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Technical Manual for SEPHIS MOD4, Version 2.11

W. S. Groenier

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MARTIN MARIETTA ENERGY SYSTEMS, INC.
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

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TECHNICAL MANUAL FOR SEPHIS MOD4, VERSION 2.11

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Robotics & Process Systems Division

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NOTICE This document contains information of a preliminary nature. It is subject to revision or correction and therefore does not represent a final report.

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ABSTRACT

SEPHIS MOD4, Version 2.11, is a significantly improved and enhanced version of the SEPHIS MOD4 calculational model for stagewise Purex and Thorex solvent extraction systems. Version 2.11 is especially suited for the casual user. All operations are carried out on a personal computer and extensive help features are included, enabling anyone familiar with liquid-liquid solvent extraction processes and personal computer operation to quickly become adept in applying the model to data analysis, flow sheet development, process monitoring, off-normal operational analysis, and studies of process response to changing inputs. This manual provides a detailed description of the conceptual and mathematical basis of the model and presents the programming logic. A listing of the code in BASIC language is included.

1. INTRODUCTION

The first computer-based calculational model for Solvent Extraction Processes Having Interacting Solutes (SEPHIS) was developed for the Purex process and published in 1972.[1] It was specific for a dilute Purex process as applied to Liquid Metal Fast Breeder Reactor (LMFBR) fuels and considered only a single extractant concentration and temperature. Many improvements to the model were made in succeeding years up to 1986. These improvements (1) incorporated new mass distribution data, (2) allowed the use of various extractant concentrations and temperatures, (3) included the effects of inextractable nitrate salts, and (4) permitted modeling of the chemical reduction of plutonium. Expansion of the model to include the Thorex process also occurred during this time path.

Significant structural changes to the model were made. The most important of these permitted calculations to be performed on a solute-free basis rather than a molar basis and improved the accuracy of modeling changing (transient) conditions. All of these modifications culminated in a version called SEPHIS MOD4. Some additional details of the model evolution are provided in the SEPHIS User's Manual.[2]

The new Version 2.11 of SEPHIS MOD4 provides additional enhancements. One of the most important is the adaptation to a personal computer and extensive user-oriented aids. Other improvements include an additional numerical integration technique, incorporation of additional mass distribution data, a better model for describing the reduction of Pu(IV) by hydroxylamine nitrate (HAN), and corrections to the estimation of solution densities.

This manual provides a complete description of the model, including the programming logic. It is intended as a companion document to the SEPHIS User's Manual.[2]

2. CONCEPTUAL AND MATHEMATICAL BASES

The chemical components considered by SEPHIS MOD4, Version 2.11, for the Purex process include nitric acid, uranium, plutonium (IV), plutonium (III), a plutonium reductant, and inextractable nitrate salts. For the Thorex process the components are nitric acid, uranium, thorium, and inextractable nitrate salts. Tri-*n*-butyl phosphate (TBP) is the organic-phase extracting agent for both systems. The organic-phase diluent is assumed to be *n*-dodecane (NDD) or an equivalent kerosene-based substance.

2.1 STAGE MODEL

The idealized stage model shown in Fig. 1 is used in the SEPHIS MOD4, Version 2.11, calculational model. Mixer-settler solvent extraction contactors are arranged in a countercurrent array. In a given stage (j), aqueous and organic streams from adjacent stages (A_{j-1} and O_{j+1}) and/or feed streams ($A_{f,j}$ and $O_{f,j}$) are well mixed in the mixer section with any liquid inventory in the mixer where all mass transfer between the phases takes place. An equilibrium contact is assumed (i.e., a perfect mixer). The mixed-phase stream then flows to a settler that consists of three tanks (zones) in series. In Fig. 1, the aqueous and organic portions of the settler are shown separately. These three zones are of equal volume and serve as liquid holdup regions between mixers. No additional mass transfer between the phases occurs in the settler zones, and the contents of each phase in each zone are assumed to be homogeneous. Aqueous and organic streams leaving the third settler zone proceed to adjacent stages (A_j and O_j) or are withdrawn as products ($A_{p,j}$ and $O_{p,j}$). Feed streams can be admitted to any stage and product streams can be withdrawn from any stage. A special routing provision is that the entire organic stream can be withdrawn from one stage and fed to any other stage.

2.2 CALCULATIONAL METHOD

The flow of solutes through the model is described by differential equations. Empirical correlations are used to distribute solutes between phases (Sect. 2.3), convert concentration units (Sect. 2.4), account for water extracted into the organic phase (Sect. 2.4), and model chemical (reductant) reactions (Sect. 2.6).

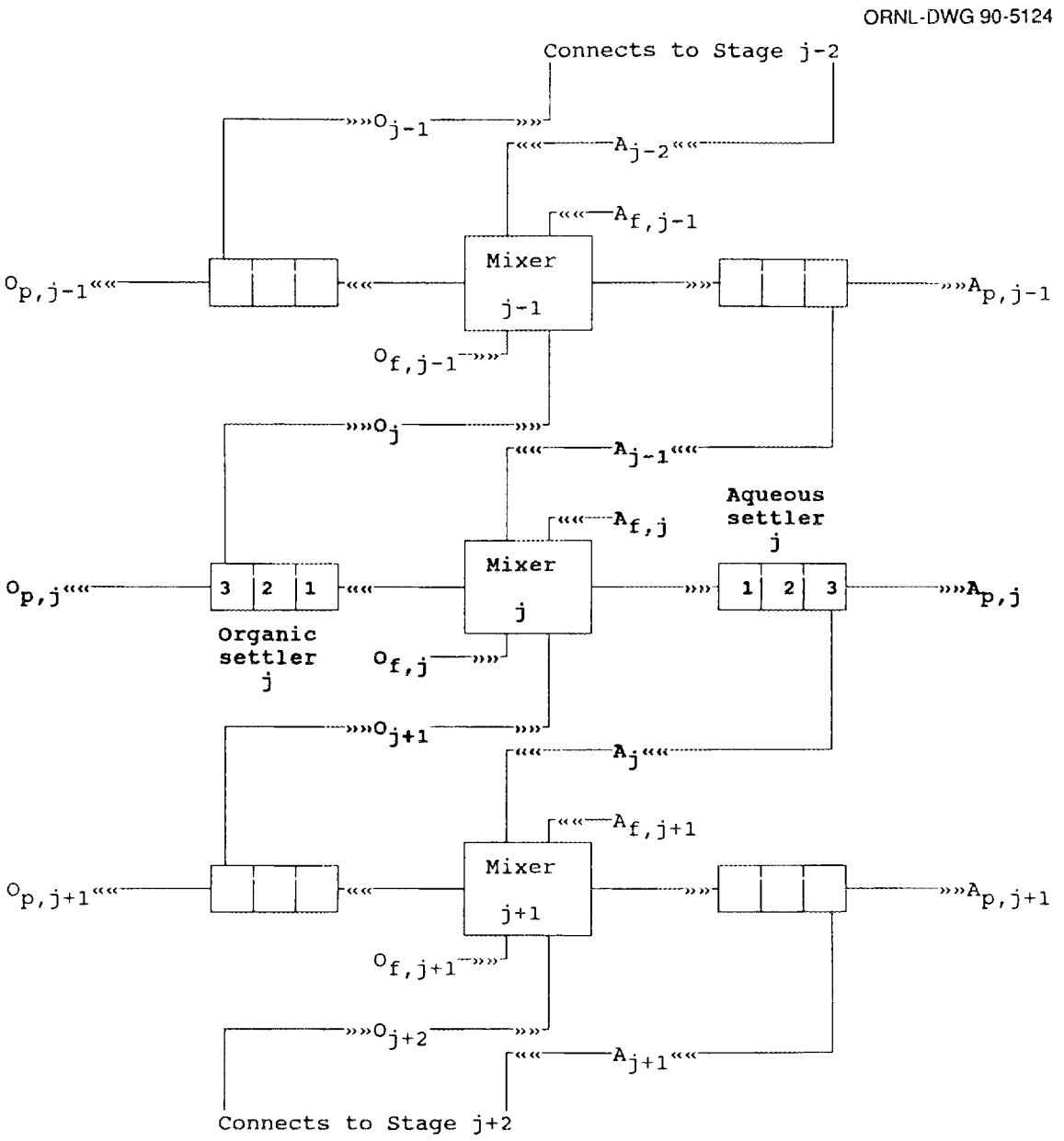


Fig. 1. Idealized mixer-settler stage model.

2.2.1 Mixers

Differential equations are used to describe the unsteady-state mass balances for the mixers of each stage. By referring to Fig. 1 and using x_i and y_i to represent concentrations of component i on a solute-free basis in the aqueous and organic phase, respectively, and using V_{maj} and V_{moj} to represent the aqueous and organic volumes in the mixer of stage j, the differential expression for an increment of time (t) is:

$$\frac{d\left[V_{maj}\, x_{i,j} + V_{moj}\, y_{i,j}\right]}{dt} = A_{j-1}\, x_{i,j-1} + O_{j+1}\, y_{i,j+1}$$

$$+ A_{f,j}\, x_{f,i,j} + O_{f,j}\, y_{f,i,j}$$

$$- (A_j + A_{p,j})\, x_{i,j} - (O_j + O_{p,j})\, y_{i,j} \quad . \tag{1}$$

For the time increment, volumes and flow rates are assumed to be constant. In addition, the solutes in the mixer are assumed to be distributed between the phases in an equilibrium ratio defined by the distribution coefficient (D_i) as follows:

$$D_i = y_{i,j} \,/\, x_{i,j} \quad . \tag{2}$$

Substitution of these simplifications in Eq. (1) yields:

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

$$- [A_j + A_{p,j} + (O_j + O_{p,j})\, D_i]\, x_{i,j}\Big] \,/\, [V_{maj} + D_i\, V_{moj}] \quad . \tag{3}$$

For the time increment, the only terms in Eq. (3) that vary are $x_{i,j}$, D_i, $x_{i,j-1}$, and $y_{i,j+1}$. Numerical integration techniques are used to determine the value of $x_{i,j}$. The value of D_i is based on the value of $x_{i,j}$ discussed in Sect. 2.3. By assuming that the remaining variables $x_{i,j-1}$ and $y_{i,j+1}$ change by only a small amount over the time increment, reasonable choices for the value of these variables can be made.

Three numerical integration techniques are available in the code for performing these calculations. Accurate modeling of transient conditions depends on the choice of the size of the time increment and on the numerical technique. The user should specify for integrations a time increment that is no more than 25% of the mean stage solution residence time if accurate results for transient conditions are needed. If only the steady-state solution is needed, a time increment of 1 min is usually satisfactory.

The three numerical integration techniques that may be specified for mixer calculations are (1) Runge-Kutta, generally the most accurate (except when chemical reduction of plutonium is occurring), (2) Trapezoidal, which will provide accurate steady-state results and consume somewhat less computer time than the Runge-Kutta technique for the same specified time increment for integrations but is not recommended for transient results, and (3) Fast, which may produce a plutonium reduction profile

that differs somewhat from profiles generated by other techniques. In the Fast technique, plutonium is reduced more slowly because of the set of concentrations used to calculate the reduction rate. When plutonium reduction is occurring, however, this is the only recommended technique for transient results.

The Fast technique will consume more computer time than the Trapezoidal for the same specified time increment for integrations but, in most cases, it is capable of handling relatively large time increments (10 min), thereby producing steady-state results very rapidly. Use the information in Table 1 as a guide when choosing the integration technique.

Table 1. Choice of numerical integration technique

	Steady-state results		Transient results	
Integration technique	No Pu reduction	Pu reduction	No Pu reduction	Pu reduction
Runge-Kutta	1*	N	R	N
Trapezoidal	R	R	N	N
Fast	1	1,2	R	R

*1 = Optional (generally consumes more computer time)
2 = Optional (plutonium profile may be in error)
R = Recommended
N = Not recommended

An iterative procedure is used as just described for each component and for every stage of the solvent extraction cascade for a given time increment. It is then repeated for the next time increment. The cascade is scanned in the opposite direction in successive time increments to offset any bias in the assumed values for $x_{i,j-1}$ and $y_{i,j+1}$ of Eq. (3). An exception is the Fast technique that scans the cascade in both directions during each time increment. Calculations continue for as many time increments as necessary to achieve the steady-state condition defined by the user, until manually stopped by the user, or until a maximum defined time limit is reached.

2.2.2 Settlers

Since no mass transfer between the phases occurs in the settler zones, calculations merely propagate the mixer concentrations through the settlers. Thus, a time delay is added between adjacent stage mixers. Differential equations to describe the unsteady-state mass balances for the settlers are formulated in the same manner as for the mixers but must consider that each settler is subdivided for each phase into three equal-volume, perfectly mixed zones. By referring again to Fig. 1 and using V_{saj} to represent the aqueous volume in the settler of stage j, the mass balance for component i in zone k of stage j is:

$$\frac{V_{saj}}{3}\frac{dx_{i,j,k}}{dt} = A_{s,j}\ (x_{i,j,k-1} - x_{i,j,k}) \quad , \tag{4}$$

where $A_{s,j}$ is the aqueous flow rate through the settler. A similar equation may be written for the organic phase. The equations are expressed in simple finite difference form and solved by the use of the Trapezoidal technique.

2.3 DISTRIBUTION COEFFICIENT CORRELATIONS

The distribution coefficients that appear in Eq. (3) are calculated by using correlations based on aqueous-phase concentrations and developed from laboratory equilibrium data.[3-8]

2.3.1 Purex Process Equilibrium Data Correlation

The following chemical reactions are assumed to apply to Purex process extractions:

$$UO_2^{2+} + 2\ NO_3^- + 2\ TBP = UO_2(NO_3)_2 \cdot TBP \quad , \tag{5}$$

$$Pu^{4+} + 4\ NO_3^- + 2\ TBP = Pu(NO_3)_4 \cdot 2TBP \quad , \tag{6}$$

$$H^+ + NO_3^- + TBP = HNO_3 \cdot TBP \quad , \tag{7}$$

$$H^+ + NO_3^- + 2TBP = HNO_3 \cdot 2TBP \quad . \tag{8}$$

Pseudo-mass-action equilibrium expressions (having embedded activity coefficient ratios) for these reactions are:

$$K'_U = \frac{[UO_2(NO_3)_2 \cdot 2TBP]}{[UO_2^{2+}]\ [NO_3^-]^2\ [TBP]^2} \quad , \tag{9}$$

$$K'_P = \frac{[Pu(NO_3)_4 \cdot 2TBP]}{[Pu^4]\ [NO_3^-]^4\ [TBP]^2} \quad , \tag{10}$$

$$K'_{H1} = \frac{[HNO_3 \cdot TBP]}{[H^+]\ [NO_3^-]\ [TBP]} \quad , \tag{11}$$

$$K'_{H2} = \frac{[HNO_3 \cdot 2TBP]}{[H^+]\ [NO_3^-]\ [TBP]^2} \quad , \tag{12}$$

where brackets [] represent molar concentrations. These are used to define the following parameters:

$$K_U = \frac{[UO_2(NO_3)_2 \cdot 2TBP]}{[UO_2^{2+}]\ [TBP]^2} = K'_U\ [NO_3^-]^2 \quad , \tag{13}$$

$$K_P = \frac{[Pu(NO_3)_4 \cdot 2TBP]}{[Pu^{4+}]\ [TBP]^2} = K'_P\ [NO_3^-]^4 \quad , \tag{14}$$

$$K_{H1} = \frac{[HNO_3 \cdot TBP]}{[H^+]\ [TBP]} = K'_{H1}\ [NO_3^-] \quad , \tag{15}$$

$$K_{H2} = \frac{[HNO_3 \cdot 2TBP]}{[H^+]\ [TBP]^2} = K'_{H2}\ [NO_3^-] \quad . \tag{16}$$

Empirical equilibrium expressions for uranium and nitric acid were derived at 100% TBP and 25°C as follows:

$$K_U^* = 3.7\ n^{1.57} + 1.4\ n^{3.9} + 0.011\ n^{7.3} \quad , \tag{17}$$

$$K_{H1}^* = 0.135\ n^{0.82} + 0.0052\ n^{3.44} \quad , \tag{18}$$

$$K_{H2}^* = K_{H1}^* \quad , \tag{19}$$

where n is the total nitrate ion concentration expressed as:

$$n = h + 2\ u + 2\ pu + 4\ pu_3 + s \quad . \tag{20}$$

The other variables are described as follows:

h = nitric acid concentration,

u = uranium concentration,

pu = plutonium(IV) concentration,

pu_3 = plutonium(III) concentration,

s = inextractable nitrate concentration.

The empirical equilibrium expression for plutonium was determined to be a function of the uranium constant as follows:

$$K_P^* = K_U^* \ (0.20 + 0.55\ F^{1.25} + 0.0074\ n^2) \quad , \tag{21}$$

where F is the TBP concentration expressed as a volume fraction.

Development of the conversion factor for TBP concentration between volume fraction and molarity follows. If T = moles of TBP per liter of organic solution (Molarity, *M*) and F = liters of TBP per liter of organic solution (volume fraction), then:

$$T = (1000\ F \rho\ )\ /\ M \quad , \tag{22}$$

where ρ is the TBP density and M is the TBP molecular weight. Since ρ = 0.9725 g/cm^3 and M = 266.3 g/mol [based on the formula $(C_4H_9)_3PO_4$],

$$T = [(1000)\ (0.9725)\ /\ 266.3]\ F = 3.65145\ F \quad . \tag{23}$$

Adjustment factors for TBP concentrations and temperatures differing from 100% and 25°C are:

$$K_U = K_U^* \ (4\ F^{-0.17} - 3)\ e^{2500\tau} \quad , \tag{24}$$

$$K_P = K_P^* \ (4\ F^{-0.17} - 3)\ e^{-200\tau} \quad , \tag{25}$$

$$K_{H1} = K_{H2} = K_{H1}^* \ (1.0 - 0.54\ e^{-15F})\ e^{340\tau} \quad , \tag{26}$$

where

$$\tau = [1\ /\ (t + 273.16)] - [1\ /\ 298.16] \quad , \tag{27}$$

and t is the temperature in °C.

Distribution coefficients are defined as:

$$D_U = \frac{[UO_2(NO_3)_2 \cdot 2TBP]}{[UO_2^{2+}]} = K_U\ [TBP]^2 \quad , \tag{28}$$

$$D_P = \frac{[Pu(NO_3)_4 \cdot 2TBP]}{[Pu^{4+}]} = K_P\ [TBP]^2 \quad , \tag{29}$$

$$D_{H1} = \frac{[HNO_3 \cdot TBP]}{[H^+]} = K_{H1}\ [TBP] \quad , \tag{30}$$

$$D_{H2} = \frac{[HNO_3 \cdot 2TBP]}{[H^+]} = K_{H2} \; [TBP]^2 \quad . \tag{31}$$

The uncomplexed, or free TBP concentration, is:

$$\begin{aligned} [TBP] = {} & [TBP]_o - 2 \; [UO_2(NO_3)_2 \cdot 2TBP] \\ & - 2 \; [Pu(NO_3)_4 \cdot 2TBP] - [HNO_3 \cdot TBP] \\ & - 2 \; [HNO_3 \cdot 2TBP] \quad , \end{aligned} \tag{32}$$

where $[TBP]_o$ is the original molar concentration of TBP.
Substitute Eqs. (28) through (31) in Eq. (32).

$$\begin{aligned} [TBP] = {} & [TBP]_o - 2 \; K_U \; [UO_2^{2+}] \; [TBP]^2 \\ & - 2 \; K_P \; [Pu^{4+}] \; [TBP]^2 - K_{H1} \; [H^+] \; [TBP] \\ & - 2 \; K_{H2} \; [H^+] \; [TBP]^2 \quad . \end{aligned} \tag{33}$$

For simplification, the following variable substitutions are made:

$$U = [UO_2^{2+}] \qquad H = [H^+]$$

$$P = [Pu^{4+}] \qquad T = [TBP]$$

By rearranging:

$$2 \; T^2 \left[K_U \; U + K_P \; P + K_{H2} \; H\right] + T \left[1 + K_{H1} \; H\right] = T_o \quad , \tag{34}$$

which is of the form:

$$a \; x^2 + b \; x + c = 0 \quad ,$$

where

$$x = T, \qquad b = 1 + K_{H1}H,$$

$$a = 2[K_uU + K_pP + K_{H2}H], \qquad c = -T_0.$$

Since the solution for x is $[-b + (b^2 - 4 \; a \; c)^{0.5}] \; / \; (2 \; a)$:

$$T = \frac{-(1 + K_{H1} H) + \left[(1 + K_{H1} H)^2 + 8 T_o (K_U U + K_P P + K_{H2} H)\right]^{0.5}}{4 (K_U U + K_P P + K_{H2} H)} . \quad (35)$$

If expressed on a solute-free basis, volume changes can be neglected. Only the positive root of Eq. (35) is used because negative values of T result from the negative root.

The method for determining distribution coefficients is as follows:

1. Assume solute-free concentration values for U, P, and H.
2. Calculate K^* values from Eqs. (17), (18), (19), and (21).
3. Calculate K values from Eqs. (24), (25), and (26).
4. Solve for T in Eq. (35).
5. Substitute values in Eqs. (28) through (31) where the D values are on a solute-free basis.

This mathematical development is the basis for the SEPHIS MOD3[9] model. Consideration of a larger body of equilibrium data for the SEPHIS MOD4 model led to the improvements shown in the equations that follow. Although not rigorous from a theoretical perspective, the equations offer an improved fit to the larger body of data. Many of the coefficients presented previously were modified:

Eq. 20: $$n = h + 2 u + 2 pu + 2 pu_3 + s , \quad (36)$$

Eq. 17: $$K_U^* = 1.130 \left[3.7 n^{1.57} + 1.4 n^{3.9} + 0.011 n^{7.3}\right] , \quad (37)$$

Eq. 21: $$K_P^* = K_U^* \left[0.135 + 0.122113 (F / 0.3)^{0.746} - 3.91 F + 0.010 n^2\right] , \quad (38)$$

Eq. 25: $$K_P = K_P^* \left[4 F^{-0.17} - 3\right] e^{-800 \tau} . \quad (39)$$

Consequently, the following method is used in SEPHIS MOD4, Version 2.11, for determining distribution coefficients. Calculate the total nitrate using Eq. (36). Make the following conversion:

Eq. 27: $$1000 \tau = [1000 / (t + 273.16)] - 3.3539 = T' . \quad (40)$$

Substitute Eq. (37) in Eq. (24):

$$K_U = \left[3.7\ n^{1.57} + 1.4\ n^{3.9} + 0.011\ n^{7.3}\right] \left[4F^{-0.17} - 3\right] (1.130)\ e^{2.5\ T'} \quad . \tag{41}$$

Substitute Eq. (38) in Eq. (39):

$$K_P = K_U^* \left[0.135 + 0.122113\ (F / 0.3)^{0.746} - 3.91\ F + 0.010\ n^2\right]\left[4\ F^{-0.17} - 3\right] e^{-0.8\ T'} \quad . \tag{42}$$

Substitute Eqs. (18) and (19) into Eq. (26):

$$K_{H1} = K_{H2} = \left[0.135\ n^{0.82} + 0.0052\ n^{3.44}\right] \left[1.0 - 0.54\ e^{-15\ F}\right] e^{0.34\ T'} \quad . \tag{43}$$

Solve for the quadratic equation coefficients:

$$a = 2\ (K_U\ U + K_P\ P + K_{H2}\ U) \quad , \tag{44}$$

$$b = 1 + K_{H1}\ H \quad , \tag{45}$$

$$c = -\ T_o \quad . \tag{46}$$

Substitute Eqs. (44) through (46) in Eq. (35):

$$T = [-b + (b^2 - 4\ a\ c)^{0.5}] / (2\ a) \quad . \tag{47}$$

Then use the result from Eq. (47) in Eqs. (28) through (31):

$$D_U = K_U\ T^2 \quad , \tag{48}$$

$$D_P = K_P\ T^2 \quad , \tag{49}$$

$$D_{H1} = K_{H1}\ T \quad , \tag{50}$$

$$D_{H2} = K_{H2}\ T^2 \quad , \tag{51}$$

$$D_H = D_{H1} + D_{H2} \quad . \tag{52}$$

For a very dilute system where the variable, a, in Eq. (44) is $<10^{-6}$, the only nitric acid-TBP complex considered is $HNO_3 \cdot TBP$. For this case:

$$T = T_o - K_{H1}\ H\ T \quad , \tag{53}$$

$$T\ (1 + K_{H1}\ H) = T_o \quad , \tag{54}$$

$$T = T_o\ /\ (1 + K_{H1}\ H) \text{ or } -c\ /\ b \quad . \tag{55}$$

Extensive tabular listings and three-dimensional graphs of Purex distribution coefficients are reported in ref. 6.

