/OV
      IF(ABS(X(I,J,1)-X(I,J,2)).GT.0.01*X(I,J,1)) ICK=1
      X(I,J,2)=X(I,J,1)
      Y(I,J,2)=Y(I,J,1)
  335 CONTINUE
      IF(ICK.EQ.0) GO TO 345
  340 CONTINUE
  345 DO 350 K=1,3
      DO 350 L=1,2
      ATS(J,K,L)=TPROF(J,1)
      OTS(J,K,L)=TPROF(J,1)
      DO 350 I=1,NSOLU
      XS(J,K,I,L)=X(I,J,1)
      YS(J,K,I,L)=Y(I,J,1)
  350 CONTINUE
  400 RETURN
C
C
 1001 FORMAT(2I2,8F8.0,I2)
 1002 FORMAT(8F10.0)
 1007 FORMAT(14X,'AQUEOUS ',I3,5X,'PRODUCT STREAM REMOVED (FLOW RATE IN
     .MOLAL UNITS)',34X,1PE10.3)
 1008 FORMAT(14X,'ORGANIC ',I3,5X,'PRODUCT STREAM REMOVED (FLOW RATE IN
     .MOLAL UNITS)',34X,1PE10.3)
 1101 FORMAT(8X,I3,2X,8('|',2X,1PE10.3,2X))
 1106 FORMAT(///7X,'STAGE |',4X,'MIXER VOLUME BY PHASE',4X,'|   SETTLER VO
     .VOLUME BY PHASE   |',7X,'MIXER FLOW RATE',7X,'|',4X,'INTERSTAGE FL
     .OW RATE')
 1107 FORMAT(8X,'NO.  ',4('|   AQUEOUS    |   ORGANIC    '))
 1108 FORMAT(13X,8('|',14X))
 2001 FORMAT(2I2,F8.0,I2)
 2101 FORMAT(2I2,2F8.0,I2)
      END
```

```
      SUBROUTINE CONVRT
C
C
C  SUBROUTINE CONVRT PRINTS THE FEED STREAM INFORMATION, AND CONVERTS THE
C  CONCENTRATIONS FROM THEIR ORIGINAL FORM TO THE MOLAL UNITS WHICH ARE
C  USED IN THE CALCULATIONS.
C
      COMMON/CONTRL/ NTOST,NSOLU,CTBP,NEWIN,NEWOUT,SPH,IPNCH,IFAST,IRXN,
     .  DTHETA,IVOLM,IVOLS,IPRO,TEMPI,ISOL(6),NSTR,ISTR,JSTR,CODUM(100)
      COMMON/CONCS/ X(6,100,2),Y(6,100,2),XS(100,3,6,2),YS(100,3,6,2)
      COMMON/MOLALC/ AQ(6),OR(6),TEMP,CONVA,CONVO,TCONC
      COMMON/STREAM/ XFD(6,100),YFD(6,100),AFDRT(100),OFDRT(100),
     .   AFDTEM(100),OFDTEM(100),ALVRT(100),OLVRT(100)
      COMMON/TEMPS/ TPROF(100,2),ATS(100,3,2),OTS(100,3,2)
C
C
C  IF NEW INPUT STREAMS HAVE BEEN GIVEN (NEWIN = 1), THIS SECTION PRINTS
C  AND CONVERTS THEM.
C
      IF(NEWIN.EQ.0) GO TO 20
      PRINT 1100
      PRINT 1101
      DO 10  J=1,NTOST
      IF(AFDRT(J)+OFDRT(J).EQ.0.0) GO TO 10
      IF(AFDRT(J).NE.0.) PRINT 1000,J,(XFD(I,J),I=1,6),AFDRT(J),
     .  AFDTEM(J)
      IF(OFDRT(J).NE.0.) PRINT 1001,CTBP,J,(YFD(I,J),I=1,6),OFDRT(J),
     .  OFDTEM(J)
C
C
C  CONVERSION TO MOLAR UNITS.
C
C
      XFD(2,J)=XFD(2,J)/238.
      YFD(2,J)=YFD(2,J)/238.
      XFD(3,J)=XFD(3,J)/239.
      YFD(3,J)=YFD(3,J)/239.
      XFD(4,J)=XFD(4,J)/239.
      YFD(4,J)=YFD(4,J)/239.
      DO 5 I=1,6
      AQ(I)=XFD(I,J)
      OR(I)=YFD(I,J)
    5 CONTINUE
      TEMP=OFDTEM(J)
C
C
C  SUBROUTINE MOLAL CALCULATES THE MOLAR TO MOLAL CONVERSION FACTORS.
C
      CALL MOLAL
      AFDRT(J)=AFDRT(J)/CONVA
      OFDRT(J)=OFDRT(J)/CONVO
      DO 10 I=1,NSOLU
      XFD(I,J)=XFD(I,J)*CONVA
      YFD(I,J)=YFD(I,J)*CONVO
   10 CONTINUE
C
C
C  IF AN INITIAL PROFILE HAS BEEN GIVEN (IPRO = 1), THIS SECTION
C  CONVERTS THE CONCENTRATIONS AND INITIALIZES THE SETTLERS.
C
   20 IF(IPRO.EQ.0) GO TO 40
      DO 30 J=1,NTOST
      X(2,J,2)=X(2,J,2)/238.
      Y(2,J,2)=Y(2,J,2)/238.
      X(3,J,2)=X(3,J,2)/239.
      Y(3,J,2)=Y(3,J,2)/239.
      X(4,J,2)=X(4,J,2)/239.
      Y(4,J,2)=Y(4,J,2)/239.
      DO 22 I=1,NSOLU
      AQ(I)=X(I,J,2)
      OR(I)=Y(I,J,2)
   22 CONTINUE
      TEMP=TPROF(J,2)
      CALL MOLAL
      DO 25 I=1,6
      AQ(I)=AQ(I)*CONVA
      OR(I)=OR(I)*CONVO
      DO 25 L=1,2
      X(I,J,L)=AQ(I)
      Y(I,J,L)=OR(I)
      DO 25 K=1,3
      XS(J,K,I,L)=AQ(I)
      YS(J,K,I,L)=OR(I)
   25 CONTINUE
   30 CONTINUE
   40 RETURN
 1000 FORMAT(14X,'AQUEOUS ',I3,7(4X,1PE10.3),3X,0PF7.1)
 1001 FORMAT(9X,2PF6.1,' % TBP ',I3,7(4X,1PE10.3),3X,0PF7.1)
 1100 FORMAT('-FEED & PRODUCT        STAGE  NITRIC ACID    URANIUM
     .PU (IV)        PU (III)       REDUCTANT    NITRATE ION     FLOW RATE
     .     TEMP')
 1101 FORMAT(' STREAM DATA              NO.       (MOL/L)         (G/L)
     . (G/L)           (G/L)           (MOL/L)         (MOL/L)         (L/MIN)
     .       (C)')
      END
```

```
      SUBROUTINE MOLAL
C
C
C  SUBROUTINE MOLAL PROVIDES THE CONVERSION FACTORS (CONVA, CONVO) BETWEEN
C  MOLAR AND MOLAL UNITS.  AQ AND OR CONTAIN THE CONCENTRATIONS TO BE
C  CONVERTED.  TCONC SIGNALS THE UNITS OF THE CONCENTRATIONS BEING PASSED.