2.3.2 Thorex Process Equilibrium Data Correlation

The following chemical reactions are assumed to apply to Thorex process extractions:

$$Th^{4+} + 4\ NO_3^- + 3\ TBP = Th(NO_3)_4 \cdot 3TBP \quad , \tag{56}$$

$$UO_2^{2+} + 2\ NO_3^- + 2\ TBP = UO_2(NO_3)_2 \cdot 2TBP \quad , \tag{57}$$

$$H^+ + NO_3^- + TBP = HNO_3 \cdot TBP \quad . \tag{58}$$

Pseudo-mass-action equilibrium expressions (having embedded activity coefficient ratios) for these reactions are:

$$K'_{Th} = \frac{[Th(NO_3)_4 \cdot 3TBP]}{[Th^{4+}]\ [NO_3^-]^4\ [TBP]^3} \quad , \tag{59}$$

$$K'_U = \frac{[UO_2(NO_3)_2 \cdot 2TBP]}{[UO_2^{2+}]\ [NO_3^-]^2\ [TBP]^2} \quad , \tag{60}$$

$$K'_H = \frac{[HNO_3 \cdot TBP]}{[H^+]\ [NO_3^-]\ [TBP]} \quad , \tag{61}$$

where brackets [] represent molar concentrations. These equilibrium constants have been correlated at 25°C with the ionic strength, z:

$$z = [H^+] + 3\ [UO_2^{2+}] + 10\ [Th^{4+}] \quad . \tag{62}$$

The correlations are:

$$K'_{Th} = C_1 + C_2\ z + C_3\ z^2 + C_4\ z^3 \quad , \tag{63}$$

$$K'_U = C_5 + C_6\ z + C_7\ z^2 + C_8\ z^3 \quad , \tag{64}$$

$$K'_H = C_9 + C_{10}\ z + C_{11}\ z^2 + C_{12}\ z^3 \quad . \tag{65}$$

where C_1 through C_{12} are empirical coefficients. A cubic equation is solved for TBP, noting that distribution coefficients are defined as follows:

$$D_{Th} = \frac{[Th(NO_3)_4 \cdot 3TBP]}{[Th^{4+}]} = K'_{Th}\ [NO_3^-]^4\ [TBP]^3 \quad , \tag{66}$$

$$D_U = \frac{[UO_2(NO_3)_2 \cdot 2TBP]}{[UO_2^{2+}]} = K'_U\ [NO_3^-]^2\ [TBP]^2 \quad , \tag{67}$$

$$D_H = \frac{[HNO_3 \cdot TBP]}{[H^+]} = K'_H\ [NO_3^-]\ [TBP] \quad . \tag{68}$$

The uncomplexed, or free TBP concentration, is:

$$[TBP] = [TBP]_o - 3\ [Th(NO_3)_4 \cdot 3TBP] - 2\ [UO_2(NO_3)_2 \cdot 2TBP] - [HNO_3 \cdot TBP] \quad , \tag{69}$$

where $[TBP]_o$ is the original molar concentration of TBP. Substitute Eqs. (66) through (68) in Eq. (69):

$$[TBP] = [TBP]_o - 3\left[K'_{Th}\ [Th^{4+}]\ [NO_3^-]^4\ [TBP]^3\right] - 2\left[K'_U\ [UO_2^{2+}]\ [NO_3^-]^2\ [TBP]^2\right] - K'_H\ [H^+]\ [NO_3^-]\ [TBP] \quad . \tag{70}$$

For simplification, the following variable substitutions are made:

$U = [UO_2^{2+}]$ $\qquad$ $R = [Th^{4+}]$

$H = [H^+]$ $\qquad$ $T = [TBP]$

$N = [NO_3^-]$

$$T^3\ [3\ K'_{Th}\ R\ N^4] + T^2\ [2\ K'_U\ U\ N^2] + T\ [1 + K'_H\ H\ N] - T_o = 0 \quad . \tag{71}$$

This is of the form: $a\ x^3 + b\ x^2 + c\ x + d = 0$,

where

$x = T,$

$a = 3\ K'_{Th}\ R\ N^4,$

$b = 2\ K'_U\ U\ N^2,$

$c = 1 + K'_H\ H\ N,$

$d = -\ T_o.$

The N terms are total nitrate, defined as:

$$N = 4\ R + 2\ U + H \quad . \tag{72}$$

A finite difference method is used to solve the cubic equation. Adjustments for temperatures other than 25°C are made as follows. Let:

$$\tau = [1 / (t + 273.16)] - [1 / 298.16] \quad , \tag{73}$$

where t is the temperature in °C. Let D′ be the distribution coefficients at 25°C:

$$D_H = D'_H\ e^{-818.802\ \tau} \quad , \tag{74}$$

$$D_U = D'_U\ e^{2500\ \tau} \quad , \tag{75}$$

$$D_{Th} = D'_{Th}\ e^{C\ \tau} \quad , \tag{76}$$

$$C = 891.664 + 879.688\ R - 1474.38\ R^2 \quad . \tag{77}$$

A check for third-phase formation is when $[Th^{4+}]$ is greater than the value of the following expression, where T is the temperature in °C and H is $[H^+]$:

$$[0.04311727 - 0.00003317647\ (T - 55.03183)^2 + 0.36719\ (H - 0.3455787)^2]^{0.5}$$

2.4 CONCENTRATION UNIT CONVERSIONS

The SEPHIS MOD4, Version 2.11, computational model performs calculations on a solute-free basis so that variations in volumetric flow rates and phase volumes from changes in solute concentration can be ignored. Molar concentrations are defined as moles of solute per unit volume of solution. Molal concentrations are usually defined as moles of solute per unit mass of solvent. The volume of a solution varies with solute concentration and with temperature. Since the mass of solvent remains constant, stagewise calculations are simplified by using molal units. Feed and product stream data, however, are usually given in molar units.

Molal concentrations may also be expressed as moles of solute per unit volume of solute-free solvent. Use of this alternate definition does not introduce a significant error since contactor temperature variations over a single time increment are very small. For the purposes of this report, the alternate molal basis is described as the solute-free basis.

The relationship between solute-free (m) and molar (*M*) units is as follows:

$$\frac{m}{M} = \frac{\text{moles of solute/L of solvent}}{\text{moles of solute/L of solution}} = \frac{\text{L of solution}}{\text{L of solvent}}$$

and the conversion between units may be calculated from (1) solution density, solvent density, and solute concentrations or (2) solute molecular volumes and solute concentrations. An equation to convert molar to solute-free units in terms of solution and solvent densities is as follows:

$$m = \frac{M \rho_z}{\rho_{soln} - \sum_{x=1}^{n} M_x \, mw_x / 1000} , \tag{78}$$

where

ρ_{soln} = the density of the solution,

ρ_z = the density of the solvent,

M_x and mw_x = the molarities and molecular weights of the solutes, respectively.

Conversely, the conversion from solute-free to molar units is:

$$M = \frac{m \, \rho_{soln}}{\rho_z + \sum_{x=1}^{n} m_x \, mw_x / 1000} , \tag{79}$$

where the m_x values are solute concentrations on a solute-free basis.

Similar equations may be obtained in terms of molecular volumes as follows:

$$m = \frac{M}{1.0 - \sum_{x=1}^{n} V_x M_x} , \tag{80}$$

$$M = \frac{m}{1.0 + \sum_{x=1}^{n} V_x \, m_x} , \tag{81}$$

where the V_x values are the molecular volumes of the solutes. The molecular volumes used in SEPHIS MOD4, Version 2.11, are listed in Table 2.

Table 2. Molecular volumes used in SEPHIS MOD4, Version 2.11

Substance	Molecular volume (mL/mol)* Aqueous phase	Organic phase
$UO_2(NO_3)_2$	72.4	97.0
$Pu(NO_3)_4$	130.0	139.0
HNO_3	30.9	43.0
Other NO_3^-	31.0	—
H_2O	—	17.4
TBP	—	273.6
NDD	—	227.5

*From ref. 10, temperature = 25°C.

Substitution of the appropriate values from Table 2 into Eq. (80) will yield a conversion factor for units conversion. For the aqueous phase of the Purex process:

$$\frac{m_a}{M_a} = \frac{1.0}{1.0 - 0.0724\ U_a - 0.13\ Pu_a - 0.0309\ H_a - 0.031\ S_a} , \tag{82}$$

where U, Pu, H, and S are molarities of uranium, plutonium, nitric acid, and inextractable nitrate salts, respectively. By letting u, pu, h, and s represent solute-free basis concentrations, Eq. (81) becomes:

$$\frac{m_a}{M_a} = 1.0 + 0.0724\ u_a + 0.13\ pu_a + 0.0309\ h_a + 0.031\ s_a . \tag{83}$$

For the organic phase of the Purex process:

$$\frac{m_o}{M_o} = \frac{1.0}{1.0 - 0.097\ U_o - 0.139\ Pu_o - 0.043\ H_o - 0.0174\ W_o} , \tag{84}$$

where W is the water concentration in the organic phase. By using solute-free concentrations:

$$\frac{m_o}{M_o} = 1.0 + 0.097\ u_o + 0.139\ pu_o + 0.043\ h_o + 0.0174\ w_o . \tag{85}$$

Since the molecular volume data are at 25°C (see Table 2), the unit conversion equations are not exact for temperatures very different from 25°C.

The values for W_o and w_o are calculated as follows:[9]

$$W_o = (3.95 - 0.0144\ t)\left[1.0 - \frac{U_o}{U_{os}} - \frac{Pu_o}{Pu_{os}} - \frac{0.65\ H_o}{H_{os}}\right] F^{1.65} \quad , \tag{86}$$

$$w_o = (4.2 - 0.015\ t)\left[1.0 - \frac{2\ u_o}{T} - \frac{2\ pu_o}{T} - \frac{0.6\ h_o}{T}\right] F^{1.69} \quad , \tag{87}$$

where the subscripts, os, refer to molar concentrations required to saturate the organic phase. The value of T is the molarity of TBP in the organic phase defined by Eq. (22), F is the volume fraction of TBP in the organic phase, and t is the temperature in °C. Saturation values are defined as follows:[9]

$$U_{os} = \frac{0.5\ T}{1.0 + 0.046\ T} \quad , \tag{88}$$

$$Pu_{os} = \frac{0.5\ T}{1.0 + 0.09\ T} \quad , \tag{89}$$

$$H_{os} = \frac{T\ [1.0 - 0.00609\ (3.95 - 0.0144\ t)\ F^{1.65}]}{1.0 - 0.043\ T} \quad . \tag{90}$$

For the Thorex process, no concentration unit conversions have been developed. Consequently, the SEPHIS MOD4, Version 2.11, model assumes that molar and solute-free basis concentrations are identical for this process.

2.5 DENSITY DATA CORRELATION

The final hard-copy printout of results from SEPHIS MOD4, Version 2.11, calculations for the Purex process includes estimates for aqueous- and organic-phase densities in each stage of the contactor. These are calculated by combining Eqs. (79) and (81):

$$\rho_{soln} = \frac{\rho_z + \sum_{x=1}^{n} m_x\ mw_x\ /\ 1000}{1.0 + \sum_{x=1}^{n} V_x\ m_x} \quad . \tag{91}$$

Since the molecular volume data are at 25°C (see Table 2), the resulting solution density values are only valid at 25°C. Based on Eq. (91), aqueous-phase solution densities are estimated as follows:

$$\rho_a = \frac{0.99707 + 0.39404\ u_a + 0.49202\ pu_a + 0.06301\ h_a + 0.2131\ s_a}{1.0 + 0.0724\ u_a + 0.13\ pu_a + 0.0309\ h_a + 0.031\ s_a} , \quad (92)$$

where $\rho_z = 0.99707$, the density of water at 25°C. Organic-phase solution densities are estimated as follows:

$$\rho_o = \frac{\rho_{zo} + 0.01802\ w_o + 0.3904\ u_o + 0.49202\ pu_o + 0.06301\ h_o}{1.0 + 0.0174\ w_o + 0.097\ u_o + 0.139\ pu_o + 0.043\ h_o} , \quad (93)$$

where w_o is as defined by Eq. (87), ρ_{zo} is

$$\rho_{zo} = \frac{mw_{TBP}}{V_{TBP}} F + \frac{mw_{NDD}}{V_{NDD}} (1 - F) \quad (94)$$

and F is the volume fraction of TBP in the organic phase.

Solution density data are not estimated for the Thorex process.

2.6 CHEMICAL REDUCTION OF PLUTONIUM (Pu)

In the Purex process, the reduction of plutonium (IV) to plutonium (III) can be modeled by SEPHIS MOD4, Version 2.11, as an instantaneous reduction, reduction by uranium (IV), or reduction by HAN. The chemical reactions are assumed to occur entirely within the aqueous phase. They may occur in the mixer, in the aqueous portion of the settler zones, or both, depending on the time constant of the reaction and the relative quantities of reactants.

2.6.1 Instantaneous Reduction of Pu(IV)

The assumed reaction is:

$$Pu^{4+} + \text{Reductant} = Pu^{3+} \quad . \quad (95)$$

Of the initial solute quantities ($SOLAMT_{1,i}$), if W is the quantity of Pu(IV) present and WW is the quantity of reductant present, then the amount of Pu(IV) reduced (RXNAMT) will be the smaller of W or WW. The solute amounts after reaction ($SOLAMT_{2,i}$) will be as follows:

$$SOLAMT_{2,i} = SOLAMT_{1,i} + (RXNAMT)\ (STOIC_i) \quad . \quad (96)$$

For HNO_3,	$i = 1$, $STOIC_1 = 0$		For Pu(III),	$i = 4$, $STOIC_4 = +1$
U,	$i = 2$, $STOIC_2 = 0$		Reductant,	$i = 5$, $STOIC_5 = -1$
Pu(IV),	$i = 3$, $STOIC_3 = -1$		Nitrate,	$i = 6$, $STOIC_6 = 0$

2.6.2 Reduction of Pu(IV) by U(IV)

The assumed reaction is

$$2\ Pu^{4+} + U^{4+} + 2\ H_2O = 2\ Pu^{3+} + UO_2^{2+} + 4\ H^+ \quad , \tag{97}$$

with the following rate equation:

$$-d[Pu(IV)]\ /\ dt = k'\ [U(IV)]\ [Pu(IV)]\ /\ [HNO_3]^2 \quad , \tag{98}$$

where the rate constant (k′) is 170 *M*/min. The nitric acid concentration is assumed to be constant. Therefore,

$$-\frac{d[Pu(IV)]}{[Pu(IV)]} = \frac{170}{[HNO_3]^2}\ [U(IV)]\ dt \quad . \tag{99}$$

The extent of reaction (E) is defined as follows:

$$E = \frac{[Pu(IV)]_1 - [Pu(IV)]_2}{[Pu(IV)]_1} \quad , \tag{100}$$

where the subscripts 1 and 2 refer to the concentrations at the beginning and end of a time increment, respectively. From Eq. (100),

$$[Pu(IV)]_2 = [Pu(IV)]_1\ (1 - E) \quad . \tag{101}$$

The maximum extent of reaction (E_{max}) is limited by the amount of reductant present, by a reaction half-time of 10 s, or by the amount of Pu(IV) present.

From stoichiometry, the maximum extent limited by reductant is:

$$E_{max} = 2\ [U(IV)]_1\ /\ [Pu(IV)]_1 \quad . \tag{102}$$

From the 10-s half-time, the maximum extent is:

$$E_{max} = 1.0 - 0.5^{6t} \quad , \tag{103}$$

where t is time in minutes. If the quantity of Pu(IV) is limiting:

$$E_{max} = 1.0 \quad . \tag{104}$$

Case I - Stoichiometric Ratio of Reactants

For a stoichiometric ratio of reactants:

$$[U(IV)] = [Pu(IV)] / 2 \quad . \tag{105}$$

This condition remains throughout the time increment. Substitute Eq. (105) in Eq. (99) and form the integral.

$$-\frac{d[Pu(IV)]}{[Pu(IV)]} = \frac{170}{[HNO_3]^2} \frac{[Pu(IV)]}{2} (1 - E)\, dt \quad , \tag{106}$$

$$-\int_{[Pu(IV)]_1}^{[Pu(IV)]_2} \frac{d[Pu(IV)]}{[Pu(IV)]^2} = \frac{170}{2\,[HNO_3]^2} \int_{t_1}^{t_2} dt \quad . \tag{107}$$

By integrating:

$$\frac{1}{[Pu(IV)]_2} - \frac{1}{[Pu(IV)]_1} = \frac{170}{2\,[HNO_3]^2} (t_2 - t_1) \quad , \tag{108}$$

or

$$\frac{[Pu(IV)]_1 - [Pu(IV)]_2}{[Pu(IV)]_1\,[Pu(IV)]_2} = \frac{170}{2\,[HNO_3]^2} (t_2 - t_1) \quad . \tag{109}$$

Substitute Eqs. (100) and (101) in Eq. (109):

$$\frac{E}{[Pu(IV)]_1\,(1 - E)} = \frac{170}{2\,[HNO_3]^2} (t_2 - t_1) \quad . \tag{110}$$

Substitute Eq. (105) in Eq. (110) and solve for E:

$$\frac{E}{1 - E} = \frac{170}{[HNO_3]^2} [U(IV)]_1\,(t_2 - t_1) \quad , \tag{111}$$

$$E = \frac{170\,[U(IV)]_1\,(t_2 - t_1)}{170\,[U(IV)]_1\,(t_2 - t_1) + [HNO_3]^2} \quad . \tag{112}$$

Eq. (112) is coded as Statement 3950 (MCHEMP) or as Statement 4800 (SCHMEP) in the model:

```
EXTENT = RK/(RK + RHO)
```

where RK and RHO are equivalent to 170 $[U(IV)]_1$ $(t_2 - t_1)$ and $[HNO_3]^2$.

Case II - General Solution

For reactant ratios that are not stoichiometric, the analysis begins with Eq. (99). For simplification, the following variable substitutions are made: $H = [HNO_3]$, $U = [U(IV)]$, and $P = [Pu(IV)]$. Rewriting Eq. (99):

$$-\frac{dP}{P} = \frac{170}{H^2} U \, dt \quad . \tag{113}$$

From reaction stoichiometry:

$$U_1 - U = (P_1 - P) / 2 \quad , \tag{114}$$

or

$$U = Q \, U_1 + P / 2 \quad , \tag{115}$$

where $Q = 1 - P_1 / (2 \, U_1)$. For the stoichiometric case (Case I), $Q = 0$ and $U = P / 2$. For the general case, Eq. (115) applies. By substituting Eq. (115) in Eq.(113):

$$-\frac{dP}{P} = \frac{170}{H^2} \left[Q \, U_1 + \frac{P}{2} \right] dt \quad . \tag{116}$$

By rearranging:

$$-\frac{dP}{dt} = \frac{170 \, P}{H^2} \left[Q \, U_1 + \frac{P}{2} \right] \quad , \tag{117}$$

or

$$-\frac{dP}{dt} = P \left[\frac{170 \, Q}{H^2} U_1 + \frac{170}{2 \, H^2} P \right] \quad . \tag{118}$$

Rearrange again, and form the integral.

$$\int_{P_1}^{P_2} \frac{-\,dP}{P\,[170\,Q\,U_1\,/\,H^2 + 170\,P\,/\,(2\,H^2)]} = \int_{t_1}^{t_2} dt \quad . \tag{119}$$

By integrating:

$$\frac{H^2}{170\,Q\,U_1}\left[\ln\left[\frac{170\,Q\,U_1}{P_2\,H^2} + \frac{170}{2\,H^2}\right] - \ln\left[\frac{170\,Q\,U_1}{P_1\,H^2} + \frac{170}{2\,H^2}\right]\right] = t_2 - t_1 \quad . \tag{120}$$

By rearranging:

$$\ln\left[\frac{(340\,Q\,U_1 + 170\,P_2)\,P_1}{(340\,Q\,U_1 + 170\,P_1)\,P_2}\right] = \frac{170\,Q\,U_1}{H^2}\,(t_2 - t_1) \quad . \tag{121}$$

From the definition of Q:

$$P_1 = 2\,U_1\,(1 - Q) \quad . \tag{122}$$

By substituting Eqs. (101) and (122) in Eq. (121) and reducing:

$$\ln\frac{Q + (1 - Q)\,(1 - E)}{(1 - E)} = \frac{170\,Q\,U_1}{H^2}\,(t_2 - t_1) \quad , \tag{123}$$

or

$$\ln\frac{1 - E + E\,Q}{1 - E} = \frac{170\,Q\,U_1}{H^2}\,(t_2 - t_1) \quad , \tag{124}$$

or

$$E = \frac{1 - e^{170\,Q\,U_1\,(t_2 - t_1)\,/\,H^2}}{1 - Q - e^{170\,Q\,U_1\,(t_2 - t_1)\,/\,H^2}} \quad . \tag{125}$$

Eq. (125) is coded as Statement 3960 (MCHEMP) or Statement 4810 (SCHEMP) in the model:

```
EXTENT = (1 - REXP) / (RCU - REXP)
```

where

REXP is equivalent to $e^{170\ Q\ U1\ (t2-t1)\ /\ H2}$,

RCU is equivalent to (1 - Q).

The test made in Statements 3960 or 4810 is equivalent to comparing the absolute value of Q to 0.05. For values $-0.05 < Q < +0.05$, a stoichiometric ratio of reactants is assumed. The value of EXTENT (E) is limited by E_{max}, just discussed.

The solute amounts after reaction ($SOLAMT_{2,i}$) are calculated by using Eq. (96) and the following values for $STOIC_i$:

For HNO_3,	$i = 1$, $STOIC_1 = +2$		For Pu(III),	$i = 4$, $STOIC_4 = +1$
U,	$i = 2$, $STOIC_2 = +0.5$		Reductant,	$i = 5$, $STOIC_5 = -0.5$
Pu(IV),	$i = 3$, $STOIC_3 = -1$		Nitrate,	$i = 6$, $STOIC_6 = 0$

2.6.3 Reduction of Pu(IV) by Hydroxylamine Nitrate (HAN)

The assumed reaction is

$$2\ HAN + 2\ Pu^{4+} = 2\ Pu^{3+} + N_2 + 2\ H_2O + 4\ H^+ \quad , \tag{126}$$

with the following rate equation:

$$-\frac{d[Pu(IV)]}{dt} = k' \frac{[Pu(IV)]^2\ [HAN]^2}{[Pu(III)]^2\ [H^+]^4\ (K_d + [NO_3^-])^2} \quad , \tag{127}$$

where the rate constant (k′) is 0.029 M^5/s at 30°C, and the dissociation constant (K_d) is 0.33 *M*. The activation energy is 31 kcal/*M*. Consequently, the rate constant varies with temperature (t) as follows:

$$k' = (0.029)\ (60)\ e^z \quad . \tag{128}$$

where

$$z = \frac{31000}{1.987} \left[\frac{1}{303.16} - \frac{1}{273.16 + t} \right] \quad , \tag{129}$$

and t is in °C. The extent of reaction (E) is defined from Eq. (100). The maximum extent (E_{max}) is limited by the amount of reductant or by the amount of Pu(IV) present. The maximum extent limited by reductant is:

$$E_{max} = [HAN]_1\ /\ [Pu(IV)]_1 \quad . \tag{130}$$

If the quantity of Pu(IV) is limiting:

$$E_{max} = 1.0 \quad . \tag{131}$$

Let the term F be defined based on the ratio of Pu(IV) to HAN at the beginning of a time increment as follows:

$$F = 1 - [Pu(IV)]_1 \; / \; [HAN]_1 \quad . \tag{132}$$

Assume constant acid and nitrate concentrations. For simplification, use the following variable substitutions: $H = [H^+]$, $P = [Pu(IV)]$, $S = [Pu(III)]$, $R = [HAN]$, and $N = K_d + [NO_3^-]$. Also, define K as:

$$K = k' \; / \; (H^4 \; N^2) \quad . \tag{133}$$

Rewriting Eq. (127):

$$- \frac{dP}{dt} = K \frac{P^2 \; R^2}{S^2} \quad . \tag{134}$$

From reaction stoichiometry yields:

$$R_1 - R = P_1 - P \quad , \tag{135}$$

and

$$S - S_1 = P_1 - P \quad . \tag{136}$$

Substitute Eq. (132) in Eq. (135) and rearrange:

$$R = F \; R_1 + P \quad . \tag{137}$$

Substitute Eqs. (136) and (137) in Eq. (134), then rearrange and form the integral.

$$- \frac{dP}{dt} = K \frac{P^2 \; (F \; R_1 + P)^2}{(S_1 + P_1 - P)^2} \quad , \tag{138}$$

$$- \int_{P_1}^{P_2} \frac{(S_1 + P_1 - P)^2 \; dP}{(F \; R_1 + P)^2 \; P^2} = K \int_{t_1}^{t_2} dt \quad . \tag{139}$$

Note that for a stoichiometric ratio of reactants, F = 0. Cases to be considered include the stoichiometric ratio, a large excess of HAN, and the general case.

Case I - Stoichiometric Ratio of Reactants

For a stoichiometric ratio of reactants, F = 0 and Eq. (139) becomes:

$$-\int_{P_1}^{P_2} \frac{(S_1 + P_1 - P)^2 \, dP}{P^4} = K \int_{t_1}^{t_2} dt \quad . \tag{140}$$

By integrating:

$$\frac{(S_1 + P_1)^2}{3} \left[\frac{1}{P_2^{\,3}} - \frac{1}{P_1^{\,3}}\right] - (S_1 + P_1) \left[\frac{1}{P_2^{\,2}} - \frac{1}{P_1^{\,2}}\right]$$

$$+ \frac{1}{P_2} - \frac{1}{P_1} = K \, (t_2 - t_1) \quad . \tag{141}$$

Substitute Eq. (101) in Eq. (141) and rearrange:

$$\frac{(S_1 + P_1)^2}{3} \left[\frac{1}{(1 - E)^3} - 1\right] - P_1 \, (S_1 + P_1) \left[\frac{1}{(1 - E)^2} - 1\right]$$

$$+ P_1^{\,2} \left[\frac{1}{1 - E} - 1\right] = K \, P_1^{\,3} \, (t_2 - t_1) \quad . \tag{142}$$

Since F = 0, from Eq. (132) note that $[Pu(IV)]_1 = [HAN]_1$, or $P_1 = R_1$. By making this substitution in Eq. (142):

$$\frac{(S_1 + P_1)^2}{3} \left[\frac{1}{(1 - E)^3} - 1\right] - P_1 \, (S_1 + P_1) \left[\frac{1}{(1 - E)^2} - 1\right]$$

$$+ P_1^{\,2} \left[\frac{1}{1 - E} - 1\right] = K \, P_1 \, R_1^{\,2} \, (t_2 - t_1) \quad . \tag{143}$$

In the model, Eq. (143) is coded as Statements 3790 and 3660 (MCHEMP) or Statements 4640 and 4510 (SCHEMP):

```
AMTINT = AA * (A^3 - 1) / 3 - BB * (A^2 - 1) + CC * (A - 1)

RK = (1.74 * EXP (31000 / 1.987 * (1 / 303.16 - 1 / (273.16 +
TPROF(J,2))))) * RX(3) * DTHETA * (RX(5) / (RX(1)^2 * TOTNIT))^2
```

where AMTINT is equivalent to the left-hand side of Eq. (143) and RK is equivalent to the right-hand side of Eq. (143). Other equivalencies are:

A	$= 1/(1 - E)$	RX(1)	$= H$
AA	$= (S_1 + P_1)^2$	RX(3)	$= P_1$
BB	$= P_1(S_1 + P_1)$	RX(5)	$= R_1$
CC	$= P_1^2$	TOTNIT	$= N$
DTHETA	$= t_2 - t_1$	TPROF(J,2)	= Temperature (°C)
EXTENT	$= E$		

A binary search is used to determine the value of E.

Case II - Large Excess of Hydroxylamine Nitrate (HAN)

For a large excess of HAN, R can be considered constant and Eq. (134) is:

$$-\frac{dP}{dt} = K R^2 \frac{P^2}{S^2} \quad . \tag{144}$$

By substituting Eq. (136) in Eq. (144):

$$-\frac{dP}{dt} = K R^2 \frac{P^2}{(S_1 + P_1 - P)^2} \quad . \tag{145}$$

Rearrange and form the integral:

$$-\int_{P_1}^{P_2} \frac{(S_1 + P_1 - P)^2}{P^2} dP = K R^2 \int_{t_1}^{t_2} dt \quad . \tag{146}$$

By integrating:

$$(S_1 + P_1)^2 \left[\frac{1}{P_2} - \frac{1}{P_1}\right] + 2 (S_1 + P_1) \ln \frac{P_2}{P_1} - P_2 + P_1$$

$$= K R^2 (t_2 - t_1) \quad . \tag{147}$$

Substitute Eq. (101) in Eq. (147) and rearrange:

$$\frac{(S_1 + P_1)2\ E}{1 - E} - 2\ P_1\ (S_1 + P_1)\ \ln\left[\frac{1}{1 - E}\right] + P_1^{\ 2}\ E$$

$$= K\ P_1\ R^2\ (t_2 - t_1) \quad . \tag{148}$$

In the model, Eq. (148) is coded as Statements 3730 and 3660 (MCHEMP) or Statements 4580 and 4510 (SCHEMP):

```
AMTINT = AA * A * EXTENT - 2 * BB * LOG (A) + CC * EXTENT

RK = (1.74 * EXP (31000 / 1.987 * (1 / 303.16 - 1 / (273.16 +
TPROF(J,2))))) * RX(3) * DTHETA * (RX(5) / (RX(1)^2 * TOTNIT))^2
```

where AMTINT is equivalent to the left-hand side of Eq. (148) and RK is equivalent to the right-hand side of Eq. (148). Other equivalencies are:

A	$= 1 / (1 - E)$	RX(1)	$= H$
AA	$= (S_1 + P_1)^2$	RX(3)	$= P_1$
BB	$= P_1\ (S_1 + P_1)$	RX(5)	$= R$
CC	$= P_1^{\ 2}$	TOTNIT	$= N$
DTHETA	$= t_2 - t_1$	TPROF(J,2)	= Temperature (°C)
EXTENT	$= E$		

A binary search is used to determine the value of E.

Case III - General Solution

For a general solution, the analysis begins with Eq. (139), repeated here:

$$-\int_{P_1}^{P_2} \frac{(S_1 + P_1 - P)^2\ dP}{(F\ R_1 + P)^2\ P^2} = K \int_{t_1}^{t_2} dt \quad . \tag{149}$$

Since $R_1 = P_1 / (1 - F)$:

$$-\int_{P_1}^{P_2} \frac{(S_1 + P_1 - P)^2\ dP}{\left[\frac{F\ P_1}{1 - F} + P\right]^2 P^2} = K \int_{t_1}^{t_2} dt \quad . \tag{150}$$

By integrating:

$$\frac{(S_1 + P_1)^2}{(P_1\ f)^2} \left[\frac{P_1\ f + 2\ P_2}{(P_1\ f + P_2)\ P_2} - \frac{P_1\ f + 2\ P_1}{(P_1\ f + P_1)\ P_1} \right]$$

$$- \frac{2\ (S_1 + P_1)^2}{(P_1 f)^3} \ln \frac{(P_1\ f + P_2)\ P_1}{(P_1\ f + P_1)\ P_2}$$

$$+ \left[\frac{2\ (S_1 + P_1)}{P_1\ f} + 1 \right] \left[\frac{1}{P_1\ f + P_2} - \frac{1}{P_1\ f + P_1} \right]$$

$$- \frac{2\ (S_1 + P_1)}{(P_1\ f)^2} \ln \frac{(P_1\ f + P_2)\ P_1}{(P_1\ f + P_1)\ P_2} = K\ (t_2 - t_1) \quad , \tag{151}$$

where $f = F\ /\ (1 - F)$. Substitute Eq. (101) in Eq. (151) and rearrange:

$$\frac{(P_1 + S_1)^2}{F^2} \left[\frac{1 - F}{1 - E + E\ F} + \frac{E}{1 - E} + F - 1 \right]$$

$$- \frac{2\ (P_1 + S_1)^2\ (1 - F)}{F^3} \ln \frac{1 - E + E\ F}{1 - E}$$

$$+ \left[\frac{2\ (P_1 + S_1)\ P_1}{F} + \frac{P_1{}^2}{1 - F} \right] \left[\frac{E - E\ F}{1 - E + E\ F} \right]$$

$$- \frac{2\ (P_1 + S_1)\ P_1}{F^2} \ln \frac{1 - E + E\ F}{1 - E} = K\ P_1\ R_1{}^2\ (t_2 - t_1) \quad . \tag{152}$$

Further rearrangement yields:

$$- \left[1 - F - \frac{E}{1 - E} - \frac{1 - F}{1 - E + E\,F} + \frac{2\,(1 - F)}{F} \ln \frac{1 - E + E\,F}{1 - E} \right] \frac{(P_1 + S_1)^2}{F^2}$$

$$+ \frac{2\,P_1\,(P_1 + S_1)}{F} \left[\frac{E - E\,F}{1 - E + E\,F} - \frac{1}{F} \ln \frac{1 - E + E\,F}{1 - E} \right] + \frac{E\,P_1^{\,2}}{1 - E + E\,F}$$

$$= K\,P_1\,R_1^{\,2}\,(t_2 - t_1) \quad . \tag{153}$$

In the model, Eq. (153) is coded as Statements 3770 and 3660 (MCHEMP) or Statements 4620 and 4510 (SCHEMP).

```
AMTINT = -((FOR1 - A * EXTENT - FOR1 / B + 2 * C * FOR1 * LOG
         (A * B)) * AA * C^2) + 2 * BB * C * (FOR1 * EXTENT / B
         - C * LOG (A * B)) + CC * EXTENT / B

RK = (1.74 * EXP (31000 / 1.987 * (1 / 303.16 - 1 / (273.16 +
TPROF(J,2))))) * RX(3) * DTHETA * (RX(5) / (RX(1)^2 * TOTNIT))^2
```

where AMTINT is equivalent to the left-hand side of Eq. (153) and RK is equivalent to the right-hand side of Eq. (153). Other equivalencies are:

A	$= 1 / (1 - E)$	DTHETA	$= t_2 - t_1$
B	$= 1 - E + E\,F$	EXTENT	$= E$
C	$= 1 / F$	RX(1)	$= H$
AA	$= (P_1 + S_1)^2$	RX(3)	$= P_1$
BB	$= P_1\,(P_1 + S_1)$	RX(5)	$= R_1$
CC	$= P_1^{\,2}$	TOTNIT	$= N$
FOR1	$= 1 - F$	TPROF(J,2)	= Temperature (°C)

A binary search is used to determine the value of E.

The test made in Statements 3720 or 4570 is equivalent to evaluating F = ~1, indicating a large excess of reductant. The test made in Statements 3750 or 4600 directs the routine to use either the general solution or the stoichiometric solution (if F = ~0). The value of E is limited by E_{max}, just discussed.

The solute amounts after reaction ($SOLAMT_{2,i}$) are calculated by using Eq. (96) and the following values for $STOIC_i$:

For HNO_3,	$i = 1$,	$STOIC_1 = +2$	For Pu(III),	$i = 4$,	$STOIC_4 = +1$
U,	$i = 2$,	$STOIC_2 = 0$	Reductant,	$i = 5$,	$STOIC_5 = -1$
Pu(IV),	$i = 3$,	$STOIC_3 = -1$	Nitrate,	$i = 6$,	$STOIC_6 = 0$

2.6.4 Test of the Plutonium Reduction Models

The source code that models plutonium reduction by U(IV) or by HAN was tested for reliability. The primary objectives were (1) to evaluate whether oscillatory behavior might occur and (2) to examine the transition between the various cases described in the preceding section (the general solution, the solution for a stoichiometric ratio of reactants, and the solution for a large excess of HAN). Oscillations were evident in previous versions of SEPHIS MOD4.

For the reduction of plutonium by U(IV), 27 cases were examined for combinations of the following solute concentrations: $[HNO_3]$ = 0.01, 0.2, and 5.0 *M*; [U(VI)] = 0, 10^{-4}, and 100 g/L; and [Pu(IV)] = 10^{-7}, 10^{-4}, and 30 g/L.

The extent of reaction was calculated for a wide range of reactant ratios [Pu(IV)/U(IV)] using a 1-min reaction time and a temperature of 30°C. The calculations were made by using the same source code statements as found in subprograms MCHEMP and SCHEMP of SEPHIS MOD4, Version 2.11. Figures 2 through 4 illustrate the variation of the extent of reaction with the reactant ratio for the conditions tested. The amount of U(VI) present was found to have no effect. A smooth transition through the region of the stoichiometric ratio was evident.

For the reduction of plutonium by HAN, the same 27 cases were examined at the same conditions. Figures 5 through 10 illustrate the variation of the extent of reaction with the reactant ratio. For the HAN reduction, the amount of U(VI) present did make a difference when lower nitric acid concentrations were used. Smooth transitions through the region of the stoichiometric ratio and with the region of excess reductant were found. However, the transition from general solution to instantaneous reduction, which occurs at very low concentrations of Pu(IV) in the presence of even lower HAN concentrations, was frequently a step function. This discontinuity is considered of little importance in a practical problem.

2.7 APPROXIMATIONS AND ASSUMPTIONS

1. *Solute concentrations in the contactor change rather slowly.* Approximations made to numerically integrate the differential equations become more exact if concentrations change slowly. By specifying a small time-increment (significantly less than the mean stage residence time) over which integrations are performed, the errors are minimized. This assumption does not apply when only steady-state results are desired.

2. *Stage volumes and flow rates remain constant.* Since real liquid solutions behave in a nonideal manner (i.e., flow rates and volumes vary with solute concentrations), SEPHIS MOD4 performs calculations on a solute-free, rather than a molar, basis. This convention greatly reduces the effect of nonideal solutions. Approximate relationships are used to convert molar quantities to solute-free quantities.

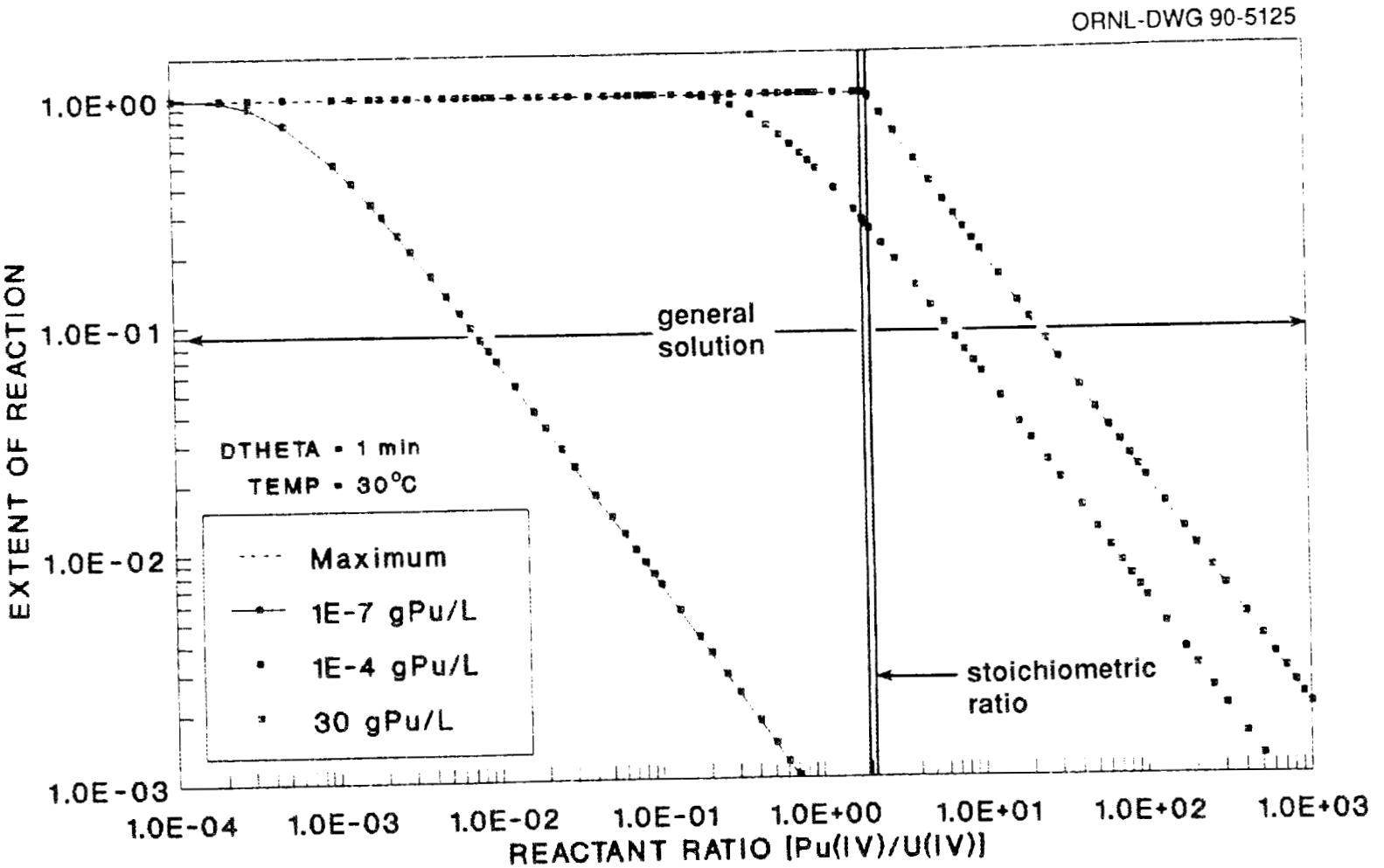


Fig. 2. Pu(IV) reduction by U(IV) [0.01 *M* HNO_3, 0–100 gU(VI)/L].

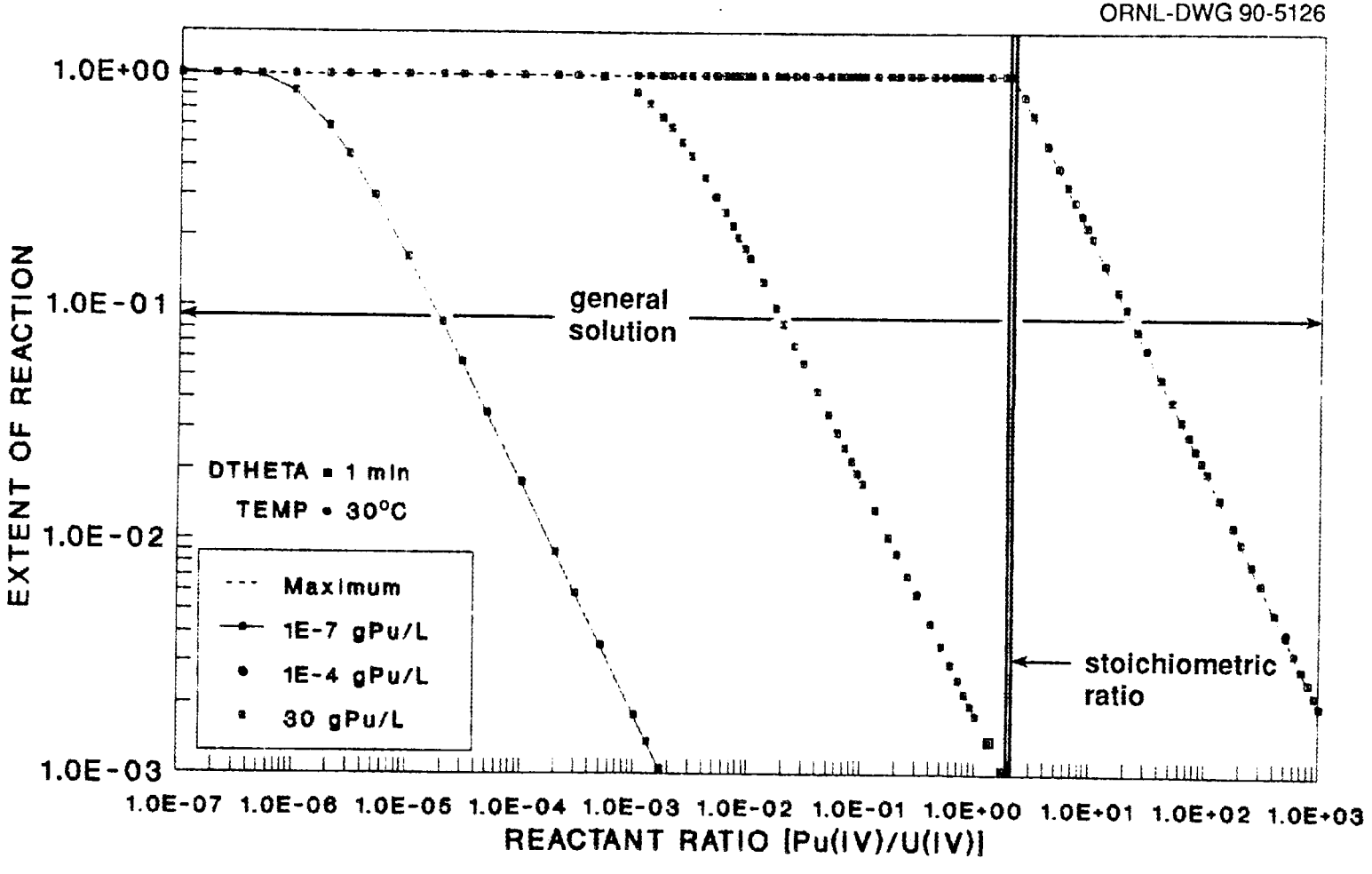


Fig. 3. Pu(IV) reduction by U(IV) [0.2 *M* HNO_3, 0-100 gU(VI)/L].

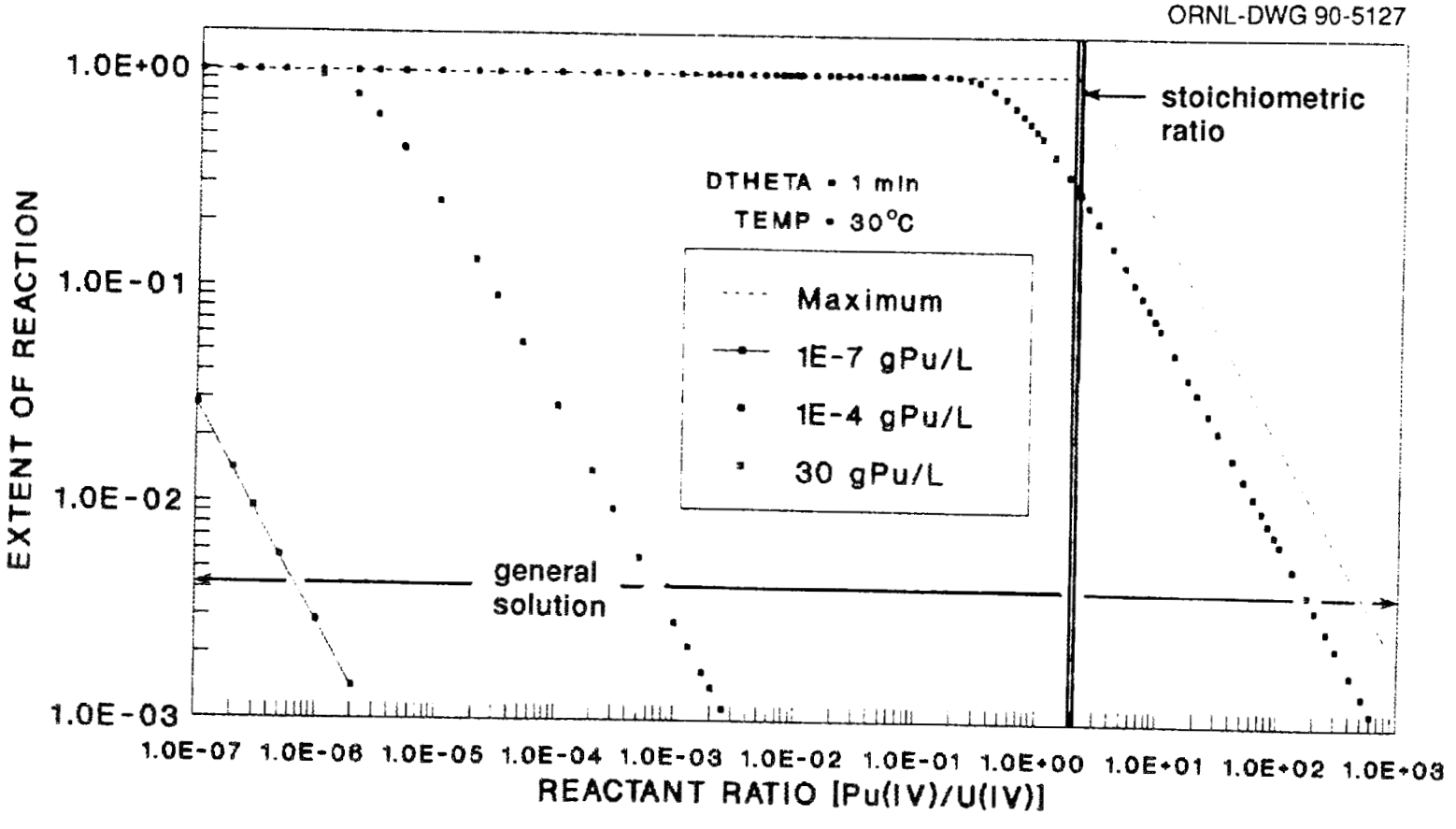


Fig. 4. Pu(IV) reduction by U(IV) [5 *M* HNO_3, 0-100 gU(VI)/L].