C              TCONC = -1.0 FOR MOLAR CONCENTRATIONS
C              TCONC =  1.0 FOR MOLAL CONCENTRATIONS
C
      COMMON/CONTRL/ NTOST,NSOLU,CTBP,NEWIN,NEWOUT,SPH,IPNCH,IFAST,IBIN,
     .  DTHETA,IVOLM,IVOLS,IPRO,TEMPI,ISOL(6),NSTR,ISTR,JSTR,CODUM(100)
      COMMON/MOLALC/ AQ(6),OR(6),TEMP,CONVA,CONVO,TCONC
      P=CTBP
      T=3.65145*P
      IF(TCONC.EQ.1.0) GO TO 5
      UOS=T/(2.0+0.092*T)
      PUOS=T/(2.0+0.18*T)
      HOS=T*(1.0-0.00609*(3.95-0.0144*TEMP)*(P**1.65))/(1.0+0.043*T)
      WO=(3.95-0.0144*TEMP)*(P**1.65)*(1.0-OR(2)/UOS-OR(3)/PUOS-
     .      0.65*OR(1)/HOS)
      GO TO 10
    5 WO=(4.2-0.015*TEMP)*(P**1.69)*(T-2.0*OR(2)-2.0*OR(3)-0.6*OR(1))/T
   10 CONVO= 1.0+TCONC*(0.097*OR(2)+0.139*OR(3)+0.043*OR(1)+0.0174*WO)
      CONVO=CONVO**TCONC
      CONVA=0.0724*AQ(2)+0.13*AQ(3)+0.0309*AQ(1)+0.031*AQ(6)
      CONVA=(1.0+TCONC*CONVA)**TCONC
      RETURN
      END
```

```
      SUBROUTINE STAGES (NDIREC)
CCCCCC
C
C
C   SUBROUTINE STAGES IS NOT COMPLICATED, BUT MODIFICATIONS TO IT SHOULD BE
C                    MADE WITH CARE.  IT EMPLOYS A FOURTH ORDER RUNGE-KUTTA
C                    INTEGRATION OF THE DIFFERENTIAL EQUATIONS GOVERNING THE
C                    CHANGES IN CONCENTRATIONS OF THE MIXERS.  CERTAIN VARIABLES
C                    IN THE EQUATIONS ARE APPROXIMATED AS CONSTANTS FOR THE
C                    TIME INTERVAL (AIN & OIN) AND DETERMINED BY RECTANGULAR
C                    METHODS HALF THE TIMES, AND BY TRAPEZOIDAL METHODS THE
C                    OTHER HALF (AS SPECIFIED BY NDIREC).
C                       SETTLER CONCENTRATIONS ARE GIVEN BY TRAPEZOIDAL
C                    METHODS RATHER THAN BY THE RUNGE-KUTTA INTEGRATION.
C                       TEMPERATURE CHANGES ARE MADE BY A SIMPLE HEAT
C                    BALANCE
C
C
C
C  DESCRIPTION OF VARIABLES
C     F(I)  AN EVALUATION OF THE DERIVATIVE IN THE INTEGRATION FOR COMPONENT I
C     PHI(I)    WEIGHTED TOTAL OF THE VARIOUS F(I) COMPUTED
C     TX(I)     TEST X FOR ITERATION BETWEEN THE CONCS AND THE DISTRIBUTION COEFF
C     AIN IS THE SOLUTE COMING IN THE AQUEOUS STREAMS
C     OIN IS THE SOLUTE COMING IN THE ORGANIC STREAMS
C     ARY       USED IN SAME WAY AS TX, SORT OF
C     DTRY      TRIAL DISTRIBUTION COEFFICIENTS
C     NDIREC CHANGES THE STREAM THAT THE CALCULATIONS ARE FOLLOWING.  ONE TIME,
C        THE CALCULATIONS WILL START WITH THE FIRST STAGE AND GO TO STAGE N
C        (FOLLOWING THE AQUEOUS PHASE).  THE NEXT TIME IT WILL START WITH
C        STAGE N, AND GO THE OTHER DIRECTION.
C
C
CCCCCC
      COMMON/CONTRL/ NTOST,NSOLU,CTBP,NEWIN,NEWOUT,SPH,IPNCH,IFAST,IRIN,
        DTHETA,IVOLM,IVOLS,IPRO,TEMPI,ISOL(6),NSTR,ISTR,JSTR,CODUM(100)
      COMMON/CONCS/ X(6,100,2),Y(6,100,2),XS(100,3,6,2),YS(100,3,6,2)
      COMMON/DISTRB/ TEMPC,ARY(6),DTRY(6)
      COMMON/FLOWS/ A(100),O(100),AT(100),OT(100)
      COMMON/MOLALC/ AQ(6),OR(6),TEMP,CONVA,CONVO,TCONC
      COMMON/STREAM/ XFD(6,100),YFD(6,100),AFDRT(100),OFDRT(100),
         AFDTEM(100),OFDTEM(100),ALVRT(100),OLVRT(100)
      COMMON/TEMPS/ TPROF(100,2),ATS(100,3,2),OTS(100,3,2)
      COMMON/VOLS/ AVOL(100),OVOL(100),ASVOL(100),OSVOL(100)
      DIMENSION F(6),PHI(6),TX(6),AIN(6),OIN(6)
      CCD=0.001
C
C
C  TCONC = 1.0 FOR THE VOLUME CONVERSIONS SINCE MOLAL CONCENTRATIONS ARE PASSED.
C
      TCONC=1.0
      DO 2 I=1,6
      F(I)=0.0
      TX(I)=0.0
      AQ(I)=0.0
      OR(I)=0.0
      ARY(I)=0.0
      AIN(I)=0.0
      OIN(I)=0.0
      PHI(I)=0.0
    2 CONTINUE
      DO 500 NSCAN=1,NTOST
      J=NSCAN
      IF(NDIREC.LT.0) J=NTOST-NSCAN+1
      JJ=J-1
      JJJ=J+1
      CODUM(J)=0.0
C
C  ALL OF THIS 'DO 5' LOOP IS CONCERNED WITH ACCUMULATING THE APPROXIMATION
C     FOR THE INPUT CONCENTRATIONS
C
      DO 5 I=1,NSOLU
      IF(ISOL(I).EQ.0) GO TO 5
C
C
C  ADDING THE SOLUTES IN THE FEED STREAMS
C
      AIN(I)=AFDRT(J)*XFD(I,J)
      OIN(I)=OFDRT(J)*YFD(I,J)
C
C
C  ADDING THE AQUEOUS SOLUTE FROM THE PRECEEDING STAGE.  IF NDIREC IS
C  POSITIVE, THE PRECEEDING STAGE HAS A VALUE FOR TWO POINTS IN TIME,
C  SO A TRAPEZOIDAL APPROXIMATION IS USED.
C
      IF(J.GT.1) AIN(I)=AIN(I)+A(JJ)*XS(JJ,3,I,1)
      IF (J*NDIREC.GT.1) AIN(I)=AIN(I)+(XS(JJ,3,I,2)-XS(JJ,3,I,1))*
        A(JJ)/2.
C
C
C  A SIMILAR PROCESS FOR THE ORGANIC SOLUTE FROM THE SUCCEEDING STAGE.