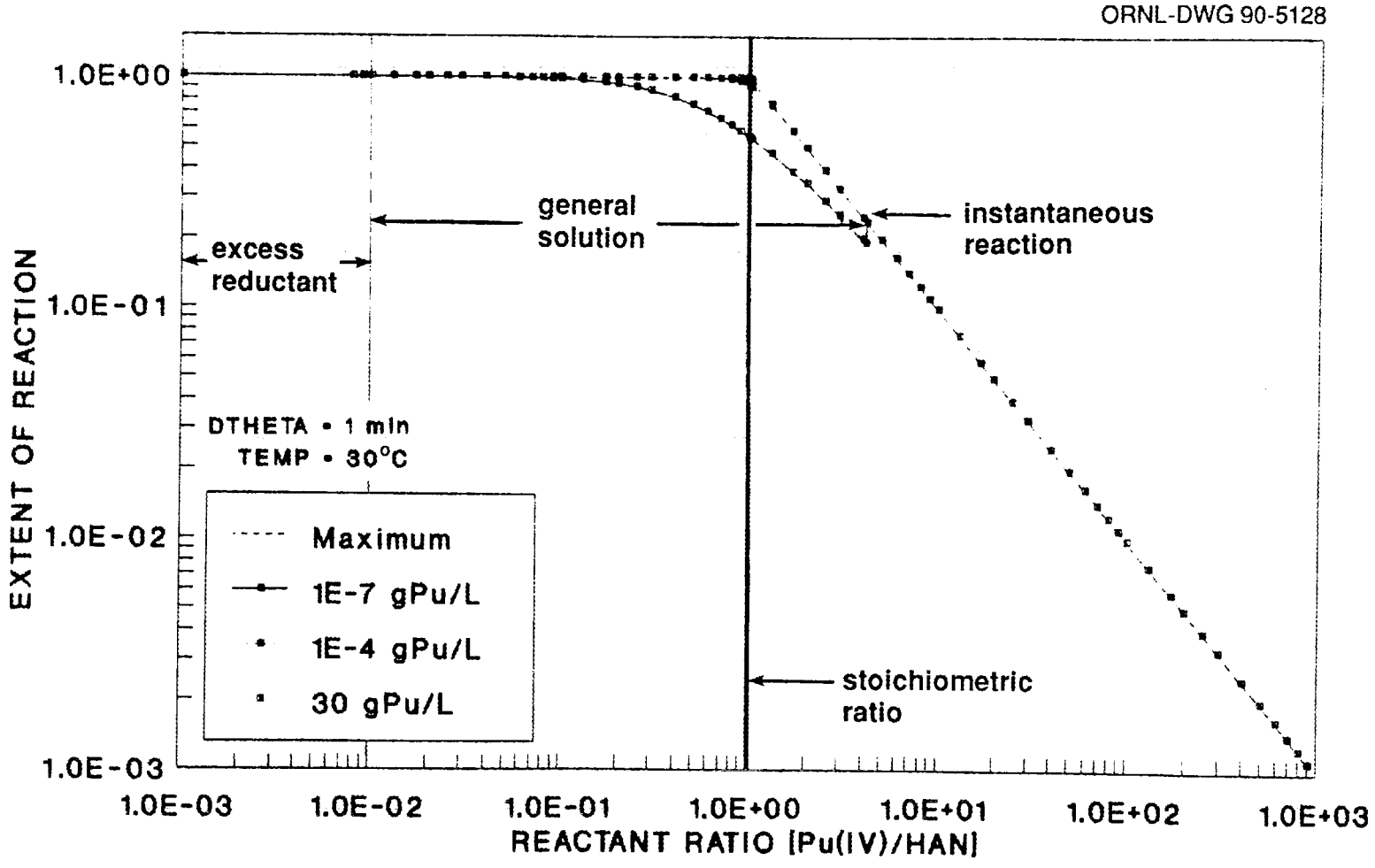


Fig. 5. Pu(IV) reduction by HAN [0.01 *M* HNO_3, <1E-4 gU/L].

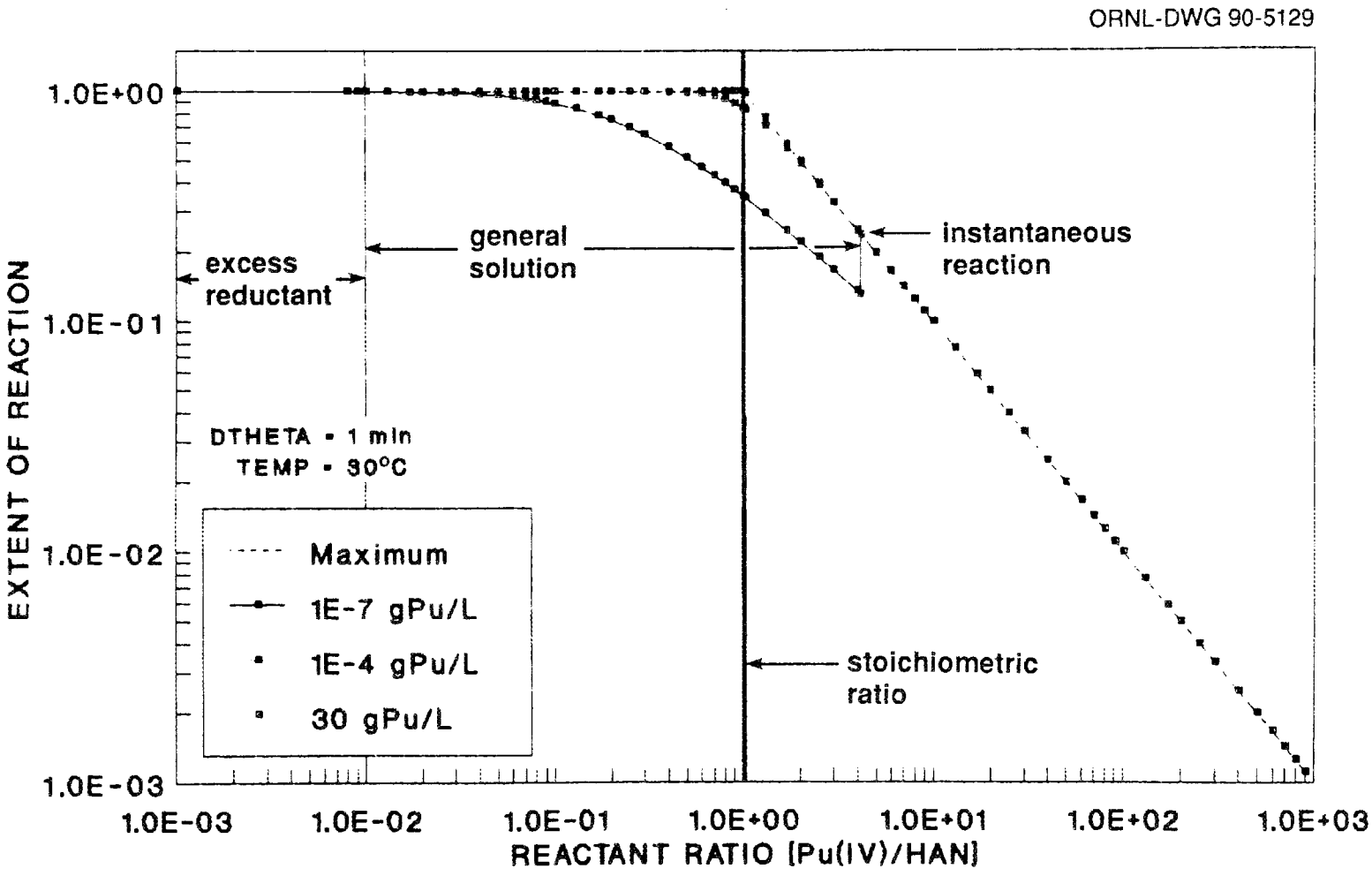


Fig. 6. Pu(IV) reduction by HAN [0.01 *M* HNO_3, 100 gU/L].

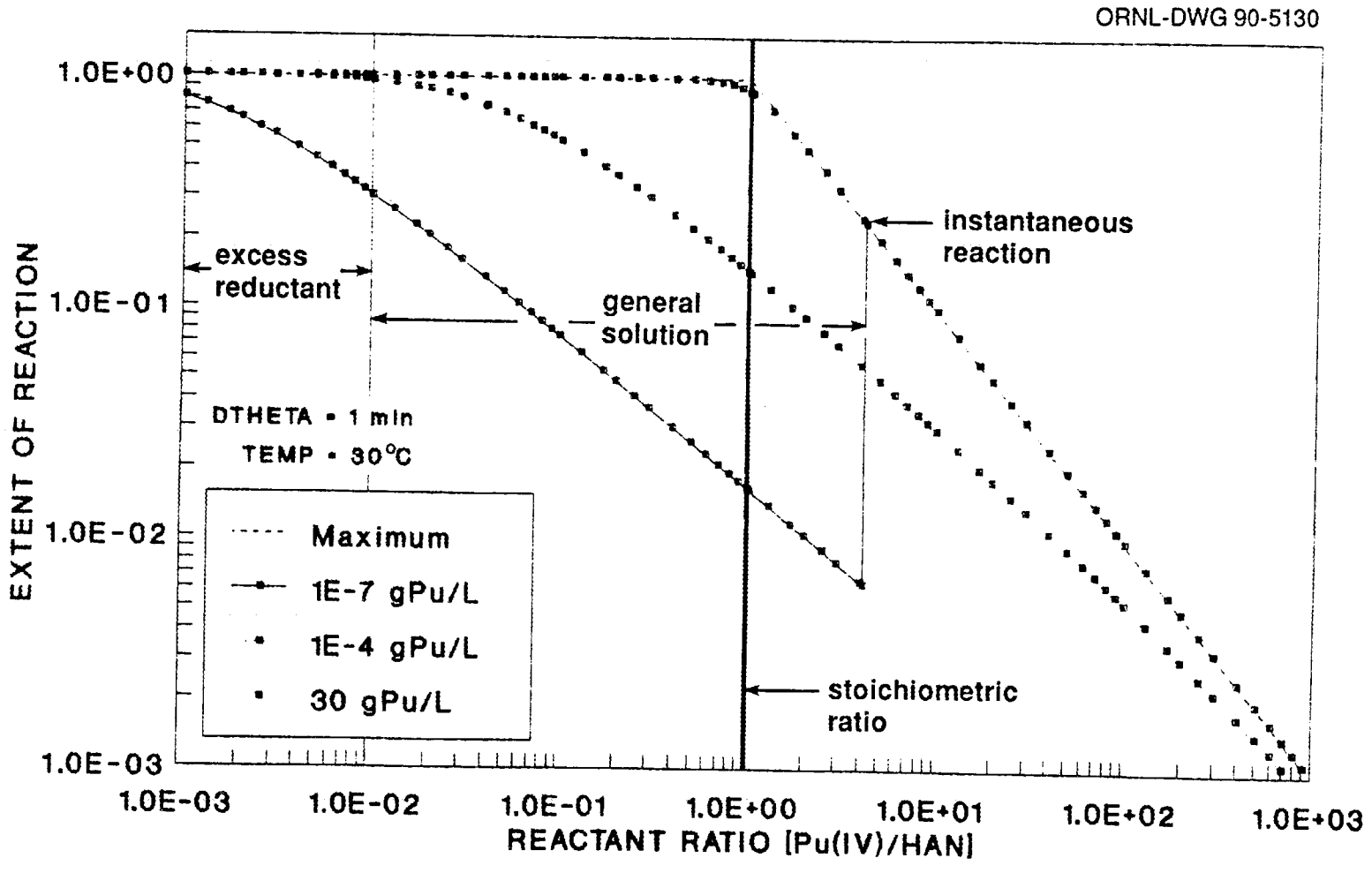


Fig. 7. Pu(IV) reduction by HAN [0.2 *M* HNO_3, <1E-4 gU/L].

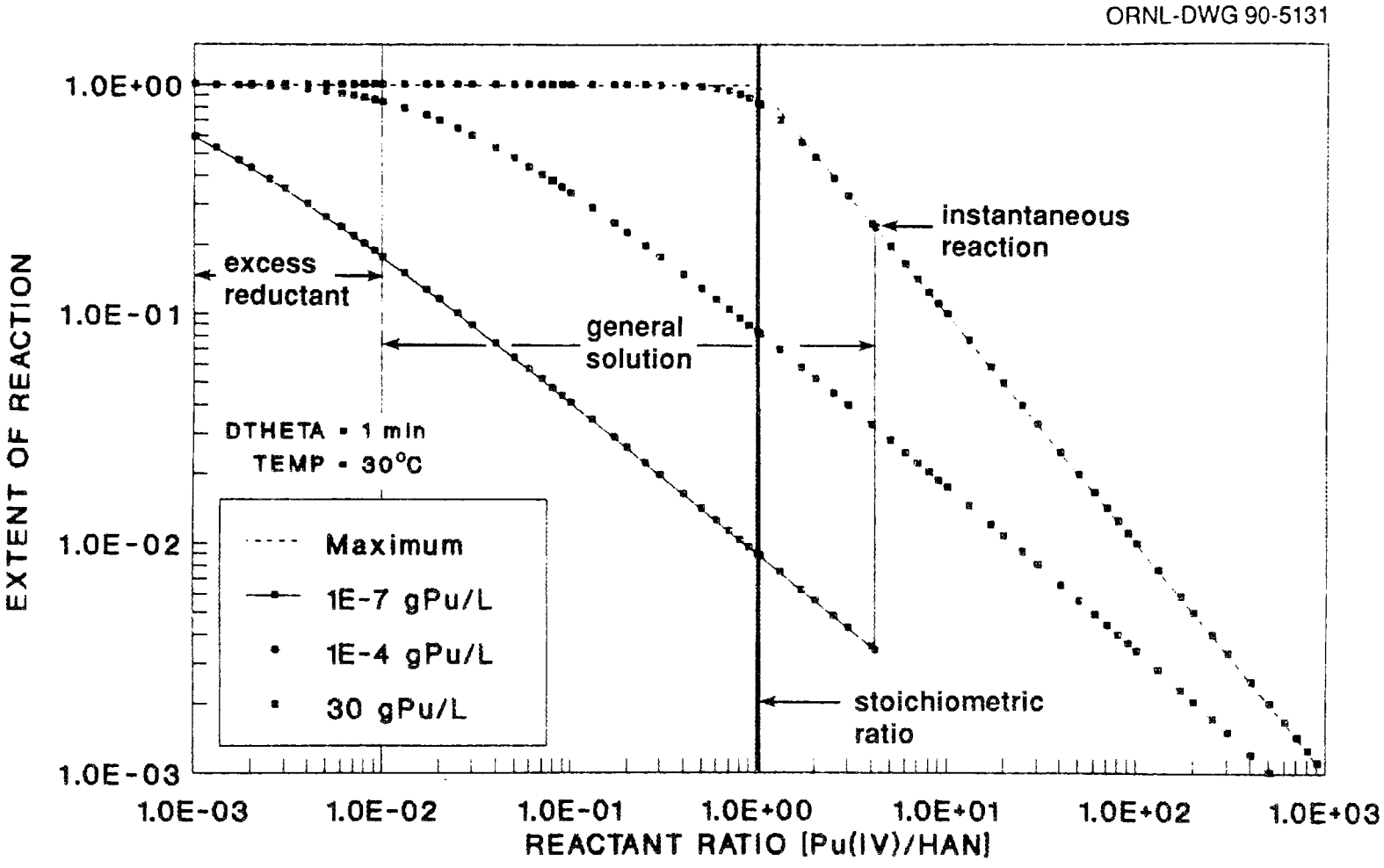


Fig. 8. Pu(IV) reduction by HAN [0.2 *M* HNO_3, 100 gU/L].

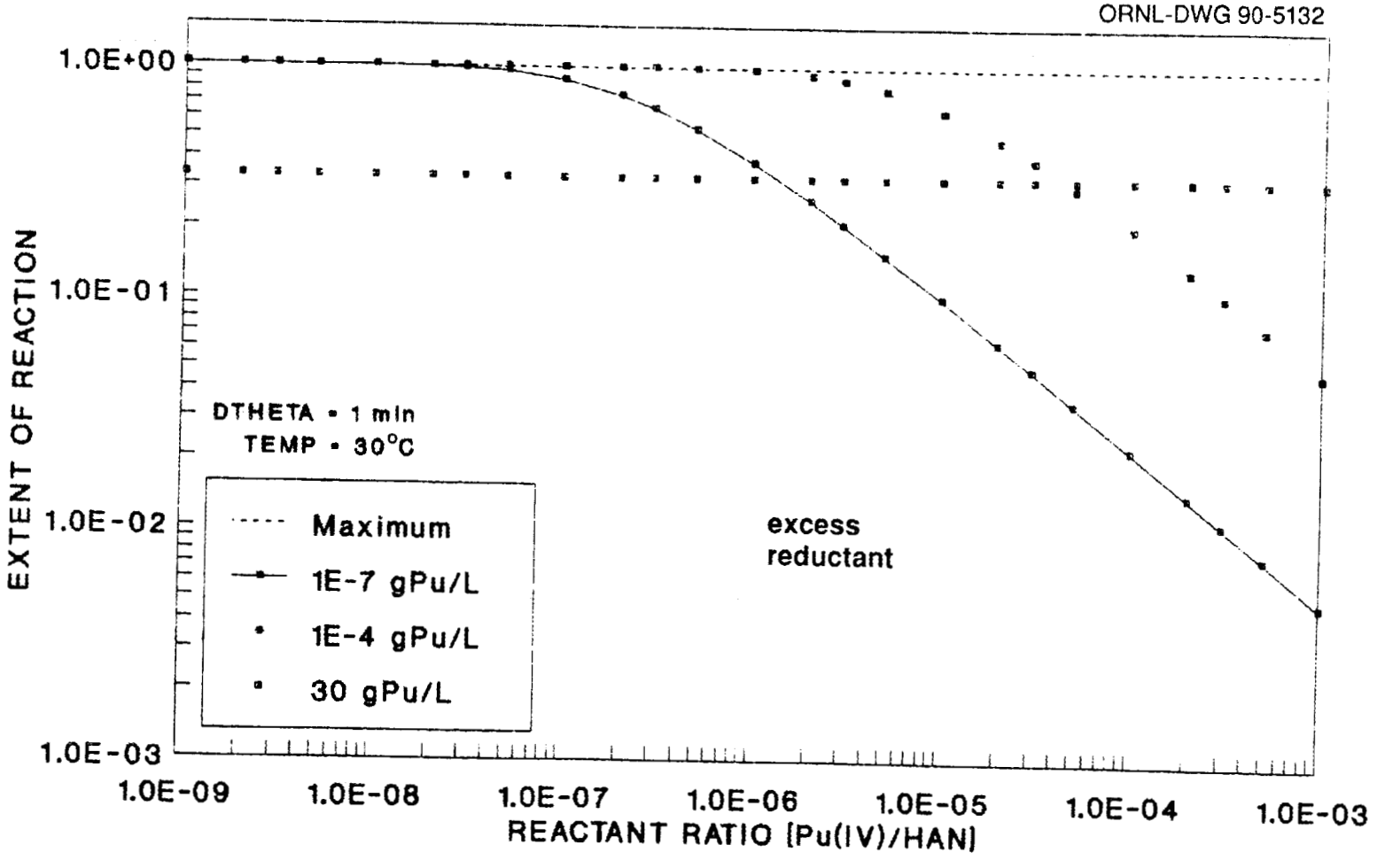


Fig. 9. Pu(IV) reduction by HAN [5 *M* HNO_3, 0–100 gU/L].

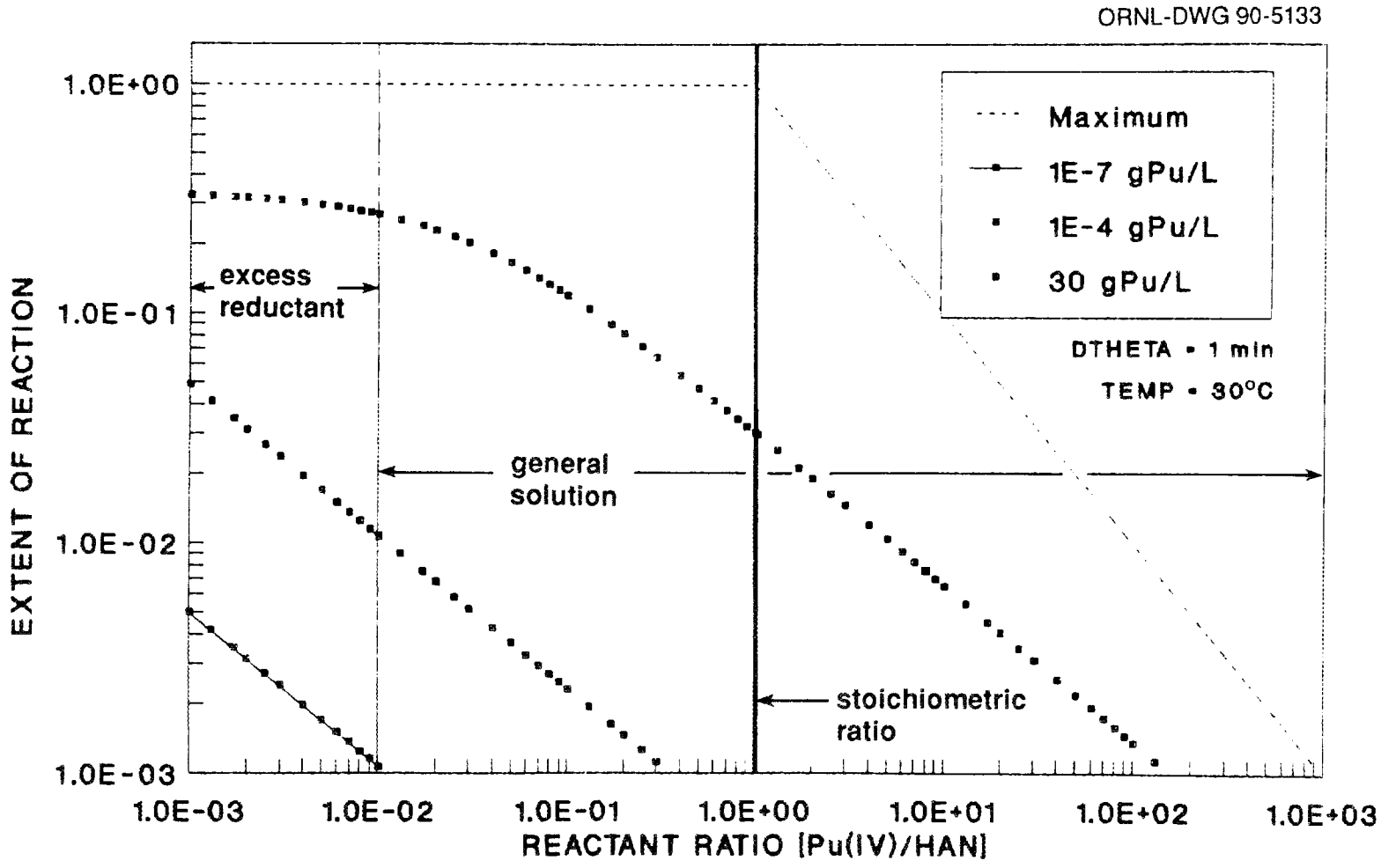


Fig. 10. Pu(IV) reduction by HAN [5 *M* HNO_3, 0-100 gU/L].

3. *The contactor operation conforms with the concept of the model.* Perfect mixing and all interphase mass transfers are assumed to occur in the mixers. The solutes are at an equilibrium distribution between the phases, as defined by using approximate correlations of laboratory distribution data. In the settlers, phases separate completely and no interphase mass transfer is allowed. Entrainment of one phase within the other is not considered. Each phase in every settler zone is homogeneous.

4. *Chemical reactions occur entirely within the aqueous phase.* Plutonium (III), the reductant, and inextractable nitrate salts remain in the aqueous phase. The extent of reactions is governed by approximate chemical reaction kinetic data and expressions.

5. *Solvent degradation products from radiolysis or chemical attack are not considered.*

6. *Nonideal heat effects are neglected.* Temperature profiles are calculated by using approximate heat capacities for the phases. Heats of mixing, heats of reaction (mass transfer), heat contributions from radiation, and heat transfer to the surrounding environment are not considered.

3. ORGANIZATION OF SEPHIS MOD4, VERSION 2.11

SEPHIS MOD4, Version 2.11, is a menu-driven set of computer programs. Source codes for the various programs were prepared by using the BASIC language. The source code programs were then compiled into machine-language routines for efficient operation by using Microsoft QuickBASIC, Version 4.0. A single 2S/2D, 5 1/4-in. floppy disk contains all of the executable files and is available for distribution by writing to the DOE National Energy Software Center, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439. Files that are included in the distribution diskette are listed in Table 3.

Table 3. Files included in the distribution diskette

File	Size	Date
SECALC.EXE	136093	07-16-90
SEPHIS.EXE	50641	07-15-90
SEPREP.EXE	97631	07-16-90
SEPRNT.EXE	74343	07-16-90

3.1 SEPHIS - THE MENU PROGRAM

The SEPHIS program contains the menu program from which the user may select any of the three companion programs or exit to the computer system. On completion of any of the three companion programs, the menu reappears. The source code for this program, SEPHIS.BAS, is provided in Appendix A.

3.2 SEPREP - PROGRAM FOR PROBLEM DEFINITION FILE PREPARATION

The SEPREP program is used to prepare the Problem Definition file. It prompts the user to provide all of the input data for a particular problem to be solved. Detailed instructions for its use are provided in the SEPHIS User's Manual.[2] The source code for this program, SEPREP.BAS, is given in Appendix B.

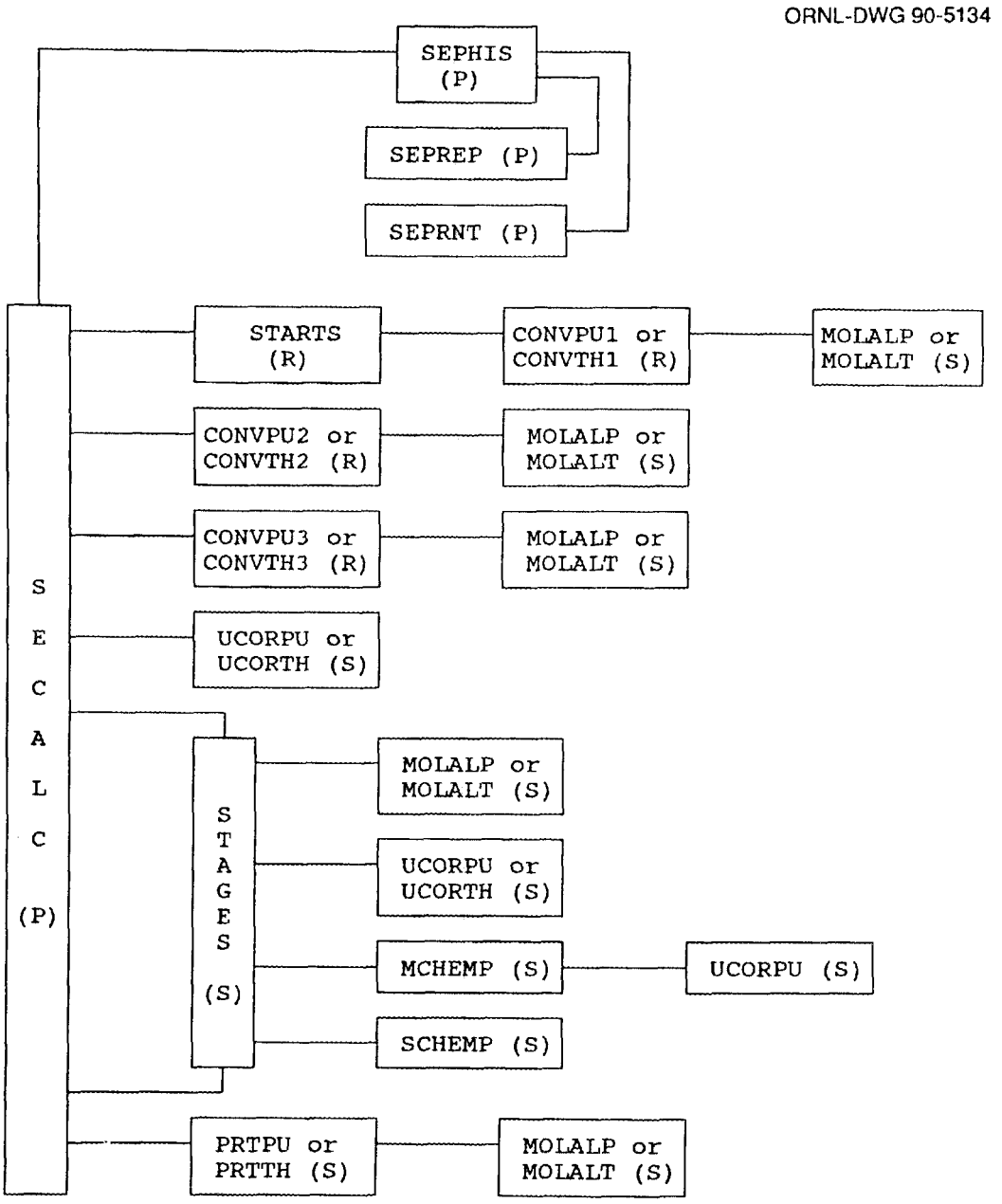
3.3 SECALC - PROGRAM FOR OBTAINING THE SOLUTION TO DEFINED PROBLEMS

The SECALC program is the calculational routine that performs all mathematical operations based on information provided through the Problem Definition file. Detailed instructions for its use are furnished in the SEPHIS User's Manual.[2] The source code appears in two modules as SECALC.BAS and SECAL1.BAS in Appendixes C and D, respectively. These modules are linked by using SECOM.BI (given as Appendix E) from which common data blocks are defined. An overall flow diagram for computations is shown in Fig. 11.

The SECALC program is composed of many subprograms and subroutines, each of which performs a specific function. General input functions based on the Problem Definition file are created and the system hydraulics are set by the STARTS routine. The conversion of units is handled through routines with titles that begin with CONV- and MOLAL-. The subprogram STAGES is the principal computational tool. It performs all stage calculations while interfacing with other routines to obtain distribution coefficients and extents of reaction. Distribution coefficient correlations are contained in routines with titles that begin with UCOR-. The chemical reduction of plutonium is performed by MCHEMP and SCHEMP. Hard-copy printouts of results are handled by routines with titles that begin with PRT-. On completion, the SECALC program prepares a Problem Results file.

3.4 SEPRNT - PROGRAM FOR RETRIEVAL OF PAST PROBLEM RESULTS

The SEPRNT program is provided to obtain hard-copy printouts of problems previously run, without the necessity of rerunning them. This feature is handy for instances where the original printout is destroyed or lost, or where additional copies are desired. Detailed instructions for its use are provided in the SEPHIS User's Manual.[2] The source code for this program, SEPRNT.BAS, is given in Appendix F.



P = Program
R = Routine within a program
S = Subprogram

Fig. 11. Overall flow diagram for computations.

4. SAMPLE PROBLEM – A THREE-CONTACTOR FLOW SHEET FOR THE RECOVERY OF URANIUM (U) AND PLUTONIUM (Pu) FROM A FAST BREEDER-TYPE SPENT FUEL SOLUTION

Several sample problems for simple solvent extraction operations are presented in the SEPHIS User's Manual.[2] To show the computational power of SEPHIS MOD4, Version 2.11, a more elaborate problem is selected herein. The system modeled consists of three solvent extraction contactors configured as shown in Fig. 12. The solvent extraction operations include co-extraction and co-scrubbing of U and Pu (A-Bank) as well as U-Pu partitioning (B-Bank) and U stripping (C-Bank). The flow sheet conditions selected are hypothetical but are based on an actual experimental flow sheet operated in the Solvent Extraction Test Facility at Oak Ridge National Laboratory (ORNL).

4.1 TRANSIENT CALCULATION

Computer output is provided in this section for the startup transient, beginning with the contactors at zero concentration. Since plutonium reduction is occurring, the Fast integration technique is used. The chosen time increment for integrations is 0.2 min, based on the flow rates shown, and stage volumes are 1.8 L for mixers and 3.0 L for settlers. For 1000 min of process time, the computational time, determined by using an upgraded IBM PC/XT (16 MHz with 32-bit processor), was 5 h 50 min. This output shows the concentration profile for each 200 min, up to a total time of 1000 min. A second computer run was made to obtain profiles for each 20 min for the first 200 min as a display of time-dependent concentrations (Sect. 4.3). Steady-state concentrations were attained in ~1400 min (<0.0001% inventory change in any stage during a 1-min time increment).

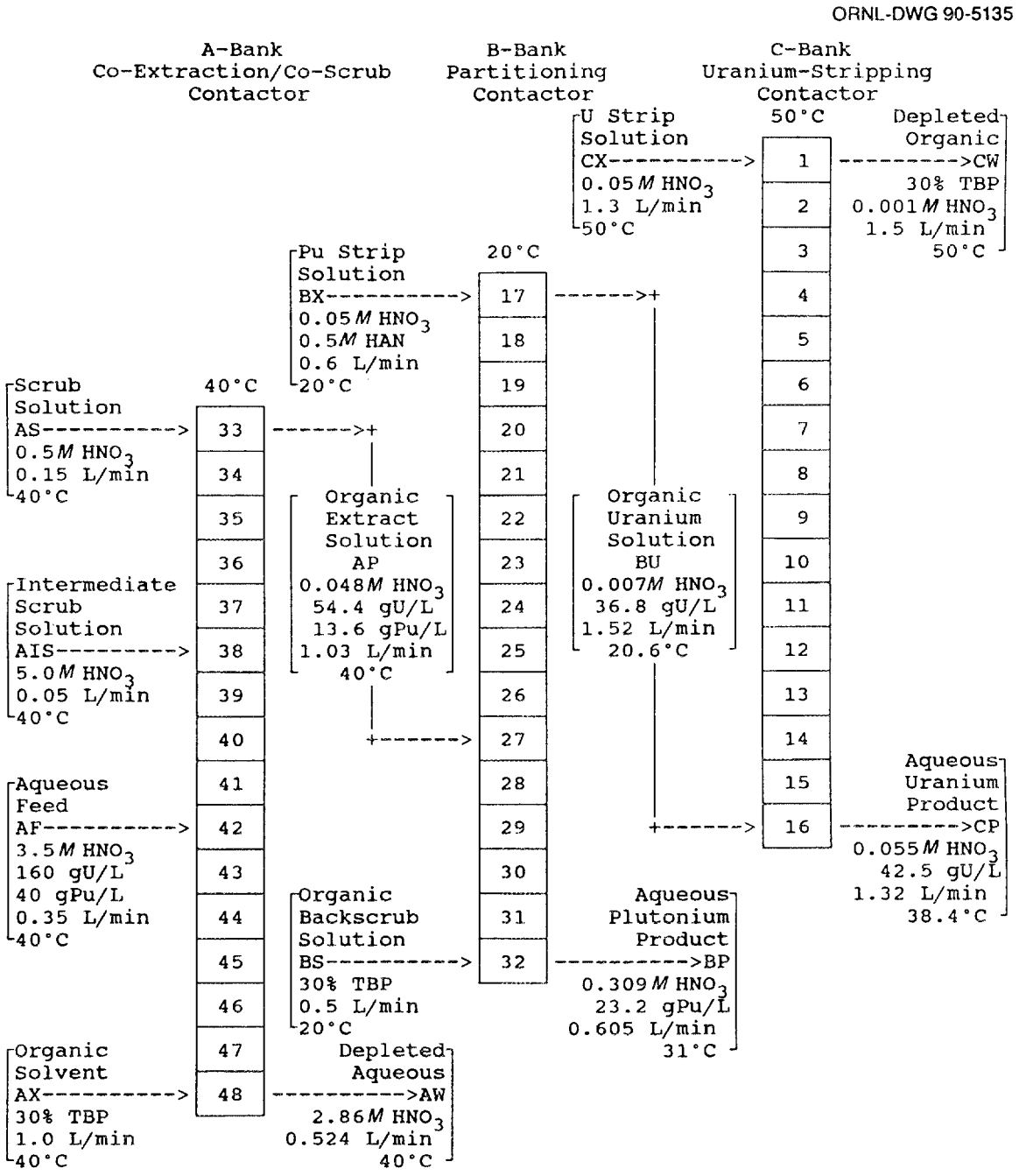


Fig. 12. A three-contactor flow sheet for the recovery of uranium and plutonium from a fast breeder-type spent fuel solution.

PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11: 06-08-1990 09:58

Problem: BREEDER FLOWSHEET EXAMPLE

PUREX PROCESS
Total stages: 48
Volume % TBP in solvent: 30.0
Initial or default temperature (°C): 40.0
Organic taken from stage 33 feeds stage 27 .
Reduction of Pu(IV) by hydroxylamine nitrate.
Minutes per time increment: 0.20
Minutes between printing of the concentration profile: 200
Calculations will stop after 5000 minutes or when a tolerance of 0.0001 % per minute is reached.
Total mixer volumes are defined (phase ratios = flow ratios).
Total settler volumes are defined (phase ratios = flow ratios).
Initial concentration profile is zero.
Fast integration will be used.
Extra product stream(s).

The FILESPEC for this Problem Definition data file is: B:EXPL_P.DAT
The FILESPEC for this Problem Results data file is: B:EXPL_R.DAT

FEED AND PRODUCT STREAM DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
AQUEOUS	1	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.30E+00	50.0
AQUEOUS	17	5.00E-02	0.00E+00	0.00E+00	0.00E+00	5.00E-01	5.00E-01	6.00E-01	20.0
30.0 % TBP	32	0.00E+00	0.00E+00	0.00E+00				5.00E-01	20.0
AQUEOUS	33	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.50E-01	40.0
AQUEOUS	38	5.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.00E-02	40.0
AQUEOUS	42	3.50E+00	1.60E+02	4.00E+01	0.00E+00	0.00E+00	0.00E+00	3.50E-01	40.0
30.0 % TBP	48	0.00E+00	0.00E+00	0.00E+00				1.00E+00	40.0
AQUEOUS	16	Product stream removed (actual flow rate to be computed)						1.30E+00	
AQUEOUS	32	Product stream removed (actual flow rate to be computed)						6.00E-01	

STAGE VOLUME AND FLOW RATE DATA (Molal basis):

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	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
2	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
3	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
4	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
5	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
6	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
7	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
8	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
9	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
10	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
11	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
12	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
13	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
14	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+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
15	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
16	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	0.00E+00	1.49E+00
17	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
18	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
19	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
20	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
21	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
22	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
23	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
24	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
25	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
26	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
27	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
28	9.78E-01	8.22E-01	1.63E+00	1.37E+00	5.90E-01	4.96E-01	5.90E-01	4.96E-01
29	9.78E-01	8.22E-01	1.63E+00	1.37E+00	5.90E-01	4.96E-01	5.90E-01	4.96E-01
30	9.78E-01	8.22E-01	1.63E+00	1.37E+00	5.90E-01	4.96E-01	5.90E-01	4.96E-01
31	9.78E-01	8.22E-01	1.63E+00	1.37E+00	5.90E-01	4.96E-01	5.90E-01	4.96E-01
32	9.78E-01	8.22E-01	1.63E+00	1.37E+00	5.90E-01	4.96E-01	0.00E+00	4.96E-01
33	2.33E-01	1.57E+00	3.89E-01	2.61E+00	1.48E-01	9.92E-01	1.48E-01	9.92E-01
34	2.33E-01	1.57E+00	3.89E-01	2.61E+00	1.48E-01	9.92E-01	1.48E-01	9.92E-01
35	2.33E-01	1.57E+00	3.89E-01	2.61E+00	1.48E-01	9.92E-01	1.48E-01	9.92E-01
36	2.33E-01	1.57E+00	3.89E-01	2.61E+00	1.48E-01	9.92E-01	1.48E-01	9.92E-01
37	2.33E-01	1.57E+00	3.89E-01	2.61E+00	1.48E-01	9.92E-01	1.48E-01	9.92E-01
38	2.89E-01	1.51E+00	4.82E-01	2.52E+00	1.90E-01	9.92E-01	1.90E-01	9.92E-01
39	2.89E-01	1.51E+00	4.82E-01	2.52E+00	1.90E-01	9.92E-01	1.90E-01	9.92E-01
40	2.89E-01	1.51E+00	4.82E-01	2.52E+00	1.90E-01	9.92E-01	1.90E-01	9.92E-01
41	2.89E-01	1.51E+00	4.82E-01	2.52E+00	1.90E-01	9.92E-01	1.90E-01	9.92E-01
42	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
43	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
44	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
45	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
46	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
47	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
48	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01

PROBLEM RESULTS FOR SEPHIS MOD4, Ver. 2.11: 06-08-1990 10:04

Problem: BREEDER FLOWSHEET EXAMPLE
(mixer concentrations shown)

TIME = 0.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
9	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
12	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
13	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
14	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
15	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
16	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
16	PRODUCT STREAM							1.30E+00	
17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
18	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
19	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
20	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
21	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
22	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
23	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
24	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
25	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
26	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
27	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
28	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
29	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
30	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
31	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
32	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
32	PRODUCT STREAM							5.90E-01	
33	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.48E-01	40.0
34	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.48E-01	40.0
35	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.48E-01	40.0
36	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.48E-01	40.0
37	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.48E-01	40.0
38	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.90E-01	40.0
39	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.90E-01	40.0
40	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.90E-01	40.0
41	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.90E-01	40.0
42	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
43	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0
44	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0
45	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0
46	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0
47	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0
48	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
9	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
12	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
13	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
14	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
15	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
16	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
18	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
19	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
20	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
21	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
22	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
23	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
24	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
25	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
26	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
27	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
28	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	5.00E-01	0.0	2.00E+02
29	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	5.00E-01	0.0	2.00E+02
30	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	5.00E-01	0.0	2.00E+02
31	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	5.00E-01	0.0	2.00E+02
32	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	5.00E-01	0.0	2.00E+02
33	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
34	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
35	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
36	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
37	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
38	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
39	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
40	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
41	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
42	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
43	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
44	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
45	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
46	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
47	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
48	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02

TIME = 200.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
2	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
3	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
4	5.00E-02	1.05E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
5	5.00E-02	2.34E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
6	5.00E-02	4.95E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
7	5.00E-02	1.04E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
8	5.01E-02	2.14E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
9	5.07E-02	3.93E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
10	5.21E-02	3.66E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.30E+00	50.0
11	5.31E-02	1.26E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.02E+00	1.31E+00	49.9
12	5.35E-02	2.35E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.03E+00	1.31E+00	49.7
13	5.34E-02	3.29E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.04E+00	1.31E+00	49.3
14	5.32E-02	4.01E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E+00	1.32E+00	48.2
15	5.31E-02	4.45E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	45.4
16	5.50E-02	4.47E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	38.5
16	PRODUCT STREAM							1.32E+00	
17	4.89E-02	1.30E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.02E-01	20.8
18	4.86E-02	1.58E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	21.6
19	4.86E-02	1.66E+01	0.00E+00	0.00E+00	4.97E-01	4.97E-01	1.11E+00	6.03E-01	22.6
20	4.88E-02	1.70E+01	0.00E+00	2.91E-05	4.97E-01	4.97E-01	1.11E+00	6.03E-01	23.7
21	4.93E-02	1.74E+01	1.67E-05	2.23E-04	4.97E-01	4.97E-01	1.11E+00	6.03E-01	24.9
22	5.11E-02	1.78E+01	1.34E-04	1.82E-03	4.97E-01	4.97E-01	1.11E+00	6.03E-01	26.3
23	5.67E-02	1.82E+01	1.06E-03	1.47E-02	4.97E-01	4.97E-01	1.11E+00	6.03E-01	27.8
24	7.42E-02	1.82E+01	8.02E-03	1.17E-01	4.96E-01	4.97E-01	1.11E+00	6.04E-01	29.5
25	1.24E-01	1.72E+01	5.59E-02	8.87E-01	4.93E-01	4.96E-01	1.12E+00	6.05E-01	31.4
26	2.37E-01	1.38E+01	3.18E-01	6.10E+00	4.69E-01	4.95E-01	1.12E+00	6.06E-01	33.5
27	3.84E-01	9.17E+00	1.34E+00	2.31E+01	3.96E-01	4.93E-01	1.15E+00	6.08E-01	35.9
28	4.05E-01	1.34E+00	5.20E-02	2.44E+01	3.92E-01	4.94E-01	1.14E+00	6.07E-01	35.9
29	4.08E-01	1.71E-01	1.01E-02	2.46E+01	3.91E-01	4.94E-01	1.14E+00	6.07E-01	35.9
30	4.06E-01	2.13E-02	2.80E-03	2.48E+01	3.91E-01	4.94E-01	1.14E+00	6.07E-01	35.7
31	3.91E-01	2.58E-03	8.17E-04	2.50E+01	3.90E-01	4.95E-01	1.14E+00	6.06E-01	34.8
32	3.20E-01	2.84E-04	2.19E-04	2.52E+01	3.90E-01	4.96E-01	1.13E+00	6.05E-01	31.5
32	PRODUCT STREAM							6.05E-01	
33	5.33E-01	3.69E+01	2.07E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.54E-01	40.0
34	6.74E-01	3.95E+01	2.40E+01	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.55E-01	40.0

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
35	9.42E-01	3.30E+01	2.01E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
36	1.36E+00	2.32E+01	1.34E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.57E-01	40.0
37	1.93E+00	1.46E+01	7.56E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.59E-01	40.0
38	2.71E+00	9.34E+00	4.06E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.08E-01	40.0
39	2.78E+00	8.88E+00	3.75E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
40	2.91E+00	8.45E+00	3.46E+00	0.00E+00	0.00E+00	0.00E+00	1.11E+00	2.10E-01	40.0
41	3.23E+00	7.77E+00	2.95E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	2.12E-01	40.0
42	4.29E+00	7.15E+00	2.08E+00	0.00E+00	0.00E+00	0.00E+00	1.15E+00	5.53E-01	40.0
43	4.36E+00	1.24E-01	4.15E-02	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
44	4.36E+00	2.00E-03	7.73E-04	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
45	4.34E+00	3.22E-05	1.44E-05	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.51E-01	40.0
46	4.27E+00	5.14E-07	2.71E-07	0.00E+00	0.00E+00	0.00E+00	1.13E+00	5.50E-01	40.0
47	3.94E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	5.44E-01	40.0
48	2.84E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	5.23E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
2	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
3	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
4	1.20E-03	4.72E-09	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
5	1.20E-03	1.06E-07	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
6	1.20E-03	2.23E-06	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	4.01E-05
7	1.20E-03	4.67E-05	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	4.28E+00
8	1.21E-03	9.72E-04	0.00E+00	5.24E-02	0.00E+00	2.78E-02	8.18E-01	1.50E+00	0.1	4.09E+00
9	1.30E-03	2.00E-02	0.00E+00	5.87E-02	0.00E+00	2.95E-02	8.18E-01	1.50E+00	0.1	3.57E+00
10	1.89E-03	3.64E-01	0.00E+00	1.15E-01	0.00E+00	4.17E-02	8.18E-01	1.50E+00	0.5	2.26E+00
11	3.17E-03	3.33E+00	0.00E+00	3.05E-01	0.00E+00	6.86E-02	8.22E-01	1.50E+00	2.8	1.26E+00
12	4.20E-03	1.13E+01	0.00E+00	5.56E-01	0.00E+00	9.03E-02	8.33E-01	1.51E+00	9.1	6.51E-01
13	4.63E-03	2.11E+01	0.00E+00	7.37E-01	0.00E+00	9.97E-02	8.46E-01	1.51E+00	16.6	3.11E-01
14	4.71E-03	2.95E+01	0.00E+00	8.48E-01	0.00E+00	1.02E-01	8.57E-01	1.52E+00	23.1	1.26E-01
15	4.65E-03	3.58E+01	0.00E+00	9.27E-01	0.00E+00	1.01E-01	8.65E-01	1.52E+00	27.9	1.52E-02
16	4.65E-03	3.97E+01	0.00E+00	1.02E+00	0.00E+00	9.75E-02	8.70E-01	1.52E+00	30.9	6.31E-02
17	6.31E-03	3.98E+01	0.00E+00	7.72E+00	0.00E+00	3.26E-01	8.70E-01	1.52E+00	31.1	1.48E-01
18	5.93E-03	4.47E+01	0.00E+00	7.15E+00	0.00E+00	3.08E-01	8.77E-01	1.52E+00	34.8	1.58E-01
19	5.87E-03	4.56E+01	0.00E+00	6.93E+00	0.00E+00	3.05E-01	8.78E-01	1.52E+00	35.5	1.61E-01
20	5.87E-03	4.57E+01	0.00E+00	6.77E+00	0.00E+00	3.05E-01	8.78E-01	1.52E+00	35.6	1.59E-01
21	5.94E-03	4.56E+01	1.15E-05	6.62E+00	1.21E-01	3.05E-01	8.78E-01	1.52E+00	35.5	1.54E-01
22	6.17E-03	4.56E+01	9.44E-05	6.46E+00	1.22E-01	3.05E-01	8.78E-01	1.52E+00	35.5	2.07E-01
23	6.88E-03	4.55E+01	7.71E-04	6.33E+00	1.23E-01	3.06E-01	8.78E-01	1.52E+00	35.6	2.44E-01
24	9.10E-03	4.55E+01	6.21E-03	6.31E+00	1.26E-01	3.10E-01	8.78E-01	1.52E+00	35.7	2.56E-01
25	1.57E-02	4.53E+01	4.90E-02	6.65E+00	1.31E-01	3.20E-01	8.78E-01	1.52E+00	36.2	2.68E-01
26	3.29E-02	4.47E+01	3.71E-01	8.14E+00	1.45E-01	3.48E-01	8.78E-01	1.53E+00	37.6	2.59E-01
27	6.07E-02	4.32E+01	2.53E+00	1.18E+01	2.60E-01	3.97E-01	8.80E-01	1.53E+00	40.6	2.21E-01
28	9.87E-02	1.11E+01	1.72E-01	6.88E+00	5.84E-03	2.02E-01	8.35E-01	5.04E-01	17.7	4.69E-01
29	1.10E-01	1.62E+00	3.83E-02	7.84E+00	1.29E-03	2.24E-01	8.23E-01	5.02E-01	11.3	4.92E-01
30	1.11E-01	2.07E-01	1.08E-02	8.03E+00	3.60E-04	2.27E-01	8.21E-01	5.02E-01	10.3	4.38E-01
31	1.07E-01	2.53E-02	3.07E-03	8.11E+00	1.02E-04	2.28E-01	8.21E-01	5.02E-01	9.8	3.52E-01
32	8.75E-02	2.77E-03	7.24E-04	8.08E+00	2.38E-05	2.27E-01	8.20E-01	5.02E-01	8.0	2.62E-01