C
      IF (J.LT.NTOST) OIN(I)=OIN(I)+O(JJJ)*YS(JJJ,3,I,1)
      IF(J.LT.NTOST.AND.NDIREC.LT.0) OIN(I)=OIN(I)+(YS(JJJ,3,I,2)-
        YS(JJJ,3,I,1))*O(JJJ)/2.
```

```
C
C  IF NSTR = 1 AN ORGANIC STREAM MUST BE TREATED IN A SPECIAL MANNER.
C
      IF(NSTR.EQ.1.AND.J.EQ.JSTR)  OIN(I)=OIN(I)+O(ISTR)*YS(ISTR,3,I,1)
      IF(NSTR.EQ.1.AND.J.EQ.JSTR.AND.NDIREC*(J-ISTR).GT.0)
     .   OIN(I)=OIN(I)+(YS(ISTR,3,I,2)-YS(ISTR,3,I,1))*O(ISTR)/2.
      IF(NSTR.EQ.1.AND.J.EQ.ISTR-1)  OIN(I)=OFDRT(J)*YFD(I,J)
C
C  THE PROGRAM WILL NOT DEAL WITH SOLUTE FLOWS SMALLER THAN THIS
C  THRESHOLD LEVEL.
C
      IF(ABS(AIN(I)).LT.1.0E-15)  AIN(I)=0.0
      IF(ABS(OIN(I)).LT.1.0E-15)  OIN(I)=0.0
      TX(I)=X(I,J,1)
      ARY(I)=X(I,J,1)
      AQ(I)=X(I,J,1)
      OR(I)=Y(I,J,1)
    5 CONTINUE
C
C  GETTING MOLAL VOLUMES
C     SOLUTE FREE VOLUMES ARE REQUIRED TO CORRECT THE UNITS OF THE VOLUMES
C     FROM REAL VOLUME UNITS TO MOLAL UNITS IN ORDER TO MAKE THE V*X VALID
C
      TEMP=TPROF(J,1)
      CALL MOLAL
      AQVOL=AVOL(J)/CONVA
      ORVOL=OVOL(J)/CONVO
      AQSVOL=ASVOL(J)/CONVA
      ORSVOL=OSVOL(J)/CONVO
C
C  THE HEAT BALANCES ARE DONE IN A WAY SIMILAR TO THE CONCENTRATIONS
C
      AHTIN=AFDRT(J)*AFDTEM(J)
      OHTIN=OFDRT(J)*OFDTEM(J)
      IF(J.GT.1)  AHTIN=AHTIN+A(JJ)*ATS(JJ,3,1)
      IF(J*NDIREC.GT.1)  AHTIN=AHTIN+(ATS(JJ,3,2)-ATS(JJ,3,1))*A(JJ)/2.
      IF(J.LT.NTOST)  OHTIN=OHTIN+O(JJJ)*OTS(JJJ,3,1)
      IF(J.LT.NTOST.AND.NDIREC.LT.0)  OHTIN=OHTIN+(OTS(JJJ,3,2)-
     .    OTS(JJJ,3,1))*O(JJJ)/2.
      IF(NSTR.EQ.1.AND.J.EQ.ISTR-1)  OHTIN=OFDRT(J)*OFDTEM(J)
      IF(NSTR.EQ.1.AND.J.EQ.JSTR)  OHTIN=OHTIN+O(ISTR)*OTS(ISTR,3,1)
      IF(NSTR.EQ.1.AND.J.EQ.JSTR.AND.NDIREC*(J-ISTR).GT.0)
     .   OHTIN=OHTIN+(OTS(ISTR,3,2)-OTS(ISTR,3,1))*O(ISTR)/2.
      TPROF(J,2)=TPROF(J,1)+DTHETA*(AHTIN+SPH*OHTIN-(AT(J)+SPH*OT(J))
     .   *TPROF(J,1))/(AQVOL+SPH*ORVOL)
      TEMPC=TPROF(J,2)
C
C
C     THIS BRANCH IS FOR THE FASTER INTEGRATION METHOD.
C
      IF(IFAST.EQ.1)  GO TO 150
CCC
C
C
C     THIS IS THE START OF THE RUNGE-KUTTA INTEGRATION
C
C
CCC
      MCK=0
C
C     GET THE DISTRIBUTION COEFF FROM THE PREVIOUS TIME
C
      CALL UCOR
   10 DO 20 I=1,NSOLU
C
C     CALCULATE THE FIRST DERIVATIVE
C
      F(I)=(AIN(I)+OIN(I)-(AT(J)+OT(J)*DTRY(I))*X(I,J,1))/
           (AQVOL+ORVOL*DTRY(I))
C
C     INCREASE X(I) BY DELTA X /2
C
   20 ARY(I)=X(I,J,1)+DTHETA*F(I)/2.
      MCK=MCK+1
C
C     GETTING A NEW DTRY WITH THE SLIGHTLY LARGER X'S
C
      CALL UCOR
C
C     ITERATING TO GET MATCHING DTRY'S AND X'S (ARY'S)
C
      MDEX=0
      DO 30 I=1,NSOLU
      IF(ABS(ARY(I)).LT.1.0E-6)  GO TO 30
      DIF=ABS((TX(I)-ARY(I))/ARY(I))
      IF(DIF.GT.CCD)  MDEX=1
   30 TX(I)=ARY(I)
      IF(MDEX.EQ.1.AND.MCK.LT.5)  GO TO 10
      DO 40 I=1,NSOLU
      X(I,J,2)=ARY(I)
   40 PHI(I)=F(I)
C
C  THIS (OR SIMILAR) PROCESS IS REPEATED WHILE ACCUMULATING PHI'S FOR THE
C     FINAL DETERMINATION OF X AT THE NEW TIME
```

```
   45 DO 50 I=1,NSOLU
      F(I)=(AIN(I)+OIN(I)-(AT(J)+OT(J)*DTRY(I))*X(I,J,2))/
     .      (AQVOL+ORVOL*DTRY(I))
   50 ARY(I)=X(I,J,1)+DTHETA*F(I)/2.
      MCK=MCK+1
      CALL UCOR
      MDEX=0
      DO 60 I=1,NSOLU
      IF(ABS(ARY(I)).LT.1.0E-6) GO TO 60
      DIF=ABS((TX(I)-ARY(I))/ARY(I))
      IF(DIF.GT.CCD)MDEX=1
   60 TX(I)=ARY(I)
      IF(MDEX.EQ.1.AND.MCK.LT.10) GO TO 45
      DO 70 I=1,NSOLU
      X(I,J,2)=ARY(I)
   70 PHI(I)=PHI(I)+2.*F(I)
   75 DO 80 I=1,NSOLU
      F(I)=(AIN(I)+OIN(I)-(AT(J)+OT(J)*DTRY(I))*X(I,J,2))/
     .      (AQVOL+ORVOL*DTRY(I))
   80 ARY(I)=X(I,J,1)+DTHETA*F(I)
      MCK=MCK+1
      CALL UCOR
      MDEX=0
      DO 90 I=1,NSOLU
      IF(ABS(ARY(I)).LT.1.0E-6) GO TO 90
      DIF=ABS((TX(I)-ARY(I))/ARY(I))
      IF(DIF.GT.CCD) MDEX=1
   90 TX(I)=ARY(I)
      IF(MDEX.EQ.1.AND.MCK.LT.15) GO TO 75
      DO 100 I=1,NSOLU
      X(I,J,2)=ARY(I)
  100 PHI(I)=PHI(I)+2.*F(I)
  105 DO 110 I=1,NSOLU
      F(I)=(AIN(I)+OIN(I)-(AT(J)+OT(J)*DTRY(I))*X(I,J,2))/
     .      (AQVOL+ORVOL*DTRY(I))