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
33	4.49E-02	5.58E+01	1.43E+01	1.01E+01	4.62E+00	5.64E-01	9.15E-01	1.03E+00	57.8	1.29E-01
34	5.20E-02	6.09E+01	1.72E+01	1.03E+01	4.77E+00	5.14E-01	9.26E-01	1.03E+00	64.6	1.77E-01
35	7.46E-02	6.09E+01	1.75E+01	1.23E+01	5.82E+00	5.27E-01	9.27E-01	1.03E+00	66.9	1.79E-01
36	1.17E-01	5.96E+01	1.68E+01	1.70E+01	8.32E+00	5.67E-01	9.25E-01	1.04E+00	69.2	1.31E-01
37	1.82E-01	5.78E+01	1.57E+01	2.58E+01	1.35E+01	6.16E-01	9.23E-01	1.04E+00	72.9	7.42E-02
38	2.73E-01	5.63E+01	1.47E+01	3.00E+01	1.80E+01	5.01E-01	9.22E-01	1.04E+00	79.3	3.47E-02
39	2.83E-01	5.58E+01	1.43E+01	3.13E+01	1.90E+01	5.07E-01	9.21E-01	1.04E+00	79.6	3.09E-02
40	2.97E-01	5.57E+01	1.42E+01	3.27E+01	2.04E+01	5.06E-01	9.21E-01	1.04E+00	80.7	2.66E-02
41	3.27E-01	5.55E+01	1.42E+01	3.51E+01	2.35E+01	4.97E-01	9.22E-01	1.04E+00	83.3	1.84E-02
42	3.99E-01	5.52E+01	1.40E+01	1.46E+01	1.27E+01	1.76E-01	9.23E-01	1.04E+00	89.5	6.19E-03
43	8.48E-01	3.81E+00	1.11E+00	5.79E+01	5.02E+01	3.65E-01	8.47E-01	1.04E+00	81.2	8.36E-03
44	8.81E-01	6.59E-02	2.21E-02	6.20E+01	5.37E+01	3.79E-01	8.42E-01	1.04E+00	80.5	1.69E-02
45	8.80E-01	1.06E-03	4.12E-04	6.20E+01	5.36E+01	3.80E-01	8.42E-01	1.04E+00	80.3	2.69E-02
46	8.71E-01	1.69E-05	7.56E-06	6.18E+01	5.24E+01	3.84E-01	8.41E-01	1.03E+00	79.5	8.45E-03
47	8.29E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.00E-01	8.40E-01	1.03E+00	75.7	1.05E-02
48	6.38E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.39E-01	8.35E-01	1.03E+00	58.2	1.23E-02

TIME = 400.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
2	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
3	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
4	5.00E-02	4.37E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
5	5.00E-02	8.81E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
6	5.00E-02	1.69E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
7	5.00E-02	3.23E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
8	5.02E-02	6.05E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
9	5.12E-02	8.99E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.30E+00	50.0
10	5.26E-02	5.76E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E+00	1.30E+00	50.0
11	5.34E-02	1.54E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.02E+00	1.31E+00	49.9
12	5.36E-02	2.55E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.03E+00	1.31E+00	49.7
13	5.36E-02	3.38E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.04E+00	1.31E+00	49.3
14	5.34E-02	3.98E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E+00	1.32E+00	48.2
15	5.34E-02	4.33E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	45.4
16	5.55E-02	4.27E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	38.4
16	PRODUCT STREAM							1.32E+00	
17	4.89E-02	1.16E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.02E-01	20.6
18	4.87E-02	1.40E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	21.4
19	4.87E-02	1.47E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	22.2
20	4.89E-02	1.52E+01	0.00E+00	2.70E-05	4.98E-01	4.98E-01	1.11E+00	6.03E-01	23.2
21	4.94E-02	1.56E+01	1.53E-05	2.06E-04	4.98E-01	4.98E-01	1.11E+00	6.03E-01	24.3
22	5.12E-02	1.61E+01	1.22E-04	1.67E-03	4.98E-01	4.98E-01	1.11E+00	6.03E-01	25.6
23	5.70E-02	1.65E+01	9.62E-04	1.35E-02	4.97E-01	4.97E-01	1.11E+00	6.03E-01	27.1
24	7.43E-02	1.67E+01	7.30E-03	1.06E-01	4.97E-01	4.97E-01	1.11E+00	6.04E-01	28.8
25	1.22E-01	1.59E+01	5.08E-02	8.07E-01	4.93E-01	4.96E-01	1.11E+00	6.04E-01	30.7
26	2.32E-01	1.30E+01	2.91E-01	5.58E+00	4.72E-01	4.95E-01	1.12E+00	6.06E-01	33.0
27	3.77E-01	8.79E+00	1.24E+00	2.19E+01	4.02E-01	4.93E-01	1.14E+00	6.08E-01	35.5

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
28	3.95E-01	1.30E+00	4.45E-02	2.31E+01	3.98E-01	4.94E-01	1.13E+00	6.07E-01	35.5
29	3.96E-01	1.70E-01	8.55E-03	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.07E-01	35.4
30	3.93E-01	2.18E-02	2.39E-03	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	35.2
31	3.77E-01	2.75E-03	7.13E-04	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	34.3
32	3.09E-01	3.14E-04	1.96E-04	2.32E+01	3.99E-01	4.96E-01	1.13E+00	6.05E-01	31.1
32	PRODUCT STREAM							6.05E-01	
33	5.54E-01	3.48E+01	1.91E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.54E-01	40.0
34	7.19E-01	3.63E+01	2.16E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
35	1.00E+00	2.98E+01	1.77E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
36	1.42E+00	2.11E+01	1.19E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.57E-01	40.0
37	1.98E+00	1.37E+01	6.95E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.59E-01	40.0
38	2.75E+00	9.07E+00	3.89E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
39	2.81E+00	8.70E+00	3.64E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
40	2.95E+00	8.33E+00	3.38E+00	0.00E+00	0.00E+00	0.00E+00	1.11E+00	2.10E-01	40.0
41	3.26E+00	7.71E+00	2.91E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	2.12E-01	40.0
42	4.31E+00	7.15E+00	2.07E+00	0.00E+00	0.00E+00	0.00E+00	1.15E+00	5.53E-01	40.0
43	4.37E+00	1.24E-01	4.11E-02	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
44	4.37E+00	1.99E-03	7.62E-04	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
45	4.36E+00	3.21E-05	1.41E-05	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
46	4.29E+00	5.12E-07	2.64E-07	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.50E-01	40.0
47	3.97E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	5.44E-01	40.0
48	2.86E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	5.24E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
2	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
3	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
4	1.20E-03	1.97E-08	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
5	1.20E-03	3.97E-07	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
6	1.20E-03	7.62E-06	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
7	1.20E-03	1.46E-04	0.00E+00	5.21E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	2.53E-01
8	1.22E-03	2.79E-03	0.00E+00	5.32E-02	0.00E+00	2.80E-02	8.18E-01	1.50E+00	0.1	2.47E-01
9	1.40E-03	5.22E-02	0.00E+00	6.69E-02	0.00E+00	3.16E-02	8.18E-01	1.50E+00	0.2	2.04E-01
10	2.23E-03	7.77E-01	0.00E+00	1.55E-01	0.00E+00	4.88E-02	8.19E-01	1.50E+00	0.8	1.26E-01
11	3.50E-03	4.98E+00	0.00E+00	3.72E-01	0.00E+00	7.55E-02	8.25E-01	1.50E+00	4.1	7.26E-02
12	4.35E-03	1.33E+01	0.00E+00	6.00E-01	0.00E+00	9.32E-02	8.35E-01	1.51E+00	10.6	4.01E-02
13	4.67E-03	2.21E+01	0.00E+00	7.52E-01	0.00E+00	1.00E-01	8.47E-01	1.51E+00	17.4	2.25E-02
14	4.73E-03	2.92E+01	0.00E+00	8.45E-01	0.00E+00	1.02E-01	8.56E-01	1.51E+00	22.9	1.32E-02
15	4.68E-03	3.44E+01	0.00E+00	9.16E-01	0.00E+00	1.01E-01	8.63E-01	1.52E+00	26.8	7.95E-03
16	4.71E-03	3.74E+01	0.00E+00	1.01E+00	0.00E+00	9.80E-02	8.67E-01	1.52E+00	29.1	4.61E-03
17	6.53E-03	3.69E+01	0.00E+00	8.00E+00	0.00E+00	3.37E-01	8.66E-01	1.52E+00	28.9	2.34E-03
18	6.17E-03	4.14E+01	0.00E+00	7.47E+00	0.00E+00	3.20E-01	8.72E-01	1.52E+00	32.3	2.39E-03
19	6.10E-03	4.23E+01	0.00E+00	7.26E+00	0.00E+00	3.17E-01	8.74E-01	1.52E+00	33.0	2.40E-03
20	6.10E-03	4.26E+01	0.00E+00	7.09E+00	0.00E+00	3.15E-01	8.74E-01	1.52E+00	33.3	2.17E-03
21	6.15E-03	4.28E+01	1.07E-05	6.92E+00	1.22E-01	3.15E-01	8.74E-01	1.52E+00	33.4	2.13E-03
22	6.38E-03	4.30E+01	8.75E-05	6.75E+00	1.23E-01	3.14E-01	8.74E-01	1.52E+00	33.6	2.01E-03
23	7.10E-03	4.32E+01	7.11E-04	6.60E+00	1.24E-01	3.15E-01	8.75E-01	1.52E+00	33.8	1.85E-03
24	9.34E-03	4.33E+01	5.71E-03	6.56E+00	1.27E-01	3.17E-01	8.75E-01	1.52E+00	34.1	1.75E-03

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
25	1.59E-02	4.34E+01	4.50E-02	6.89E+00	1.32E-01	3.27E-01	8.75E-01	1.52E+00	34.8	1.54E-03
26	3.27E-02	4.30E+01	3.40E-01	8.30E+00	1.46E-01	3.54E-01	8.76E-01	1.52E+00	36.3	1.59E-03
27	6.04E-02	4.19E+01	2.33E+00	1.20E+01	2.53E-01	4.02E-01	8.78E-01	1.53E+00	39.4	1.34E-03
28	9.60E-02	1.06E+01	1.43E-01	6.77E+00	5.12E-03	2.02E-01	8.35E-01	5.03E-01	17.0	1.95E-03
29	1.06E-01	1.57E+00	3.09E-02	7.64E+00	1.11E-03	2.22E-01	8.23E-01	5.02E-01	10.9	2.57E-03
30	1.07E-01	2.06E-01	8.74E-03	7.79E+00	3.13E-04	2.25E-01	8.21E-01	5.02E-01	9.9	2.79E-03
31	1.02E-01	2.60E-02	2.53E-03	7.84E+00	9.07E-05	2.25E-01	8.21E-01	5.02E-01	9.4	2.89E-03
32	8.33E-02	2.95E-03	6.14E-04	7.78E+00	2.20E-05	2.24E-01	8.20E-01	5.01E-01	7.6	2.98E-03
33	4.81E-02	5.45E+01	1.36E+01	1.05E+01	4.78E+00	5.81E-01	9.12E-01	1.03E+00	56.6	1.48E-03
34	5.77E-02	5.94E+01	1.64E+01	1.09E+01	5.07E+00	5.36E-01	9.23E-01	1.03E+00	63.4	2.41E-03
35	8.29E-02	5.96E+01	1.68E+01	1.33E+01	6.30E+00	5.49E-01	9.25E-01	1.03E+00	66.1	2.44E-03
36	1.26E-01	5.86E+01	1.62E+01	1.83E+01	9.02E+00	5.86E-01	9.23E-01	1.03E+00	68.9	1.87E-03
37	1.91E-01	5.72E+01	1.53E+01	2.72E+01	1.44E+01	6.28E-01	9.22E-01	1.04E+00	73.0	1.16E-03
38	2.79E-01	5.60E+01	1.45E+01	3.07E+01	1.86E+01	5.04E-01	9.21E-01	1.04E+00	79.5	5.63E-04
39	2.87E-01	5.57E+01	1.43E+01	3.18E+01	1.95E+01	5.08E-01	9.21E-01	1.04E+00	79.9	5.24E-04
40	3.01E-01	5.56E+01	1.42E+01	3.31E+01	2.08E+01	5.06E-01	9.21E-01	1.04E+00	81.0	4.74E-04
41	3.30E-01	5.55E+01	1.41E+01	3.53E+01	2.38E+01	4.96E-01	9.22E-01	1.04E+00	83.5	3.40E-04
42	4.00E-01	5.52E+01	1.40E+01	1.46E+01	1.28E+01	1.75E-01	9.23E-01	1.04E+00	89.6	1.27E-04
43	8.50E-01	3.81E+00	1.11E+00	5.79E+01	5.05E+01	3.65E-01	8.47E-01	1.04E+00	81.4	1.47E-04
44	8.83E-01	6.59E-02	2.19E-02	6.20E+01	5.40E+01	3.79E-01	8.42E-01	1.04E+00	80.6	2.33E-04
45	8.82E-01	1.06E-03	4.06E-04	6.20E+01	5.38E+01	3.80E-01	8.42E-01	1.04E+00	80.5	5.80E-04
46	8.74E-01	1.69E-05	7.40E-06	6.19E+01	5.27E+01	3.83E-01	8.41E-01	1.03E+00	79.8	2.02E-04
47	8.33E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.99E-01	8.40E-01	1.03E+00	76.0	2.38E-04
48	6.42E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.39E-01	8.35E-01	1.03E+00	58.6	2.93E-04

TIME = 600.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
2	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
3	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
4	5.00E-02	3.24E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
5	5.00E-02	6.54E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
6	5.00E-02	1.26E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
7	5.00E-02	2.42E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
8	5.02E-02	4.57E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
9	5.10E-02	7.13E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.30E+00	50.0
10	5.25E-02	5.05E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E+00	1.30E+00	50.0
11	5.34E-02	1.44E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.02E+00	1.31E+00	49.9
12	5.36E-02	2.47E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.03E+00	1.31E+00	49.7
13	5.36E-02	3.32E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.04E+00	1.31E+00	49.3
14	5.34E-02	3.94E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E+00	1.32E+00	48.2
15	5.34E-02	4.30E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	45.4
16	5.55E-02	4.25E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	38.4
16	PRODUCT STREAM							1.32E+00	
17	4.89E-02	1.16E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.02E-01	20.6
18	4.87E-02	1.40E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	21.4
19	4.87E-02	1.47E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	22.2

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
20	4.89E-02	1.52E+01	0.00E+00	2.70E-05	4.98E-01	4.98E-01	1.11E+00	6.03E-01	23.2
21	4.94E-02	1.56E+01	1.53E-05	2.06E-04	4.98E-01	4.98E-01	1.11E+00	6.03E-01	24.3
22	5.12E-02	1.61E+01	1.22E-04	1.67E-03	4.98E-01	4.98E-01	1.11E+00	6.03E-01	25.6
23	5.70E-02	1.65E+01	9.61E-04	1.35E-02	4.97E-01	4.97E-01	1.11E+00	6.03E-01	27.0
24	7.43E-02	1.66E+01	7.29E-03	1.06E-01	4.97E-01	4.97E-01	1.11E+00	6.04E-01	28.7
25	1.22E-01	1.58E+01	5.08E-02	8.07E-01	4.93E-01	4.96E-01	1.11E+00	6.04E-01	30.7
26	2.32E-01	1.30E+01	2.91E-01	5.58E+00	4.72E-01	4.95E-01	1.12E+00	6.06E-01	32.9
27	3.77E-01	8.78E+00	1.24E+00	2.19E+01	4.02E-01	4.93E-01	1.14E+00	6.08E-01	35.5
28	3.95E-01	1.30E+00	4.45E-02	2.31E+01	3.98E-01	4.94E-01	1.13E+00	6.07E-01	35.5
29	3.96E-01	1.70E-01	8.56E-03	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.07E-01	35.4
30	3.93E-01	2.18E-02	2.39E-03	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	35.2
31	3.77E-01	2.74E-03	7.14E-04	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	34.2
32	3.09E-01	3.13E-04	1.97E-04	2.31E+01	3.99E-01	4.96E-01	1.13E+00	6.05E-01	31.0
32	PRODUCT STREAM							6.05E-01	
33	5.55E-01	3.47E+01	1.91E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.54E-01	40.0
34	7.20E-01	3.62E+01	2.16E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
35	1.01E+00	2.98E+01	1.77E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
36	1.43E+00	2.11E+01	1.18E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.57E-01	40.0
37	1.99E+00	1.37E+01	6.95E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.59E-01	40.0
38	2.75E+00	9.06E+00	3.89E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
39	2.81E+00	8.70E+00	3.64E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
40	2.95E+00	8.32E+00	3.37E+00	0.00E+00	0.00E+00	0.00E+00	1.11E+00	2.10E-01	40.0
41	3.26E+00	7.71E+00	2.91E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	2.12E-01	40.0
42	4.31E+00	7.14E+00	2.07E+00	0.00E+00	0.00E+00	0.00E+00	1.15E+00	5.53E-01	40.0
43	4.37E+00	1.24E-01	4.11E-02	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
44	4.37E+00	1.99E-03	7.61E-04	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
45	4.36E+00	3.21E-05	1.41E-05	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
46	4.29E+00	5.12E-07	2.64E-07	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.50E-01	40.0
47	3.97E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	5.44E-01	40.0
48	2.86E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	5.24E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
2	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
3	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
4	1.20E-03	1.46E-08	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
5	1.20E-03	2.95E-07	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
6	1.20E-03	5.68E-06	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
7	1.20E-03	1.09E-04	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	6.11E-02
8	1.22E-03	2.09E-03	0.00E+00	5.29E-02	0.00E+00	2.79E-02	8.18E-01	1.50E+00	0.1	5.92E-02
9	1.36E-03	3.95E-02	0.00E+00	6.39E-02	0.00E+00	3.08E-02	8.18E-01	1.50E+00	0.2	4.99E-02
10	2.11E-03	6.18E-01	0.00E+00	1.41E-01	0.00E+00	4.64E-02	8.19E-01	1.50E+00	0.7	3.10E-02
11	3.40E-03	4.37E+00	0.00E+00	3.49E-01	0.00E+00	7.32E-02	8.24E-01	1.50E+00	3.7	1.77E-02
12	4.29E-03	1.25E+01	0.00E+00	5.82E-01	0.00E+00	9.21E-02	8.34E-01	1.51E+00	10.0	9.57E-03
13	4.65E-03	2.14E+01	0.00E+00	7.42E-01	0.00E+00	9.99E-02	8.46E-01	1.51E+00	16.8	5.23E-03
14	4.73E-03	2.87E+01	0.00E+00	8.40E-01	0.00E+00	1.02E-01	8.56E-01	1.51E+00	22.5	2.81E-03
15	4.68E-03	3.41E+01	0.00E+00	9.14E-01	0.00E+00	1.01E-01	8.63E-01	1.52E+00	26.6	1.51E-03
16	4.72E-03	3.72E+01	0.00E+00	1.01E+00	0.00E+00	9.80E-02	8.67E-01	1.52E+00	29.0	6.61E-04

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
17	6.53E-03	3.68E+01	0.00E+00	8.00E+00	0.00E+00	3.37E-01	8.66E-01	1.52E+00	28.9	5.02E-05
18	6.18E-03	4.14E+01	0.00E+00	7.48E+00	0.00E+00	3.20E-01	8.72E-01	1.52E+00	32.3	2.60E-05
19	6.11E-03	4.23E+01	0.00E+00	7.26E+00	0.00E+00	3.17E-01	8.73E-01	1.52E+00	33.0	1.15E-04
20	6.10E-03	4.26E+01	0.00E+00	7.10E+00	0.00E+00	3.16E-01	8.74E-01	1.52E+00	33.2	1.79E-05
21	6.16E-03	4.28E+01	1.07E-05	6.93E+00	1.22E-01	3.15E-01	8.74E-01	1.52E+00	33.4	4.94E-05
22	6.38E-03	4.29E+01	8.74E-05	6.76E+00	1.23E-01	3.14E-01	8.74E-01	1.52E+00	33.5	2.86E-04
23	7.10E-03	4.31E+01	7.11E-04	6.61E+00	1.24E-01	3.15E-01	8.75E-01	1.52E+00	33.7	3.16E-04
24	9.34E-03	4.33E+01	5.71E-03	6.57E+00	1.27E-01	3.18E-01	8.75E-01	1.52E+00	34.1	1.57E-04
25	1.59E-02	4.33E+01	4.50E-02	6.90E+00	1.32E-01	3.27E-01	8.75E-01	1.52E+00	34.7	3.64E-05
26	3.27E-02	4.30E+01	3.40E-01	8.31E+00	1.46E-01	3.54E-01	8.76E-01	1.52E+00	36.2	4.16E-05
27	6.04E-02	4.18E+01	2.33E+00	1.20E+01	2.53E-01	4.02E-01	8.78E-01	1.53E+00	39.4	3.94E-05
28	9.60E-02	1.06E+01	1.43E-01	6.77E+00	5.12E-03	2.02E-01	8.35E-01	5.03E-01	17.0	8.23E-05
29	1.06E-01	1.57E+00	3.09E-02	7.64E+00	1.11E-03	2.22E-01	8.23E-01	5.02E-01	10.9	2.03E-04
30	1.07E-01	2.05E-01	8.74E-03	7.79E+00	3.13E-04	2.25E-01	8.21E-01	5.02E-01	9.9	2.03E-04
31	1.02E-01	2.60E-02	2.54E-03	7.84E+00	9.09E-05	2.25E-01	8.21E-01	5.02E-01	9.4	2.46E-04
32	8.32E-02	2.94E-03	6.15E-04	7.78E+00	2.20E-05	2.24E-01	8.20E-01	5.01E-01	7.6	2.95E-04
33	4.81E-02	5.44E+01	1.36E+01	1.05E+01	4.78E+00	5.81E-01	9.12E-01	1.03E+00	56.6	3.39E-05
34	5.78E-02	5.94E+01	1.64E+01	1.09E+01	5.08E+00	5.36E-01	9.23E-01	1.03E+00	63.4	5.01E-05
35	8.30E-02	5.96E+01	1.68E+01	1.33E+01	6.31E+00	5.49E-01	9.24E-01	1.03E+00	66.1	5.71E-05
36	1.26E-01	5.86E+01	1.62E+01	1.83E+01	9.03E+00	5.86E-01	9.23E-01	1.03E+00	68.9	4.04E-05
37	1.91E-01	5.72E+01	1.53E+01	2.72E+01	1.44E+01	6.28E-01	9.22E-01	1.04E+00	73.0	1.06E-04
38	2.79E-01	5.60E+01	1.45E+01	3.08E+01	1.86E+01	5.04E-01	9.21E-01	1.04E+00	79.5	5.82E-05
39	2.88E-01	5.57E+01	1.43E+01	3.18E+01	1.95E+01	5.08E-01	9.21E-01	1.04E+00	79.9	4.22E-05
40	3.01E-01	5.56E+01	1.42E+01	3.31E+01	2.08E+01	5.06E-01	9.21E-01	1.04E+00	81.0	4.01E-05
41	3.30E-01	5.55E+01	1.41E+01	3.53E+01	2.38E+01	4.96E-01	9.22E-01	1.04E+00	83.5	3.02E-05
42	4.00E-01	5.52E+01	1.40E+01	1.46E+01	1.28E+01	1.75E-01	9.23E-01	1.04E+00	89.6	0.00E+00
43	8.50E-01	3.81E+00	1.11E+00	5.79E+01	5.05E+01	3.65E-01	8.47E-01	1.04E+00	81.4	0.00E+00
44	8.83E-01	6.59E-02	2.19E-02	6.20E+01	5.40E+01	3.79E-01	8.42E-01	1.04E+00	80.6	0.00E+00
45	8.82E-01	1.06E-03	4.06E-04	6.20E+01	5.38E+01	3.80E-01	8.42E-01	1.04E+00	80.5	0.00E+00
46	8.74E-01	1.69E-05	7.40E-06	6.19E+01	5.28E+01	3.83E-01	8.41E-01	1.03E+00	79.8	0.00E+00
47	8.33E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.99E-01	8.40E-01	1.03E+00	76.0	0.00E+00
48	6.42E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.39E-01	8.35E-01	1.03E+00	58.6	0.00E+00