  110 ARY(I)=X(I,J,1)+(PHI(I)+F(I))*DTHETA/6.
      MCK=MCK+1
      CALL UCOR
      MDEX=0
      DO 120 I=1,NSOLU
      IF(ABS(ARY(I)).LT.1.0E-6) GO TO 120
      DIF=ABS((TX(I)-ARY(I))/ARY(I))
      IF(DIF.GT.CCD) MDEX=1
  120 TX(I)=ARY(I)
      IF(MDEX.EQ.1.AND.MCK.LT.20) GO TO 105
      DO 130 I=1,NSOLU
      IF(ABS(ARY(I)).LE.1.E-20) ARY(I)=0.0
      Y(I,J,2)=DTRY(I)*ARY(I)
  130 X(I,J,2)=ARY(I)
C
C  THIS COMPLETES THE INTEGRATION.  ARY(I) (FROM STM 110) BECOMES THE NEW
C     AQUEOUS CONCENTRATIONS
C     AND NOW THE SETTLER VALUES ARE CALCULATED WITH A TRAPEZOIDAL METHOD
C
      GO TO 180
CCC
C
C
C     THIS IS THE FASTER INTEGRATION METHOD.  IT IS VERY SIMILAR TO ONE
C     OF THE SEGMENTS OF THE RUNGE-KUTTA INTEGRATION.  IT USES A SIMPLER
C     FINITE DIFFERENCE METHOD TO EVALUATE THE CONCENTRATIONS IN THE
C     MIXERS.  ALL OTHER CALCULATIONS ARE DONE IN THE SAME WAY AS FOR
C     THE RUNGE-KUTTA INTEGRATION
C
CCC
  150 MCK=0
  160 MDEX=0
      CALL UCOR
      DO 170 I=1,NSOLU
      IF(ISOL(I).EQ.0) GO TO 170
      DVOLS=AQVOL+DTRY(I)*ORVOL
      DFLOS=AT(J)+DTRY(I)*OT(J)
      X(I,J,2)=(AQVOL*X(I,J,1)+ORVOL*Y(I,J,1)+DTHETA*(AIN(I)+OIN(I)-
     .      (AT(J)*X(I,J,1)+OT(J)*Y(I,J,1))/2.))/(DVOLS+DTHETA*DFLOS/2.)
      Y(I,J,2)=X(I,J,2)*DTRY(I)
      IF(ABS(X(I,J,2)).LT.1.E-09) GO TO 165
      DIF=ABS((X(I,J,2)-ARY(I))/X(I,J,2))
      IF(DIF.GE.CCD) MDEX=1
  165 ARY(I)=X(I,J,2)
  170 CONTINUE
      MCK=MCK+1
      IF(MDEX.EQ.1.AND.MCK.LE.20) GO TO 160
C
  180 FACTA=0.0
      FACTO=0.0
      IF(IRXN.EQ.0) GO TO 185
C
C
C  SUBROUTINE MCHEM DEALS WITH ANY CHEMICAL REACTIONS OCCURING IN THE MIXERS.
C
      CALL MCHEM(J,AQVOL,ORVOL)
  185 CONTINUE
C
C
```

```
      IF(AQSVOL.GT.0.0)  FACTA=1.5*AT(J)*DTHETA/AQSVOL
      IF(ORSVOL.GT.0.0)  FACTO=1.5*OT(J)*DTHETA/ORSVOL
      ATS(J,1,2)=ATS(J,1,1)+FACTA*(TPROF(J,2)+TPROF(J,1)-ATS(J,1,1))
      ATS(J,1,2)=ATS(J,1,2)/(1.+FACTA)
      OTS(J,1,2)=OTS(J,1,1)+FACTO*(TPROF(J,2)+TPROF(J,1)-OTS(J,1,1))
      OTS(J,1,2)=OTS(J,1,2)/(1.+FACTO)
      DO 200 I=1,NSOLU
      IF(ISOL(I).EQ.0)  GO TO 200
      CNGINV=0.0
      IF(X(I,J,2)+Y(I,J,2).GT.1.0E-6)  CNGINV=(AVOL(J)*(X(I,J,2)-X(I,J,1)
     .)+OVOL(J)*(Y(I,J,2)-Y(I,J,1)))/(DTHETA*(AVOL(J)*X(I,J,2)+OVOL(J)*
     .Y(I,J,2)))
      CNGINV=100*ABS(CNGINV)
      CODUM(J)=AMAX1(CODUM(J),CNGINV)
      XS(J,1,I,2)=(XS(J,1,I,1)+FACTA*(X(I,J,2)+X(I,J,1)-XS(J,1,I,1)))/
     .      (1.+FACTA)
      YS(J,1,I,2)=(YS(J,1,I,1)+FACTO*(Y(I,J,2)+Y(I,J,1)-YS(J,1,I,1)))/
     .      (1.+FACTO)
  200 CONTINUE
      DO 300 KZ=2,3
      KZB=KZ-1
      ATS(J,KZ,2)=(ATS(J,KZ,1)+FACTA*(ATS(J,KZB,2)+ATS(J,KZB,1)-
     .      ATS(J,KZ,1)))/(1.+FACTA)
      OTS(J,KZ,2)=(OTS(J,KZ,1)+FACTO*(OTS(J,KZB,2)+OTS(J,KZB,1)-
     .      OTS(J,KZ,1)))/(1.+FACTO)
      DO 300 I=1,NSOLU
      XS(J,KZ,I,2)=(XS(J,KZ,I,1)+FACTA*(XS(J,KZB,I,2)+XS(J,KZB,I,1)-
     .      XS(J,KZ,I,1)))/(1.+FACTA)
      YS(J,KZ,I,2)=(YS(J,KZ,I,1)+FACTO*(YS(J,KZB,I,2)+YS(J,KZB,I,1)-
     .      YS(J,KZ,I,1)))/(1.+FACTO)
  300 CONTINUE
      IF(IRXN.EQ.0)  GO TO 500
C
C
C  SUBROUTINE SCHEM DEALS WITH ANY CHEMICAL REACTIONS OCCURING IN THE
C  SETTLERS.  THESE REACTIONS ARE SIMPLER SINCE NO PHASE TRANSFER IS
C  POSSIBLE.
C
      CALL SCHEM(J,AQSVOL,ORSVOL)
C
C
  500 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE UCOR
      COMMON/CONTRL/ NTOST,NSOLU,CTBP,NEWIN,NEWOUT,SPH,IPNCH,IFAST,IRXN,
     .  DTHETA,IVOLM,IVOLS,IPRO,TEMPI,ISOL(6),NSTR,ISTR,JSTR,CODUM(100)
      COMMON/DISTRB/ TEMPC,ARY(6),DTRY(6)
C
C
C  UCOR RETURNS A VALUE OF THE DISTRIBUTION COEFFICIENT = Y/X FOR EACH
C    VALUE OF X TRIED
C
      PUTOT=ARY(3)+ARY(4)
      F=CTBP
      HAM = ARY(1)
      UAM = ARY(2)
      PUAM = ARY(3)
      SNITR = ARY(6)
      IF(UAM.LT.0) UAM = 0.