TIME = 800.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
2	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
3	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
4	5.00E-02	3.04E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
5	5.00E-02	6.16E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
6	5.00E-02	1.19E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
7	5.00E-02	2.28E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
8	5.02E-02	4.32E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
9	5.10E-02	6.81E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.30E+00	50.0
10	5.24E-02	4.91E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E+00	1.30E+00	50.0
11	5.33E-02	1.42E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.02E+00	1.31E+00	49.9
12	5.36E-02	2.45E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.03E+00	1.31E+00	49.7

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
13	5.36E-02	3.30E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.04E+00	1.31E+00	49.3
14	5.34E-02	3.93E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E+00	1.32E+00	48.2
15	5.34E-02	4.29E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	45.4
16	5.55E-02	4.25E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	38.4
16	PRODUCT STREAM							1.32E+00	
17	4.89E-02	1.16E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.02E-01	20.6
18	4.87E-02	1.40E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	21.4
19	4.87E-02	1.47E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	22.2
20	4.89E-02	1.52E+01	0.00E+00	2.70E-05	4.98E-01	4.98E-01	1.11E+00	6.03E-01	23.2
21	4.94E-02	1.56E+01	1.53E-05	2.06E-04	4.98E-01	4.98E-01	1.11E+00	6.03E-01	24.3
22	5.12E-02	1.61E+01	1.22E-04	1.67E-03	4.98E-01	4.98E-01	1.11E+00	6.03E-01	25.6
23	5.70E-02	1.65E+01	9.61E-04	1.35E-02	4.97E-01	4.97E-01	1.11E+00	6.03E-01	27.0
24	7.43E-02	1.66E+01	7.29E-03	1.06E-01	4.97E-01	4.97E-01	1.11E+00	6.04E-01	28.7
25	1.22E-01	1.58E+01	5.08E-02	8.07E-01	4.93E-01	4.96E-01	1.11E+00	6.04E-01	30.7
26	2.32E-01	1.30E+01	2.91E-01	5.58E+00	4.72E-01	4.95E-01	1.12E+00	6.06E-01	32.9
27	3.77E-01	8.78E+00	1.24E+00	2.19E+01	4.02E-01	4.93E-01	1.14E+00	6.08E-01	35.5
28	3.95E-01	1.30E+00	4.45E-02	2.31E+01	3.98E-01	4.94E-01	1.13E+00	6.07E-01	35.5
29	3.96E-01	1.70E-01	8.56E-03	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.07E-01	35.4
30	3.93E-01	2.18E-02	2.39E-03	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	35.2
31	3.77E-01	2.74E-03	7.14E-04	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	34.2
32	3.09E-01	3.13E-04	1.97E-04	2.31E+01	3.99E-01	4.96E-01	1.13E+00	6.05E-01	31.0
32	PRODUCT STREAM							6.05E-01	
33	5.55E-01	3.47E+01	1.91E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.54E-01	40.0
34	7.20E-01	3.62E+01	2.16E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
35	1.01E+00	2.98E+01	1.77E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
36	1.43E+00	2.11E+01	1.18E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.57E-01	40.0
37	1.99E+00	1.37E+01	6.95E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.59E-01	40.0
38	2.75E+00	9.06E+00	3.89E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
39	2.81E+00	8.70E+00	3.64E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
40	2.95E+00	8.32E+00	3.37E+00	0.00E+00	0.00E+00	0.00E+00	1.11E+00	2.10E-01	40.0
41	3.26E+00	7.71E+00	2.91E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	2.12E-01	40.0
42	4.31E+00	7.14E+00	2.07E+00	0.00E+00	0.00E+00	0.00E+00	1.15E+00	5.53E-01	40.0
43	4.37E+00	1.24E-01	4.11E-02	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
44	4.37E+00	1.99E-03	7.61E-04	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
45	4.36E+00	3.21E-05	1.41E-05	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
46	4.29E+00	5.12E-07	2.64E-07	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.50E-01	40.0
47	3.97E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	5.44E-01	40.0
48	2.86E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	5.24E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
2	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
3	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
4	1.20E-03	1.37E-08	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
5	1.20E-03	2.78E-07	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
6	1.20E-03	5.35E-06	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
7	1.20E-03	1.03E-04	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	1.06E-02
8	1.21E-03	1.98E-03	0.00E+00	5.29E-02	0.00E+00	2.79E-02	8.18E-01	1.50E+00	0.1	1.03E-02

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
9	1.36E-03	3.74E-02	0.00E+00	6.34E-02	0.00E+00	3.07E-02	8.18E-01	1.50E+00	0.2	8.75E-03
10	2.09E-03	5.90E-01	0.00E+00	1.38E-01	0.00E+00	4.60E-02	8.19E-01	1.50E+00	0.6	5.42E-03
11	3.37E-03	4.26E+00	0.00E+00	3.44E-01	0.00E+00	7.27E-02	8.24E-01	1.50E+00	3.6	3.10E-03
12	4.28E-03	1.23E+01	0.00E+00	5.79E-01	0.00E+00	9.18E-02	8.34E-01	1.51E+00	9.9	1.67E-03
13	4.65E-03	2.13E+01	0.00E+00	7.40E-01	0.00E+00	9.98E-02	8.46E-01	1.51E+00	16.7	9.03E-04
14	4.73E-03	2.86E+01	0.00E+00	8.39E-01	0.00E+00	1.02E-01	8.56E-01	1.51E+00	22.4	5.23E-04
15	4.68E-03	3.40E+01	0.00E+00	9.14E-01	0.00E+00	1.01E-01	8.63E-01	1.52E+00	26.5	2.77E-04
16	4.72E-03	3.72E+01	0.00E+00	1.01E+00	0.00E+00	9.80E-02	8.67E-01	1.52E+00	29.0	8.78E-05
17	6.53E-03	3.68E+01	0.00E+00	8.00E+00	0.00E+00	3.37E-01	8.66E-01	1.52E+00	28.9	0.00E+00
18	6.18E-03	4.14E+01	0.00E+00	7.48E+00	0.00E+00	3.20E-01	8.72E-01	1.52E+00	32.3	0.00E+00
19	6.11E-03	4.23E+01	0.00E+00	7.27E+00	0.00E+00	3.17E-01	8.73E-01	1.52E+00	33.0	0.00E+00
20	6.10E-03	4.26E+01	0.00E+00	7.10E+00	0.00E+00	3.16E-01	8.74E-01	1.52E+00	33.2	0.00E+00
21	6.16E-03	4.28E+01	1.07E-05	6.93E+00	1.22E-01	3.15E-01	8.74E-01	1.52E+00	33.4	0.00E+00
22	6.38E-03	4.29E+01	8.74E-05	6.76E+00	1.23E-01	3.14E-01	8.74E-01	1.52E+00	33.5	0.00E+00
23	7.10E-03	4.31E+01	7.11E-04	6.61E+00	1.24E-01	3.15E-01	8.75E-01	1.52E+00	33.7	0.00E+00
24	9.34E-03	4.33E+01	5.71E-03	6.57E+00	1.27E-01	3.18E-01	8.75E-01	1.52E+00	34.1	0.00E+00
25	1.59E-02	4.33E+01	4.50E-02	6.90E+00	1.32E-01	3.27E-01	8.75E-01	1.52E+00	34.7	0.00E+00
26	3.27E-02	4.30E+01	3.40E-01	8.31E+00	1.46E-01	3.54E-01	8.76E-01	1.52E+00	36.2	0.00E+00
27	6.04E-02	4.18E+01	2.33E+00	1.20E+01	2.53E-01	4.02E-01	8.78E-01	1.53E+00	39.4	0.00E+00
28	9.60E-02	1.06E+01	1.43E-01	6.77E+00	5.12E-03	2.02E-01	8.35E-01	5.03E-01	17.0	0.00E+00
29	1.06E-01	1.57E+00	3.09E-02	7.64E+00	1.11E-03	2.22E-01	8.23E-01	5.02E-01	10.9	0.00E+00
30	1.07E-01	2.05E-01	8.74E-03	7.79E+00	3.13E-04	2.25E-01	8.21E-01	5.02E-01	9.9	0.00E+00
31	1.02E-01	2.60E-02	2.54E-03	7.84E+00	9.09E-05	2.25E-01	8.21E-01	5.02E-01	9.4	0.00E+00
32	8.32E-02	2.94E-03	6.15E-04	7.78E+00	2.20E-05	2.24E-01	8.20E-01	5.01E-01	7.6	0.00E+00
33	4.81E-02	5.44E+01	1.36E+01	1.05E+01	4.78E+00	5.81E-01	9.12E-01	1.03E+00	56.6	0.00E+00
34	5.78E-02	5.94E+01	1.64E+01	1.09E+01	5.08E+00	5.36E-01	9.23E-01	1.03E+00	63.4	0.00E+00
35	8.30E-02	5.96E+01	1.68E+01	1.33E+01	6.31E+00	5.49E-01	9.24E-01	1.03E+00	66.1	0.00E+00
36	1.26E-01	5.86E+01	1.62E+01	1.83E+01	9.03E+00	5.86E-01	9.23E-01	1.03E+00	68.9	0.00E+00
37	1.91E-01	5.72E+01	1.53E+01	2.72E+01	1.44E+01	6.28E-01	9.22E-01	1.04E+00	73.0	0.00E+00
38	2.79E-01	5.60E+01	1.45E+01	3.08E+01	1.86E+01	5.04E-01	9.21E-01	1.04E+00	79.5	0.00E+00
39	2.88E-01	5.57E+01	1.43E+01	3.18E+01	1.95E+01	5.08E-01	9.21E-01	1.04E+00	79.9	0.00E+00
40	3.01E-01	5.56E+01	1.42E+01	3.31E+01	2.08E+01	5.06E-01	9.21E-01	1.04E+00	81.0	0.00E+00
41	3.30E-01	5.55E+01	1.41E+01	3.53E+01	2.38E+01	4.96E-01	9.22E-01	1.04E+00	83.5	0.00E+00
42	4.00E-01	5.52E+01	1.40E+01	1.46E+01	1.28E+01	1.75E-01	9.23E-01	1.04E+00	89.6	0.00E+00
43	8.50E-01	3.81E+00	1.11E+00	5.79E+01	5.05E+01	3.65E-01	8.47E-01	1.04E+00	81.4	0.00E+00
44	8.83E-01	6.59E-02	2.19E-02	6.20E+01	5.40E+01	3.79E-01	8.42E-01	1.04E+00	80.6	0.00E+00
45	8.82E-01	1.06E-03	4.06E-04	6.20E+01	5.38E+01	3.80E-01	8.42E-01	1.04E+00	80.5	0.00E+00
46	8.74E-01	1.69E-05	7.40E-06	6.19E+01	5.28E+01	3.83E-01	8.41E-01	1.03E+00	79.8	0.00E+00
47	8.33E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.99E-01	8.40E-01	1.03E+00	76.0	0.00E+00
48	6.42E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.39E-01	8.35E-01	1.03E+00	58.6	0.00E+00

TIME = 1000.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
2	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
3	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
4	5.00E-02	3.01E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
5	5.00E-02	6.10E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
6	5.00E-02	1.18E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
7	5.00E-02	2.26E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
8	5.02E-02	4.28E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
9	5.10E-02	6.75E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.30E+00	50.0
10	5.24E-02	4.89E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E+00	1.30E+00	50.0
11	5.33E-02	1.42E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.02E+00	1.31E+00	49.9
12	5.36E-02	2.45E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.03E+00	1.31E+00	49.7
13	5.36E-02	3.30E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.04E+00	1.31E+00	49.3
14	5.34E-02	3.93E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E+00	1.32E+00	48.2
15	5.34E-02	4.29E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	45.4
16	5.55E-02	4.25E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	38.4
16	PRODUCT STREAM							1.32E+00	
17	4.89E-02	1.16E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.02E-01	20.6
18	4.87E-02	1.40E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	21.4
19	4.87E-02	1.47E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	22.2
20	4.89E-02	1.52E+01	0.00E+00	2.70E-05	4.98E-01	4.98E-01	1.11E+00	6.03E-01	23.2
21	4.94E-02	1.56E+01	1.53E-05	2.06E-04	4.98E-01	4.98E-01	1.11E+00	6.03E-01	24.3
22	5.12E-02	1.61E+01	1.22E-04	1.67E-03	4.98E-01	4.98E-01	1.11E+00	6.03E-01	25.6
23	5.70E-02	1.65E+01	9.61E-04	1.35E-02	4.97E-01	4.97E-01	1.11E+00	6.03E-01	27.0
24	7.43E-02	1.66E+01	7.29E-03	1.06E-01	4.97E-01	4.97E-01	1.11E+00	6.04E-01	28.7
25	1.22E-01	1.58E+01	5.08E-02	8.07E-01	4.93E-01	4.96E-01	1.11E+00	6.04E-01	30.7
26	2.32E-01	1.30E+01	2.91E-01	5.58E+00	4.72E-01	4.95E-01	1.12E+00	6.06E-01	32.9
27	3.77E-01	8.78E+00	1.24E+00	2.19E+01	4.02E-01	4.93E-01	1.14E+00	6.08E-01	35.5
28	3.95E-01	1.30E+00	4.45E-02	2.31E+01	3.98E-01	4.94E-01	1.13E+00	6.07E-01	35.5
29	3.96E-01	1.70E-01	8.56E-03	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.07E-01	35.4
30	3.93E-01	2.18E-02	2.39E-03	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	35.2
31	3.77E-01	2.74E-03	7.14E-04	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	34.2
32	3.09E-01	3.13E-04	1.97E-04	2.31E+01	3.99E-01	4.96E-01	1.13E+00	6.05E-01	31.0
32	PRODUCT STREAM							6.05E-01	
33	5.55E-01	3.47E+01	1.91E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.54E-01	40.0
34	7.20E-01	3.62E+01	2.16E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
35	1.01E+00	2.98E+01	1.77E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
36	1.43E+00	2.11E+01	1.18E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.57E-01	40.0
37	1.99E+00	1.37E+01	6.95E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.59E-01	40.0
38	2.75E+00	9.06E+00	3.89E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
39	2.81E+00	8.70E+00	3.64E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
40	2.95E+00	8.32E+00	3.37E+00	0.00E+00	0.00E+00	0.00E+00	1.11E+00	2.10E-01	40.0
41	3.26E+00	7.71E+00	2.91E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	2.12E-01	40.0
42	4.31E+00	7.14E+00	2.07E+00	0.00E+00	0.00E+00	0.00E+00	1.15E+00	5.53E-01	40.0
43	4.37E+00	1.24E-01	4.11E-02	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
44	4.37E+00	1.99E-03	7.61E-04	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
45	4.36E+00	3.21E-05	1.41E-05	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
46	4.29E+00	5.12E-07	2.64E-07	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.50E-01	40.0
47	3.97E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	5.44E-01	40.0
48	2.86E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	5.24E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
2	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
3	1.20E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
4	1.20E-03	1.36E-08	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
5	1.20E-03	2.75E-07	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
6	1.20E-03	5.30E-06	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
7	1.20E-03	1.02E-04	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	1.82E-03
8	1.21E-03	1.96E-03	0.00E+00	5.29E-02	0.00E+00	2.79E-02	8.18E-01	1.50E+00	0.1	1.75E-03
9	1.36E-03	3.71E-02	0.00E+00	6.33E-02	0.00E+00	3.07E-02	8.18E-01	1.50E+00	0.2	1.45E-03
10	2.09E-03	5.85E-01	0.00E+00	1.38E-01	0.00E+00	4.59E-02	8.19E-01	1.50E+00	0.6	8.63E-04
11	3.37E-03	4.24E+00	0.00E+00	3.43E-01	0.00E+00	7.26E-02	8.24E-01	1.50E+00	3.6	5.12E-04
12	4.28E-03	1.23E+01	0.00E+00	5.78E-01	0.00E+00	9.18E-02	8.34E-01	1.51E+00	9.8	2.80E-04
13	4.65E-03	2.12E+01	0.00E+00	7.40E-01	0.00E+00	9.98E-02	8.46E-01	1.51E+00	16.7	1.66E-04
14	4.72E-03	2.86E+01	0.00E+00	8.39E-01	0.00E+00	1.02E-01	8.55E-01	1.51E+00	22.4	9.01E-05
15	4.68E-03	3.40E+01	0.00E+00	9.13E-01	0.00E+00	1.01E-01	8.63E-01	1.52E+00	26.5	4.56E-05
16	4.72E-03	3.72E+01	0.00E+00	1.01E+00	0.00E+00	9.80E-02	8.67E-01	1.52E+00	29.0	0.00E+00
17	6.53E-03	3.68E+01	0.00E+00	8.00E+00	0.00E+00	3.37E-01	8.66E-01	1.52E+00	28.9	0.00E+00
18	6.18E-03	4.14E+01	0.00E+00	7.48E+00	0.00E+00	3.20E-01	8.72E-01	1.52E+00	32.3	0.00E+00
19	6.11E-03	4.23E+01	0.00E+00	7.27E+00	0.00E+00	3.17E-01	8.73E-01	1.52E+00	33.0	0.00E+00
20	6.10E-03	4.26E+01	0.00E+00	7.10E+00	0.00E+00	3.16E-01	8.74E-01	1.52E+00	33.2	0.00E+00
21	6.16E-03	4.28E+01	1.07E-05	6.93E+00	1.22E-01	3.15E-01	8.74E-01	1.52E+00	33.4	0.00E+00
22	6.38E-03	4.29E+01	8.74E-05	6.76E+00	1.23E-01	3.14E-01	8.74E-01	1.52E+00	33.5	0.00E+00
23	7.10E-03	4.31E+01	7.11E-04	6.61E+00	1.24E-01	3.15E-01	8.75E-01	1.52E+00	33.7	0.00E+00
24	9.34E-03	4.33E+01	5.71E-03	6.57E+00	1.27E-01	3.18E-01	8.75E-01	1.52E+00	34.1	0.00E+00
25	1.59E-02	4.33E+01	4.50E-02	6.90E+00	1.32E-01	3.27E-01	8.75E-01	1.52E+00	34.7	0.00E+00
26	3.27E-02	4.30E+01	3.40E-01	8.31E+00	1.46E-01	3.54E-01	8.76E-01	1.52E+00	36.2	0.00E+00
27	6.04E-02	4.18E+01	2.33E+00	1.20E+01	2.53E-01	4.02E-01	8.78E-01	1.53E+00	39.4	0.00E+00
28	9.60E-02	1.06E+01	1.43E-01	6.77E+00	5.12E-03	2.02E-01	8.35E-01	5.03E-01	17.0	0.00E+00
29	1.06E-01	1.57E+00	3.09E-02	7.64E+00	1.11E-03	2.22E-01	8.23E-01	5.02E-01	10.9	0.00E+00
30	1.07E-01	2.05E-01	8.74E-03	7.79E+00	3.13E-04	2.25E-01	8.21E-01	5.02E-01	9.9	0.00E+00
31	1.02E-01	2.60E-02	2.54E-03	7.84E+00	9.09E-05	2.25E-01	8.21E-01	5.02E-01	9.4	0.00E+00
32	8.32E-02	2.94E-03	6.15E-04	7.78E+00	2.20E-05	2.24E-01	8.20E-01	5.01E-01	7.6	0.00E+00
33	4.81E-02	5.44E+01	1.36E+01	1.05E+01	4.78E+00	5.81E-01	9.12E-01	1.03E+00	56.6	0.00E+00
34	5.78E-02	5.94E+01	1.64E+01	1.09E+01	5.08E+00	5.36E-01	9.23E-01	1.03E+00	63.4	0.00E+00
35	8.30E-02	5.96E+01	1.68E+01	1.33E+01	6.31E+00	5.49E-01	9.24E-01	1.03E+00	66.1	0.00E+00
36	1.26E-01	5.86E+01	1.62E+01	1.83E+01	9.03E+00	5.86E-01	9.23E-01	1.03E+00	68.9	0.00E+00
37	1.91E-01	5.72E+01	1.53E+01	2.72E+01	1.44E+01	6.28E-01	9.22E-01	1.04E+00	73.0	0.00E+00
38	2.79E-01	5.60E+01	1.45E+01	3.08E+01	1.86E+01	5.04E-01	9.21E-01	1.04E+00	79.5	0.00E+00
39	2.88E-01	5.57E+01	1.43E+01	3.18E+01	1.95E+01	5.08E-01	9.21E-01	1.04E+00	79.9	0.00E+00
40	3.01E-01	5.56E+01	1.42E+01	3.31E+01	2.08E+01	5.06E-01	9.21E-01	1.04E+00	81.0	0.00E+00
41	3.30E-01	5.55E+01	1.41E+01	3.53E+01	2.38E+01	4.96E-01	9.22E-01	1.04E+00	83.5	0.00E+00
42	4.00E-01	5.52E+01	1.40E+01	1.46E+01	1.28E+01	1.75E-01	9.23E-01	1.04E+00	89.6	0.00E+00
43	8.50E-01	3.81E+00	1.11E+00	5.79E+01	5.05E+01	3.65E-01	8.47E-01	1.04E+00	81.4	0.00E+00
44	8.83E-01	6.59E-02	2.19E-02	6.20E+01	5.40E+01	3.79E-01	8.42E-01	1.04E+00	80.6	0.00E+00
45	8.82E-01	1.06E-03	4.06E-04	6.20E+01	5.38E+01	3.80E-01	8.42E-01	1.04E+00	80.5	0.00E+00
46	8.74E-01	1.69E-05	7.40E-06	6.19E+01	5.28E+01	3.83E-01	8.41E-01	1.03E+00	79.8	0.00E+00
47	8.33E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.99E-01	8.40E-01	1.03E+00	76.0	0.00E+00
48	6.42E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.39E-01	8.35E-01	1.03E+00	58.6	0.00E+00

4.2 STEADY-STATE CALCULATION

The steady-state concentration profiles were obtained in a parallel run by using the Trapezoidal integration technique. The output is reproduced in this section. This run was made using an IBM-compatible personal computer (8 MHz with 16-bit processor). Steady-state was achieved in 1467 min and required 2 h 59 min of computer time.

Steady-state concentration profiles are shown in Figs. 13 through 15 and the profile for degree of saturation of the TBP extractant is shown in Fig. 16. These figures were prepared directly from the ASCII Problem Results file by using commercial graphics software.

PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11: 06-08-1990 09:58

Problem: BREEDER FLOWSHEET EXAMPLE

PUREX PROCESS
Total stages: 48
Volume % TBP in solvent: 30.0
Initial or default temperature (°C): 40.0
Organic taken from stage 33 feeds stage 27 .
Reduction of Pu(IV) by hydroxylamine nitrate.
Minutes per time increment: 1.00
Minutes between printing of the concentration profile: 1000
Calculations will stop after 5000 minutes or when a tolerance of 0.0001 % per minute is reached.
Total mixer volumes are defined (phase ratios = flow ratios).
Total settler volumes are defined (phase ratios = flow ratios).
Initial concentration profile is zero.
Trapezoidal integration will be used.
Extra product stream(s).