      IF(PUAM.LT.0) PUAM = 0.
      IF(HAM.LT.0) HAM = 0.
      IF(SNITR.LT.0) SNITR = 0.
      PUIII = PUTOT - PUAM
      IF(PUIII.LT.0) PUIII = 0.
      TNM = HAM + 2.*UAM + 2.*PUAM + SNITR  + 4.*PUIII
      IF (TNM.EQ.0.0) TNM = 1.0
      TEMPRK = 1000./(TEMPC + 273.16)
      DRT = TEMPRK - 3.3539
      UK = 3.7*TNM**1.57 + 1.4*TNM**3.9 + 0.011*TNM**7.3
      UK = UK*(4.*F**(-0.17) - 3.)
      PUK = UK*(.20 + .55*F**1.25 + .0074*TNM**2)
      HK1 = 0.135*TNM**0.82 + 0.0052*TNM**3.44
      IF (F.LT.1.) HK1 = HK1*(1. - 0.54*EXP(-15.*F))
      IF (TEMPC.NE.25.) UK = UK*EXP(2.5*DRT)
      IF (TEMPC.NE.25.) PUK = PUK*EXP(-.2*DRT)
      IF (TEMPC.NE.25.) HK1 = HK1*EXP(0.34*DRT)
      HK2 = HK1
      A = 2.*(UK*UAM + PUK*PUAM + HK2*HAM)
      B = HK1*HAM + 1.
      C=-3.65145*CTBP
      IF(A.GE.1.E-6) GO TO 10
      TP=-C/B
      GO TO 15
 10   CONTINUE
      TP = (-B + SQRT(B**2 -4.*A*C))/(2.*A)
 15   CONTINUE
      DH1 = HK1*TP
      DH2 = HK2*TP**2
      DH = DH1 + DH2
      DU = UK*TP**2
      DPU = PUK*TP**2
      DTRY(1) = DH
      DTRY(2) = DU
      DTRY(3) = DPU
      DTRY(4)=0.0
      DTRY(5)=0.0
      DTRY(6)=0.0
 20   RETURN
      END
```

```
      SUBROUTINE MCHEM (J,AQVOL,ORVOL)
C
C
C  SUBROUTINE MCHEM HANDLES THE CHEMICAL REACTIONS IN THE SYSTEM.  PRESENTLY,
C  INSTANTANEOUS REDUCTION OF PLUTONIUM, REDUCTION BY U(IV), AND REDUCTION
C  BY HYDROXYLAMINE ARE AVAILABLE AS REACTIONS.  THE SUBROUTINE CAN EASILY
C  BE ADAPTED TO CONSIDER ANY INTEGRATED RATE EQUATION, WITH ANY DESIRED
C  STOICHIOMETRY.
C  THE SUBROUTINE ASSUMES THE REACTION IS TOTALLY IN THE AQUEOUS PHASE, BUT
C  THAT THE SOLUTE IN THE ORGANIC PHASE ALSO AIDS IN MAINTAINING THE
C  AQUEOUS CONCENTRATION.  THE INTEGRATED RATE EQUATION DETERMINES THE
C  EXTENT OF REACTION.  THE ROUTINE THEN SPLITS THE RESULTING SOLUTES
C  BETWEEN THE PHASES.
C
C  IRXN INDICATES WHICH REACTION RATE IS TO BE USED.
C  SOLAMT IS THE TOTAL AMOUNT OF SOLUTE IN THE MIXER
C  SOLVOL IS A PSEUDO-VOLUME SO THAT THE SOLUTE IS ENTIRELY IN THE AQUEOUS PHASE
C  RX IS THE AQUEOUS COMPOSITION USED TO DETERMINE THE REACTION RATE
C  RXNAMT IS THE AMOUNT OF REACTED SOLUTE USING SOME COMPONENT AS A BASIS
C  RK IS A REACTION RATE CONSTANT
C  EXTENT = THE EXTENT OF REACTION, BASED ON THE FRACTION OF
C           SOME COMPONENT CONSUMED BY THE REACTION.
C
C
      COMMON/CONTRL/ NTOST,NSOLU,CTBP,NEWIN,NEWOUT,SPH,IPNCH,IFAST,IRXN,
     .  DTHETA,IVOLM,IVOLS,IPRO,TEMPI,ISOL(6),NSTR,ISTR,JSTR,CODUM(100)
      COMMON/CONCS/ X(6,100,2),Y(6,100,2),XS(100,3,6,2),YS(100,3,6,2)
      COMMON/DISTRB/ TEMPC,ARY(6),DTRY(6)
      COMMON/TEMPS/ TPROF(100,2),ATS(100,3,2),OTS(100,3,2)
      DIMENSION RX(6),SOLAMT(6),SOLVOL(6)
      REAL STOIC(6,3)/0.0,0.0,-1.0,1.0,-1.0,0.0,
     .                2.0,0.5,-1.0,1.0,-0.5,0.0,
     .                2.0,0.0,-1.0,1.0,-1.0,0.0/
      IF(ISOL(5).EQ.0) GO TO 300
      DO 10 I=1,6
      SOLAMT(I)=AQVOL*X(I,J,2)+ORVOL*Y(I,J,2)
      SOLVOL(I)=AQVOL+DTRY(I)*ORVOL
      RX(I)=X(I,J,2)
   10 CONTINUE
      GO TO (90,80,70,60,50,40,30,20),IRXN
   20 CONTINUE
   30 CONTINUE
   40 CONTINUE
   50 CONTINUE
   60 CONTINUE
      GO TO 90
   70 CONTINUE
C
C
C  IRXN = 3  REACTION BETWEEN PU(IV) AND HYDROXYLAMINE
C     FOR = RATIO OF PU(IV) TO REDUCTANT
C     RK = RATE CONSTANT
C     EXTMAX = MAXIMUM EXTENT OF REACTION (BASED ON PU (IV))
C     EXTINC = INCREMENT IN SEARCH FOR EXTENT
C     AMTINT = THE INTEGRATED CHANGE IN EXTENT (EQUAL TO RK)
C
      IF(RX(1).LT.1.0E-10.OR.RX(3).LT.1.0E-10.OR.RX(5).LT.1.0E-10)
     .     GO TO 90
      FOR=SOLAMT(3)/SOLAMT(5)
      TOTNIT=RX(1)+2.*RX(2)+4.*RX(3)+3.*RX(4)+RX(6)+0.33
      RK=1.74*EXP(31000./1.987*(1.0/303.16-1.0/(273.16+TPROF(J,2))))
      RK=RK*RX(3)*DTHETA*(RX(5)/(RX(1)*RX(1)*TOTNIT))**2.0
      EXTMAX=AMIN1(1.0,1.0/FOR)
C
C
C     THIS IS A BINARY SEARCH FOR THE CORRECT EXTENT OF REACTION
C
      EXTINC=0.25*EXTMAX
      EXTENT=0.5*EXTMAX
      B=SOLAMT(3)/SOLVOL(4)
      A=RX(4)+B
      AA=A*A
      BB=A*B
      CC=B*B
      DO 78 I=1,10
      A=1.0/(1.0-EXTENT)
      IF(FOR.GT.0.01) GO TO 72
C
C
C     THIS INTEGRATED FORM ASSUMES A LARGE EXCESS OF THE REDUCTANT
C
      AMTINT=AA*A*EXTENT-2.0*BB*ALOG(A)+CC*EXTENT
      GO TO 76
   72 IF(ABS(1.0-FOR).LT.0.01) GO TO 74
C
C
C     THIS INTEGRATED RATE EQUATION IS THE GENERAL CASE
C
      B=1.0-FOR*EXTENT
      C=1.0/(1.0-FOR)
      AMTINT=(FOR-A*EXTENT-FOR/B+2.0*C*FOR*ALOG(A*B))*AA*C*C
      AMTINT=AMTINT-2.0*BB*C*(FOR*EXTENT/B-C*ALOG(A*B))-CC*EXTENT/B
      AMTINT=-AMTINT
      GO TO 76
```

```
C
C
C     THIS INTEGRATED FORM ASSUMES A STOICHIOMETRIC AMOUNT OF REDUCTANT
C
   74 AMTINT=AA*(A*A*A-1.0)/3.0-BB*(A*A-1.0)+CC*(A-1.0)
   76 CONTINUE
      IF(AMTINT.GT.RK) EXTENT=EXTENT-EXTINC
      IF(AMTINT.LT.RK) EXTENT=EXTENT+EXTINC
      EXTINC=EXTINC/2.0
   78 CONTINUE
      RXNAMT=EXTENT*SOLAMT(3)
      GO TO 100
   80 CONTINUE
C
C
C  IRXN = 2  REACTION BETWEEN PU (IV) AND U (IV)
C     RK = RATE CONSTANT
C     RCU = RATIO OF PU (IV) TO REDUCTANT
C     EXTMAX = MAXIMUM EXTENT BASED ON PU (IV) AND A TEN SECOND HALF TIME
C
      IF(RX(3).LT.1.0E-10.OR.RX(5).LT.1.0E-10) GO TO 90
      EXTMAX=AMIN1(1.0,1.0-0.5**(6.0*DTHETA),2.0*SOLAMT(5)/SOLAMT(3))
      RK=170.0
      RK=RK*DTHETA*RX(5)
      RCU=SOLAMT(3)/(2.0*SOLAMT(5))
      RHO=RX(1)*RX(1)
      REXP=1.0E40
      IF(RK*(1.0-RCU).LT.100.0*RHO) REXP=EXP(RK*(1.0-RCU)/RHO)
      EXTENT=RK/(RK+RHO)
      IF(ABS(1.0-RCU).GT.0.05) EXTENT=(1.0-REXP)/(RCU-REXP)
      EXTENT=AMIN1(EXTENT,EXTMAX)
      RXNAMT=SOLAMT(3)*EXTENT
      GO TO 100
   90 CONTINUE
C
C
C  IRXN = 1  INSTATANEOUS REDUCTION OF PU (IV)
C     THIS MECHANISM IS USED BY ALL REDUCTION REACTIONS WHEN THE
C     CONCENTRATIONS FALL BELOW A THRESHHOLD LEVEL
C
      RXNAMT=AMIN1(-SOLAMT(3)/STOIC(3,IRXN),-SOLAMT(5)/STOIC(5,IRXN))
  100 DO 110 I=1,6
      SOLAMT(I)=SOLAMT(I)+RXNAMT*STOIC(I,IRXN)
      IF(SOLAMT(I).LT.0.0) SOLAMT(I)=0.0
      ARY(I)=SOLAMT(I)/SOLVOL(I)
      IF(SOLAMT(I).NE.0.0) ISOL(I)=1
      IF(ISOL(I).EQ.1.AND.NSOLU.LT.I) NSOLU=I
  110 CONTINUE
C
C
C  DIVIDING THE RESULTING SOLUTES BETWEEN THE PHASES
C
      DO 125 ITRY=1,5
      ICK=0
      CALL UCOR
      DO 120 I=1,NSOLU
      X(I,J,2)=SOLAMT(I)/(AQVOL+DTRY(I)*ORVOL)
      IF(ABS(X(I,J,2)-ARY(I)).GT.0.0001*X(I,J,2)) ICK=1
      ARY(I)=X(I,J,2)
      IF(X(I,J,2).LE.1.E-20) X(I,J,2)=0.0
      Y(I,J,2)=X(I,J,2)*DTRY(I)
  120 CONTINUE
      IF(ICK.EQ.0) GO TO 130
  125 CONTINUE
  130 CONTINUE
  300 RETURN
      END
```

```
      SUBROUTINE SCHEM(J,AQSVOL,ORSVOL)
C
C
C  SUBROUTINE SCHEM WORKS SIMILAR TO MCHEM, BUT THE PHASES ARE KEPT SEPARATE
C  AT ALL TIMES.
C
C  IRXN INDICATES WHICH REACTION RATE IS TO BE USED.
C  RK IS A REACTION RATE CONSTANT
C  EXTENT = THE EXTENT OF REACTION, BASED ON THE FRACTION OF
C           SOME COMPONENT CONSUMED BY THE REACTION.
C
C
C
      COMMON/CONTRL/ NTOST,NSOLU,CTBP,NEWIN,NEWOUT,SPH,IPNCH,IFAST,IRXN,
     . DTHETA,IVOLM,IVOLS,IPRO,TEMPI,ISOL(6),NSTR,ISTR,JSTR,CODUM(100)
      COMMON/CONCS/ X(6,100,2),Y(6,100,2),XS(100,3,6,2),YS(100,3,6,2)
      COMMON/TEMPS/ TPROF(100,2),ATS(100,3,2),OTS(100,3,2)
      REAL STCICX(6,3)/0.0,0.0,-1.0,1.0,-1.0,0.0,
                       2.0,0.5,-1.0,1.0,-0.5,0.0,
                       2.0,0.0,-1.0,1.0,-1.0,0.0/
      REAL STOICY(6,3)/0.0,0.0,0.0,0.0,0.0,0.0,12*0.0/
      DIMENSION RX(6),RY(6)
      IF(ISOL(5).EQ.0) GO TO 300
      DO 150 KZ=1,3
      DO 10 I=1,6
      RX(I)=XS(J,KZ,I,2)
      RY(I)=YS(J,KZ,I,2)
   10 CONTINUE
      GO TO (90,80,70,60,50,40,30,20),IRXN
   20 CONTINUE
   30 CONTINUE
   40 CONTINUE
   50 CONTINUE
   60 CONTINUE
      GO TO 90
   70 CONTINUE
C
C
C  IRXN = 3  REACTION BETWEEN PU(IV) AND HYDROXYLAMINE
C     FOR = RATIO OF PU(IV) TO REDUCTANT
C     RK = RATE CONSTANT
C     EXTMAX = MAXIMUM EXTENT OF REACTION (BASED ON PU (IV))
C     EXTINC = INCREMENT IN SEARCH FOR EXTENT
C     AMTINT = THE INTEGRATED CHANGE IN EXTENT (EQUAL TO RK)
C
      IF(RX(1).LT.1.0E-10.OR.RX(3).LT.1.0E-10.OR.RX(5).LT.1.0E-10)
           GO TO 90
      FOR=RX(3)/RX(5)
      TOTNIT=RX(1)+2.*RX(2)+4.*RX(3)+3.*RX(4)+RX(6)+0.33
      RK=1.74*EXP(31000./1.987*(1.0/303.16-1.0/(273.16+TPROF(J,2))))
      RK=RK*RX(3)*DTHETA*(RX(5)/(RX(1)*RX(1)*TOTNIT))**2.0
      EXTMAX=AMIN1(1.0,1.0/FOR)
C
C
C     THIS IS A BINARY SEARCH FOR THE CORRECT EXTENT OF REACTION
C
      EXTINC=0.25*EXTMAX
      EXTENT=0.5*EXTMAX
      B=RX(3)
      A=RX(4)+B
      AA=A*A
      BB=A*B
      CC=B*B
      DO 78 I=1,10
      A=1.0/(1.0-EXTENT)
      IF(FOR.GT.0.01) GO TO 72
      AMTINT=AA*A*EXTENT-2.0*BB*ALOG(A)+CC*EXTENT
      GO TO 76
   72 IF(ABS(1.0-FOR).LT.0.01) GO TO 74
      B=1.0-FOR*EXTENT
      C=1.0/(1.0-FOR)
      AMTINT=(FOR-A*EXTENT-FOR/B+2.0*C*FOR*ALOG(A*B))*AA*C*C
      AMTINT=AMTINT-2.0*BB*C*(FOR*EXTENT/B-C*ALOG(A*B))-CC*EXTENT/B
      AMTINT=-AMTINT
      GO TO 76
   74 AMTINT=AA*(A*A*A-1.0)/3.0-BB*(A*A-1.0)+CC*(A-1.0)
   76 CONTINUE
      IF(AMTINT.GT.RK) EXTENT=EXTENT-EXTINC
      IF(AMTINT.LT.RK) EXTENT=EXTENT+EXTINC
      EXTINC=EXTINC/2.0
   78 CONTINUE
      DELTAX=RX(3)*EXTENT
      DELTAY=0.0
      GO TO 100
```

```
   80 CONTINUE
C
C
C  IRXN = 2  REACTION BETWEEN PU (IV) AND U (IV)
C     RK = RATE CONSTANT
C     RCU = RATIO OF PU (IV) TO REDUCTANT
C     EXTMAX = MAXIMUM EXTENT BASED ON PU (IV) AND A TEN SECOND HALF TIME
C
      IF(RX(3).LT.1.0E-10.OR.RX(5).LT.1.0E-10) GO TO 90
      EXTMAX=AMIN1(1.0,1.0-0.5**(6.0*DTHETA),2.0*RX(5)/RX(3))
      RK=170.0
      RK=RK*DTHETA*RX(5)
      RCU=RX(3)/(2.0*RX(5))
      RHO=RX(1)*RX(1)
      REXP=1.0E40
      IF(RK*(1.0-RCU).LT.100.0*RHO) REXP=EXP(RK*(1.0-RCU)/RHO)
      EXTENT=RK/(RK+RHO)
      IF(ABS(1.0-RCU).GT.0.05) EXTENT=(1.0-REXP)/(RCU-REXP)
      EXTENT=AMIN1(EXTENT,EXTMAX)
      DELTAX=RX(3)*EXTENT
      DELTAY=0.0
      GO TO 100
   90 CONTINUE
C
C
C  IRXN = 1  INSTATANEOUS REDUCTION OF PU (IV)
C     THIS MECHANISM IS USED BY ALL REDUCTION REACTIONS WHEN THE
C     CONCENTRATIONS FALL BELOW A THRESHHOLD LEVEL
C
      DELTAX=AMIN1(-RX(3)/STOICX(3,IRXN),-RX(5)/STOICX(5,IRXN))
      DELTAY=0.0
  100 CONTINUE
      DO 105 I=1,6
      XS(J,KZ,I,2)=XS(J,KZ,I,2)+STOICX(I,IRXN)*DELTAX
      YS(J,KZ,I,2)=YS(J,KZ,I,2)+STOICY(I,IRXN)*DELTAY
      IF(XS(J,KZ,I,2).LE.1.E-20) XS(J,KZ,I,2)=0.0
      IF(YS(J,KZ,I,2).LE.1.E-20) YS(J,KZ,I,2)=0.0
      IF(XS(J,KZ,I,2).NE.0.0) ISOL(I)=1
      IF(YS(J,KZ,I,2).NE.0.0) ISOL(I)=1
      IF(ISOL(I).EQ.1.AND.NSOLU.LT.I) NSOLU=I
  105 CONTINUE
  150 CONTINUE
  300 RETURN
      END
```

```
      SUBROUTINE PRTOUT
C
C
C  PRTOUT CONVERTS THE CONCENTRATIONS FROM THE MOLAL FORM USED BY THE PROGRAM
C  TO THE MORE COMMON UNITS IN THE OUTPUT.  IN ORDER TO GET THE PROPER
C  HEADINGS FOR THE PUREX SYSTEM, THE SUBPROGRAM ALSO PRINTS THE PROFILES.
C
      COMMON/CONTRL/ NTOST,NSOLU,CTBP,NEWIN,NEWOUT,SPH,IPNCH,IFAST,IRXN,
     .  DTHETA,IVOLM,IVOLS,IPRO,TEMPI,ISOL(6),NSTR,ISTR,JSTR,CODUM(100)
      COMMON/CONCS/ X(6,100,2),Y(6,100,2),XS(100,3,6,2),YS(100,3,6,2)
      COMMON/FLOWS/ A(100),O(100),AT(100),OT(100)
      COMMON/MOLALC/ AQ(6),OR(6),TEMP,CONVA,CONVO,TCONC
      COMMON/STREAM/ XFD(6,100),YFD(6,100),AFDRT(100),OFDRT(100),
     .   AFDTEM(100),OFDTEM(100),ALVRT(100),OLVRT(100)
      COMMON/TEMPS/ TPROF(100,2),ATS(100,3,2),OTS(100,3,2)
      DIMENSION AOUT(100),OOUT(100)
      TCONC=1.0
      PRINT 1101
      PRINT 1102
      PRINT 1103
      PRINT 1104
      DO 20 J=1,NTOST
      DO 10 I=1,NSOLU
      AQ(I)=X(I,J,2)
      OR(I)=Y(I,J,2)
   10 CONTINUE
      TEMP=TPROF(J,2)
      CALL MOLAL
      ADEN=(1000.-72.4*AQ(2)-130.*(AQ(3)+AQ(4))-30.9*AQ(1)-31.*AQ(6))/
     .      (1000./0.99707)+0.39404*AQ(2)+0.49202*(AQ(3)+AQ(4))
     .      +0.06301*AQ(1)+0.213*AQ(6)
      AOUT(J)=AT(J)*CONVA
      OOUT(J)=OT(J)*CONVO
      DO 15 I=1,NSOLU
      X(I,J,2)=AQ(I)/CONVA
      Y(I,J,2)=OR(I)/CONVO
   15 CONTINUE
      X(2,J,2)=X(2,J,2)*238.
      Y(2,J,2)=Y(2,J,2)*238.
      X(3,J,2)=X(3,J,2)*239.
      Y(3,J,2)=Y(3,J,2)*239.
      X(4,J,2)=X(4,J,2)*239.
      Y(4,J,2)=Y(4,J,2)*239.
      PRINT 1000,J,(X(I,J,2),I=1,6),ADEN,AOUT(J),TPROF(J,2)
      IF(ALVRT(J).EQ.0.0) GO TO 20
      CONVA=CONVA*ALVRT(J)
      PRINT 1001,J,CONVA
   20 CONTINUE
      PRINT 1105
      PRINT 1106
      PRINT 1107
      PRINT 1104
      DO 30 J=1,NTOST
      EXH=0.0
      EXU=0.0
      EXPU=0.0
      IF(AOUT(J).LE.0.0) GO TO 25
      EXH=OOUT(J)/AOUT(J)
      IF(X(2,J,2).GT.0.0) EXU=EXH*Y(2,J,2)/X(2,J,2)
      IF(X(3,J,2)+X(4,J,2).GT.0.0) EXPU=EXH*(Y(3,J,2)+Y(4,J,2))/
     .      (X(3,J,2)+X(4,J,2))
      IF(X(1,J,2).GT.0.0) EXH=EXH*Y(1,J,2)/X(1,J,2)
      IF(X(1,J,2).LE.0.0) EXH=0.0
   25 CONTINUE
      ODEN=(1000.-17.4*0.29-97.*Y(2,J,1)-139.*(Y(3,J,1)+Y(4,J,1))
     .      -43.*Y(1,J,1))*(1.0+1.8)/((273.6/266.32+227.5/170.34*1.8)
     .      *1000.)+0.01802*.29+.39404*Y(2,J,1)+.49202*(Y(3,J,1)
     .      +Y(4,J,1))+.06301*Y(1,J,1)
      PRINT 1000,J,(Y(I,J,2),I=1,3),EXU,EXPU,EXH,ODEN,OOUT(J),CODUM(J)
      IF(OLVRT(J).EQ.0.0) GO TO 30
      CONVO=OLVRT(J)*OOUT(J)/OT(J)
      PRINT 1001,J,CONVO
   30 CONTINUE
      RETURN
 1000 FORMAT(12X,I3,1X,9('| ',1PE10.3,1X))
 1001 FORMAT(12X,I3,' | PRODUCT STREAM ',74X,'| ',1PE10.3,' |')
 1101 FORMAT(5X,'AQUEOUS PHASE')
 1102 FORMAT(10X,'STAGE | NITRIC ACID|  URANIUM   |  PU (IV)   |  PU (II
     .I)  | REDUCTANT  | NITRATE ION|  DENSITY   | MIXER FLOW |TEMPERATU
     .RE')
 1103 FORMAT(11X,'NO.  |   (MOL/L)  |   (G/L)    |   (G/L)    |   (G/L)
     .   |  (MOL/L)   |  (MOL/L)   |   (G/ML)   |  (L/MIN)   |(CENTIGRAD
     .E)')
 1104 FORMAT(16X,9('|',12X))
 1105 FORMAT('0    ORGANIC PHASE')
 1106 FORMAT(10X,'STAGE | NITRIC ACID|  URANIUM   |  PU(IV)    |U EXTRAC
     .TION| PU EXTRACT |HNO3 EXTRACT|  DENSITY   | FLOW RATE  | INVENTOR
     .Y')
 1107 FORMAT(10X,' NO.  |  (MOL/L)   |   (G/L)    |   (G/L)    |   FACTO
     .R   |   FACTOR   |   FACTOR   |   (G/ML)   |  (L/MIN)   | CHANGE (
     .%) ')
      END
```

APPENDIX B. TABLE OF NOMENCLATURE

Variables

A	Aqueous flow rate (liters/min)
D	Distribution coefficient
K	Pseudo mass equilibrium constant
K'	Pseudo mass equilibrium constant
K_d	Dissociation constant for $PuNO_3^{3+}$
k'	Reaction rate constant
O	Organic flow rate (liters/min)
t	Time (min)
V	Volume (liters)
x	Aqueous-phase solute concentration
y	Organic-phase solute concentration
τ	Residence time

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

ORNL-5471
Dist. Category UC-79c

Internal Distribution

1. C. W. Alexander
2-6. M. Anthony
7. J. E. Bigelow
8. W. D. Burch
9. E. D. Collins
10. D. J. Crouse
11. W. S. Groenier
12. R. T. Jubin
13. F. A. Kappelmann
14. L. J. King
15. C. E. Lamb
16. R. E. Leuze
17-21. A. P. Malinauskas
22. B. F. Maskewitz
23-32. A. D. Mitchell
33-37. R. H. Rainey
38. F. M. Scheitlin
39. D. P. Stevens
40. D. W. Tedder
41. V. C. A. Vaughen
42. B. L. Vondra
43. S. B. Watson
44. M. E. Whatley
45. R. G. Wymer
46-47. Central Research Library
48-52. Laboratory Records
53. Laboratory Records, R.C.
54. ORNL Y-12 Technical Library Document Reference Section
55. ORNL Patent Section

External Distribution

56. Director, Nuclear Research and Development Division, DOE-ORO, P. O. Box E, Oak Ridge, TN 37830
57-58. Director, Division of Nuclear Power Development, DOE, Washington, D.C. 20545
59-60. Director, Division of Reactor Research and Technology, DOE, Washington, D.C. 20545
61. Manson Benedict, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139
62. G. E. Bennedict, General Atomic Corporation, P. O. Box 81608, San Diego, CA 92138
63. J. E. Bennett, ECE Department, Clemson University, Clemson, SC 29631
64. M. L. Bleiberg, Westinghouse Electric Corporation, Advanced Reactors Division, Waltz Mill Site, P. O. Box 158, Madison, PA 15663
65. D. E. Clayton, Battelle Pacific Northwest Laboratory, P. O. Box 999, Richland, WA 99352
66. Casey Durst, Allied Chemical Corporation, 550 Second Street, Idaho Falls, ID 83401
67. Dennis Engler, General Atomic Corporation, P. O. Box 81608, San Diego, CA 92138
68. Martin Freidland, Gulf and Western Advanced Development and Engineering Center, 101 Chester Road, Swarthmore, PA 19081
69. F. J. Jones, Bechtel Corporation, P. O. Box 3965, San Francisco, CA 94119
70. B. F. Judson, Vice-President and Manager, GEUMCO-Engineering, 175 Curtner Avenue, Mail Code 858, San Jose, CA 95125
71. R. S. Karinen, Programmed and Remote Systems Corporation, 3640 Lexington Avenue, St. Paul, MN 55112

72. R. H. Karlsson, Rockwell International, Atomics International Division, Rocky Flats Plant, P. O. Box 464, Golden, CO 80401
73. Ralph Leonard, Argonne National Laboratory, Building 205, 9700 South Cass Avenue, Argonne, IL 60439
74. R. E. Mullen, Aerojet Manufacturing Company, 601 South Placentia Avenue, P. O. Box 4210, Fullerton, CA 92634
75. L. A. Neimark, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439
76. G. L. Richardson, Hanford Engineering Development Laboratory, P. O. Box 1970, Richland, WA 99352
77. Alfred Schneider, School of Nuclear Engineering, Georgia Institute of Technology, Atlanta, GA 30332
78. Major Thompson, Savannah River Laboratory, Aiken, SC 29801
79. D. E. Wood, Kaman Sciences Corporation, 1500 Garden of the Gods Road, P. O. Box 7463, Colorado Springs, CO 80933
80. Office of Assistant Manager, Energy Research and Development, DOE-ORO, P. O. Box E, Oak Ridge, TN 37830

81-321. Given distribution as shown in TID-4500 under UC-79c, Fuel Recycle Category (Applied)