The FILESPEC for this Problem Definition data file is: B:EXPL_2P.DAT
The FILESPEC for this Problem Results data file is: B:EXPL_2R.DAT

FEED AND PRODUCT STREAM DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
AQUEOUS	1	5.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.30E+00	50.0
AQUEOUS	17	5.00E-02	0.00E+00	0.00E+00	0.00E+00	5.00E-01	5.00E-01	6.00E-01	20.0
30.0 % TBP	32	0.00E+00	0.00E+00	0.00E+00				5.00E-01	20.0
AQUEOUS	33	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.50E-01	40.0
AQUEOUS	38	5.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.00E-02	40.0
AQUEOUS	42	3.50E+00	1.60E+02	4.00E+01	0.00E+00	0.00E+00	0.00E+00	3.50E-01	40.0
30.0 % TBP	48	0.00E+00	0.00E+00	0.00E+00				1.00E+00	40.0
AQUEOUS	16	Product stream removed (actual flow rate to be computed)						1.30E+00	
AQUEOUS	32	Product stream removed (actual flow rate to be computed)						6.00E-01	

STAGE VOLUME AND FLOW RATE DATA (Molal basis):

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	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
2	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
3	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
4	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
5	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
6	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
7	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
8	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
9	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
10	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
11	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
12	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
13	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
14	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+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
15	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	1.30E+00	1.49E+00
16	8.39E-01	9.61E-01	1.40E+00	1.60E+00	1.30E+00	1.49E+00	0.00E+00	1.49E+00
17	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
18	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
19	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
20	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
21	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
22	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
23	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
24	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
25	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
26	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
27	5.11E-01	1.29E+00	8.52E-01	2.15E+00	5.90E-01	1.49E+00	5.90E-01	1.49E+00
28	9.78E-01	8.22E-01	1.63E+00	1.37E+00	5.90E-01	4.96E-01	5.90E-01	4.96E-01
29	9.78E-01	8.22E-01	1.63E+00	1.37E+00	5.90E-01	4.96E-01	5.90E-01	4.96E-01
30	9.78E-01	8.22E-01	1.63E+00	1.37E+00	5.90E-01	4.96E-01	5.90E-01	4.96E-01
31	9.78E-01	8.22E-01	1.63E+00	1.37E+00	5.90E-01	4.96E-01	5.90E-01	4.96E-01
32	9.78E-01	8.22E-01	1.63E+00	1.37E+00	5.90E-01	4.96E-01	0.00E+00	4.96E-01
33	2.33E-01	1.57E+00	3.89E-01	2.61E+00	1.48E-01	9.92E-01	1.48E-01	9.92E-01
34	2.33E-01	1.57E+00	3.89E-01	2.61E+00	1.48E-01	9.92E-01	1.48E-01	9.92E-01
35	2.33E-01	1.57E+00	3.89E-01	2.61E+00	1.48E-01	9.92E-01	1.48E-01	9.92E-01
36	2.33E-01	1.57E+00	3.89E-01	2.61E+00	1.48E-01	9.92E-01	1.48E-01	9.92E-01
37	2.33E-01	1.57E+00	3.89E-01	2.61E+00	1.48E-01	9.92E-01	1.48E-01	9.92E-01
38	2.89E-01	1.51E+00	4.82E-01	2.52E+00	1.90E-01	9.92E-01	1.90E-01	9.92E-01
39	2.89E-01	1.51E+00	4.82E-01	2.52E+00	1.90E-01	9.92E-01	1.90E-01	9.92E-01
40	2.89E-01	1.51E+00	4.82E-01	2.52E+00	1.90E-01	9.92E-01	1.90E-01	9.92E-01
41	2.89E-01	1.51E+00	4.82E-01	2.52E+00	1.90E-01	9.92E-01	1.90E-01	9.92E-01
42	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
43	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
44	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
45	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
46	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
47	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01
48	5.85E-01	1.22E+00	9.75E-01	2.03E+00	4.77E-01	9.92E-01	4.77E-01	9.92E-01

PROBLEM RESULTS FOR SEPHIS MOD4, Ver. 2.11: 06-09-1990 11:14

Problem: BREEDER FLOWSHEET EXAMPLE
(mixer concentrations shown)

TIME = 0.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
9	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
12	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
13	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
14	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
15	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
16	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.30E+00	40.0
16	PRODUCT STREAM							1.30E+00	
17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
18	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
19	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
20	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
21	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
22	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
23	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
24	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
25	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
26	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
27	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
28	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
29	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
30	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
31	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
32	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	5.90E-01	40.0
32	PRODUCT STREAM							5.90E-01	
33	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.48E-01	40.0
34	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.48E-01	40.0
35	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.48E-01	40.0
36	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.48E-01	40.0
37	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.48E-01	40.0
38	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.90E-01	40.0
39	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.90E-01	40.0
40	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.90E-01	40.0
41	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.90E-01	40.0
42	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
43	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0
44	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0
45	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0
46	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0
47	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0
48	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	4.77E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
9	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
12	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
13	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
14	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
15	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
16	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
17	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
18	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
19	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
20	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
21	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
22	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
23	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
24	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
25	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
26	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
27	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.50E+00	0.0	2.00E+02
28	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	5.00E-01	0.0	2.00E+02
29	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	5.00E-01	0.0	2.00E+02
30	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	5.00E-01	0.0	2.00E+02
31	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	5.00E-01	0.0	2.00E+02
32	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	5.00E-01	0.0	2.00E+02
33	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
34	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
35	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
36	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
37	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
38	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
39	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
40	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
41	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
42	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
43	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
44	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
45	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
46	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
47	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02
48	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	1.00E+00	0.0	2.00E+02

TIME = 1000.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	5.00E-02	4.18E-11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
2	5.00E-02	8.45E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
3	5.00E-02	1.63E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
4	5.00E-02	3.14E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
5	5.00E-02	6.04E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
6	5.00E-02	1.16E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
7	5.00E-02	2.23E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
8	5.02E-02	4.23E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
9	5.10E-02	6.69E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.30E+00	50.0
10	5.24E-02	4.86E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E+00	1.30E+00	50.0
11	5.33E-02	1.42E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.02E+00	1.31E+00	49.9
12	5.36E-02	2.45E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.03E+00	1.31E+00	49.7
13	5.36E-02	3.30E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.04E+00	1.31E+00	49.3
14	5.34E-02	3.92E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E+00	1.32E+00	48.2
15	5.34E-02	4.29E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	45.4
16	5.35E-02	4.25E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	38.4
16	PRODUCT STREAM							1.32E+00	
17	4.89E-02	1.16E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.02E-01	20.6
18	4.87E-02	1.40E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	21.4
19	4.87E-02	1.47E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	22.2
20	4.87E-02	1.52E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	23.2
21	4.91E-02	1.56E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	24.3
22	5.02E-02	1.61E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	25.6
23	5.38E-02	1.66E+01	0.00E+00	0.00E+00	4.97E-01	4.97E-01	1.11E+00	6.03E-01	27.0
24	6.50E-02	1.69E+01	0.00E+00	2.86E-12	4.97E-01	4.97E-01	1.11E+00	6.03E-01	28.7
25	9.88E-02	1.68E+01	1.35E-12	7.43E-07	4.97E-01	4.97E-01	1.11E+00	6.04E-01	30.7
26	1.94E-01	1.51E+01	2.91E-07	1.82E-01	4.95E-01	4.95E-01	1.11E+00	6.05E-01	32.9
27	3.87E-01	8.62E+00	3.68E-02	2.30E+01	3.97E-01	4.93E-01	1.14E+00	6.08E-01	35.5
28	3.96E-01	1.27E+00	8.63E-03	2.31E+01	3.98E-01	4.94E-01	1.13E+00	6.07E-01	35.5
29	3.96E-01	1.66E-01	2.41E-03	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.07E-01	35.4
30	3.93E-01	2.12E-02	7.35E-04	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	35.2
31	3.77E-01	2.67E-03	2.25E-04	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	34.2
32	3.09E-01	3.05E-04	6.25E-05	2.32E+01	3.99E-01	4.96E-01	1.13E+00	6.05E-01	31.0
32	PRODUCT STREAM							6.05E-01	
33	5.55E-01	3.47E+01	1.91E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.54E-01	40.0
34	7.20E-01	3.62E+01	2.16E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
35	1.01E+00	2.98E+01	1.77E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
36	1.43E+00	2.11E+01	1.18E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.57E-01	40.0
37	1.99E+00	1.37E+01	6.95E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.59E-01	40.0
38	2.75E+00	9.06E+00	3.89E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
39	2.81E+00	8.70E+00	3.64E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
40	2.95E+00	8.32E+00	3.37E+00	0.00E+00	0.00E+00	0.00E+00	1.11E+00	2.10E-01	40.0
41	3.26E+00	7.71E+00	2.91E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	2.12E-01	40.0
42	4.31E+00	7.14E+00	2.07E+00	0.00E+00	0.00E+00	0.00E+00	1.15E+00	5.53E-01	40.0
43	4.37E+00	1.24E-01	4.11E-02	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
44	4.37E+00	1.99E-03	7.61E-04	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
45	4.36E+00	3.22E-05	1.41E-05	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
46	4.29E+00	5.21E-07	2.69E-07	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.50E-01	40.0
47	3.97E+00	8.71E-09	5.73E-09	0.00E+00	0.00E+00	0.00E+00	1.12E+00	5.44E-01	40.0
48	2.86E+00	1.90E-10	2.04E-10	0.00E+00	0.00E+00	0.00E+00	1.09E+00	5.24E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.20E-03	1.88E-12	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
2	1.20E-03	3.81E-11	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
3	1.20E-03	7.35E-10	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
4	1.20E-03	1.41E-08	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
5	1.20E-03	2.72E-07	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
6	1.20E-03	5.24E-06	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	7.50E-06
7	1.20E-03	1.01E-04	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	5.99E-03
8	1.21E-03	1.94E-03	0.00E+00	5.29E-02	0.00E+00	2.79E-02	8.18E-01	1.50E+00	0.1	5.78E-03
9	1.36E-03	3.66E-02	0.00E+00	6.32E-02	0.00E+00	3.06E-02	8.18E-01	1.50E+00	0.2	4.86E-03
10	2.08E-03	5.80E-01	0.00E+00	1.37E-01	0.00E+00	4.58E-02	8.19E-01	1.50E+00	0.6	2.82E-03
11	3.36E-03	4.22E+00	0.00E+00	3.42E-01	0.00E+00	7.25E-02	8.24E-01	1.50E+00	3.5	1.39E-03
12	4.28E-03	1.23E+01	0.00E+00	5.77E-01	0.00E+00	9.18E-02	8.34E-01	1.51E+00	9.8	6.98E-04
13	4.65E-03	2.12E+01	0.00E+00	7.39E-01	0.00E+00	9.98E-02	8.46E-01	1.51E+00	16.7	3.65E-04
14	4.72E-03	2.86E+01	0.00E+00	8.39E-01	0.00E+00	1.02E-01	8.55E-01	1.51E+00	22.4	1.78E-04
15	4.68E-03	3.40E+01	0.00E+00	9.13E-01	0.00E+00	1.01E-01	8.63E-01	1.52E+00	26.5	9.13E-05
16	4.72E-03	3.72E+01	0.00E+00	1.01E+00	0.00E+00	9.80E-02	8.67E-01	1.52E+00	29.0	3.51E-05
17	6.53E-03	3.68E+01	0.00E+00	8.01E+00	0.00E+00	3.37E-01	8.66E-01	1.52E+00	28.9	0.00E+00
18	6.17E-03	4.14E+01	0.00E+00	7.48E+00	0.00E+00	3.20E-01	8.72E-01	1.52E+00	32.3	0.00E+00
19	6.10E-03	4.23E+01	0.00E+00	7.27E+00	0.00E+00	3.17E-01	8.73E-01	1.52E+00	33.0	0.00E+00
20	6.09E-03	4.26E+01	0.00E+00	7.10E+00	0.00E+00	3.16E-01	8.74E-01	1.52E+00	33.2	0.00E+00
21	6.11E-03	4.28E+01	0.00E+00	6.92E+00	0.00E+00	3.15E-01	8.74E-01	1.52E+00	33.4	0.00E+00
22	6.24E-03	4.29E+01	0.00E+00	6.74E+00	0.00E+00	3.14E-01	8.74E-01	1.52E+00	33.5	0.00E+00
23	6.69E-03	4.31E+01	0.00E+00	6.57E+00	0.00E+00	3.14E-01	8.75E-01	1.52E+00	33.7	0.00E+00
24	8.12E-03	4.33E+01	0.00E+00	6.45E+00	0.00E+00	3.15E-01	8.75E-01	1.52E+00	34.0	0.00E+00
25	1.26E-02	4.35E+01	1.13E-12	6.54E+00	3.84E-06	3.21E-01	8.75E-01	1.52E+00	34.5	0.00E+00
26	2.60E-02	4.34E+01	2.95E-07	7.23E+00	4.08E-06	3.36E-01	8.75E-01	1.52E+00	35.6	0.00E+00
27	6.34E-02	4.27E+01	7.21E-02	1.24E+01	7.84E-03	4.11E-01	8.76E-01	1.53E+00	38.6	0.00E+00
28	9.65E-02	1.04E+01	2.78E-02	6.80E+00	9.99E-04	2.02E-01	8.34E-01	5.03E-01	16.8	4.81E-06
29	1.06E-01	1.53E+00	8.72E-03	7.65E+00	3.12E-04	2.22E-01	8.23E-01	5.02E-01	10.9	0.00E+00
30	1.07E-01	2.00E-01	2.69E-03	7.80E+00	9.63E-05	2.25E-01	8.21E-01	5.02E-01	9.9	0.00E+00
31	1.02E-01	2.53E-02	8.00E-04	7.84E+00	2.86E-05	2.25E-01	8.21E-01	5.02E-01	9.4	0.00E+00
32	8.33E-02	2.86E-03	1.95E-04	7.78E+00	6.99E-06	2.24E-01	8.20E-01	5.01E-01	7.6	0.00E+00

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
33	4.81E-02	5.44E+01	1.36E+01	1.05E+01	4.78E+00	5.81E-01	9.12E-01	1.03E+00	56.6	0.00E+00
34	5.78E-02	5.94E+01	1.64E+01	1.09E+01	5.08E+00	5.36E-01	9.23E-01	1.03E+00	63.4	0.00E+00
35	8.30E-02	5.96E+01	1.68E+01	1.33E+01	6.31E+00	5.49E-01	9.24E-01	1.03E+00	66.1	0.00E+00
36	1.26E-01	5.86E+01	1.62E+01	1.83E+01	9.03E+00	5.86E-01	9.23E-01	1.03E+00	68.9	0.00E+00
37	1.91E-01	5.72E+01	1.53E+01	2.72E+01	1.44E+01	6.28E-01	9.22E-01	1.04E+00	73.0	0.00E+00
38	2.79E-01	5.60E+01	1.45E+01	3.08E+01	1.86E+01	5.04E-01	9.21E-01	1.04E+00	79.5	0.00E+00
39	2.88E-01	5.57E+01	1.43E+01	3.18E+01	1.95E+01	5.08E-01	9.21E-01	1.04E+00	79.9	0.00E+00
40	3.01E-01	5.56E+01	1.42E+01	3.31E+01	2.08E+01	5.06E-01	9.21E-01	1.04E+00	81.0	0.00E+00
41	3.30E-01	5.55E+01	1.41E+01	3.53E+01	2.38E+01	4.96E-01	9.22E-01	1.04E+00	83.5	0.00E+00
42	4.00E-01	5.52E+01	1.40E+01	1.46E+01	1.28E+01	1.75E-01	9.23E-01	1.04E+00	89.6	0.00E+00
43	8.50E-01	3.81E+00	1.11E+00	5.79E+01	5.05E+01	3.65E-01	8.47E-01	1.04E+00	81.4	0.00E+00
44	8.83E-01	6.59E-02	2.19E-02	6.20E+01	5.40E+01	3.79E-01	8.42E-01	1.04E+00	80.6	0.00E+00
45	8.82E-01	1.06E-03	4.06E-04	6.20E+01	5.39E+01	3.80E-01	8.42E-01	1.04E+00	80.5	0.00E+00
46	8.74E-01	1.71E-05	7.54E-06	6.19E+01	5.28E+01	3.83E-01	8.41E-01	1.03E+00	79.8	0.00E+00
47	8.33E-01	2.77E-07	1.43E-07	6.05E+01	4.74E+01	3.99E-01	8.40E-01	1.03E+00	76.0	0.00E+00
48	6.42E-01	4.52E-09	2.94E-09	4.65E+01	2.81E+01	4.39E-01	8.35E-01	1.03E+00	58.6	0.00E+00

TIME = 1467.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	5.00E-02	4.20E-11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
2	5.00E-02	8.51E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
3	5.00E-02	1.64E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
4	5.00E-02	3.16E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
5	5.00E-02	6.08E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
6	5.00E-02	1.17E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
7	5.00E-02	2.25E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
8	5.02E-02	4.25E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.99E-01	1.30E+00	50.0
9	5.10E-02	6.72E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.30E+00	50.0
10	5.24E-02	4.87E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E+00	1.30E+00	50.0
11	5.33E-02	1.42E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.02E+00	1.31E+00	49.9
12	5.36E-02	2.45E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.03E+00	1.31E+00	49.7
13	5.36E-02	3.30E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.04E+00	1.31E+00	49.3
14	5.34E-02	3.92E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E+00	1.32E+00	48.2
15	5.34E-02	4.29E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	45.4
16	5.55E-02	4.25E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E+00	1.32E+00	38.4
16	PRODUCT STREAM							1.32E+00	
17	4.89E-02	1.16E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.02E-01	20.6
18	4.87E-02	1.40E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	21.4
19	4.87E-02	1.47E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	22.2
20	4.87E-02	1.52E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	23.2
21	4.91E-02	1.56E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	24.3
22	5.02E-02	1.61E+01	0.00E+00	0.00E+00	4.98E-01	4.98E-01	1.11E+00	6.03E-01	25.6
23	5.38E-02	1.66E+01	0.00E+00	0.00E+00	4.97E-01	4.97E-01	1.11E+00	6.03E-01	27.0
24	6.50E-02	1.69E+01	0.00E+00	2.86E-12	4.97E-01	4.97E-01	1.11E+00	6.03E-01	28.7
25	9.88E-02	1.68E+01	1.35E-12	7.43E-07	4.97E-01	4.97E-01	1.11E+00	6.04E-01	30.7
26	1.94E-01	1.51E+01	2.91E-07	1.82E-01	4.95E-01	4.95E-01	1.11E+00	6.05E-01	32.9
27	3.87E-01	8.62E+00	3.68E-02	2.30E+01	3.97E-01	4.93E-01	1.14E+00	6.08E-01	35.5

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
28	3.96E-01	1.27E+00	8.63E-03	2.31E+01	3.98E-01	4.94E-01	1.13E+00	6.07E-01	35.5
29	3.96E-01	1.66E-01	2.41E-03	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.07E-01	35.4
30	3.93E-01	2.12E-02	7.35E-04	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	35.2
31	3.77E-01	2.67E-03	2.25E-04	2.31E+01	3.98E-01	4.95E-01	1.13E+00	6.06E-01	34.2
32	3.09E-01	3.05E-04	6.25E-05	2.32E+01	3.99E-01	4.96E-01	1.13E+00	6.05E-01	31.0
32	PRODUCT STREAM							6.05E-01	
33	5.55E-01	3.47E+01	1.91E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.54E-01	40.0
34	7.20E-01	3.62E+01	2.16E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
35	1.01E+00	2.98E+01	1.77E+01	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.55E-01	40.0
36	1.43E+00	2.11E+01	1.18E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.57E-01	40.0
37	1.99E+00	1.37E+01	6.95E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.59E-01	40.0
38	2.75E+00	9.06E+00	3.89E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
39	2.81E+00	8.70E+00	3.64E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	2.09E-01	40.0
40	2.95E+00	8.32E+00	3.37E+00	0.00E+00	0.00E+00	0.00E+00	1.11E+00	2.10E-01	40.0
41	3.26E+00	7.71E+00	2.91E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	2.12E-01	40.0
42	4.31E+00	7.14E+00	2.07E+00	0.00E+00	0.00E+00	0.00E+00	1.15E+00	5.53E-01	40.0
43	4.37E+00	1.24E-01	4.11E-02	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
44	4.37E+00	1.99E-03	7.61E-04	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
45	4.36E+00	3.22E-05	1.41E-05	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.52E-01	40.0
46	4.29E+00	5.21E-07	2.69E-07	0.00E+00	0.00E+00	0.00E+00	1.14E+00	5.50E-01	40.0
47	3.97E+00	8.71E-09	5.73E-09	0.00E+00	0.00E+00	0.00E+00	1.12E+00	5.44E-01	40.0
48	2.86E+00	1.90E-10	2.04E-10	0.00E+00	0.00E+00	0.00E+00	1.09E+00	5.24E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.20E-03	1.89E-12	0.00E+00	0.00E+00	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
2	1.20E-03	3.83E-11	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
3	1.20E-03	7.39E-10	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
4	1.20E-03	1.42E-08	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
5	1.20E-03	2.74E-07	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
6	1.20E-03	5.27E-06	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	0.00E+00
7	1.20E-03	1.01E-04	0.00E+00	5.20E-02	0.00E+00	2.77E-02	8.18E-01	1.50E+00	0.1	8.66E-05
8	1.21E-03	1.95E-03	0.00E+00	5.29E-02	0.00E+00	2.79E-02	8.18E-01	1.50E+00	0.1	9.77E-05
9	1.36E-03	3.68E-02	0.00E+00	6.32E-02	0.00E+00	3.06E-02	8.18E-01	1.50E+00	0.2	7.41E-05
10	2.09E-03	5.63E-01	0.00E+00	1.38E-01	0.00E+00	4.59E-02	8.19E-01	1.50E+00	0.6	7.18E-05
11	3.37E-03	4.23E+00	0.00E+00	3.43E-01	0.00E+00	7.26E-02	8.24E-01	1.50E+00	3.5	4.44E-05
12	4.28E-03	1.23E+01	0.00E+00	5.78E-01	0.00E+00	9.18E-02	8.34E-01	1.51E+00	9.8	3.45E-05
13	4.65E-03	2.12E+01	0.00E+00	7.40E-01	0.00E+00	9.98E-02	8.46E-01	1.51E+00	16.7	1.22E-05
14	4.72E-03	2.86E+01	0.00E+00	8.39E-01	0.00E+00	1.02E-01	8.55E-01	1.51E+00	22.4	1.04E-05
15	4.68E-03	3.40E+01	0.00E+00	9.13E-01	0.00E+00	1.01E-01	8.63E-01	1.52E+00	26.5	0.00E+00
16	4.72E-03	3.72E+01	0.00E+00	1.01E+00	0.00E+00	9.80E-02	8.67E-01	1.52E+00	29.0	6.88E-06
17	6.53E-03	3.68E+01	0.00E+00	8.01E+00	0.00E+00	3.37E-01	8.66E-01	1.52E+00	28.9	0.00E+00
18	6.17E-03	4.14E+01	0.00E+00	7.48E+00	0.00E+00	3.20E-01	8.72E-01	1.52E+00	32.3	0.00E+00
19	6.10E-03	4.23E+01	0.00E+00	7.27E+00	0.00E+00	3.17E-01	8.73E-01	1.52E+00	33.0	0.00E+00
20	6.09E-03	4.26E+01	0.00E+00	7.10E+00	0.00E+00	3.16E-01	8.74E-01	1.52E+00	33.2	0.00E+00
21	6.11E-03	4.28E+01	0.00E+00	6.92E+00	0.00E+00	3.15E-01	8.74E-01	1.52E+00	33.4	0.00E+00
22	6.24E-03	4.29E+01	0.00E+00	6.74E+00	0.00E+00	3.14E-01	8.74E-01	1.52E+00	33.5	0.00E+00
23	6.69E-03	4.31E+01	0.00E+00	6.57E+00	0.00E+00	3.14E-01	8.75E-01	1.52E+00	33.7	0.00E+00
24	8.12E-03	4.33E+01	0.00E+00	6.45E+00	0.00E+00	3.15E-01	8.75E-01	1.52E+00	34.0	0.00E+00

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
25	1.26E-02	4.35E+01	1.13E-12	6.54E+00	3.84E-06	3.21E-01	8.75E-01	1.52E+00	34.5	0.00E+00
26	2.60E-02	4.34E+01	2.95E-07	7.23E+00	4.08E-06	3.36E-01	8.75E-01	1.52E+00	35.6	0.00E+00
27	6.34E-02	4.27E+01	7.21E-02	1.24E+01	7.84E-03	4.11E-01	8.76E-01	1.53E+00	38.6	0.00E+00
28	9.65E-02	1.04E+01	2.78E-02	6.80E+00	9.99E-04	2.02E-01	8.34E-01	5.03E-01	16.8	4.81E-06
29	1.06E-01	1.53E+00	8.72E-03	7.65E+00	3.12E-04	2.22E-01	8.23E-01	5.02E-01	10.9	0.00E+00
30	1.07E-01	2.00E-01	2.69E-03	7.80E+00	9.63E-05	2.25E-01	8.21E-01	5.02E-01	9.9	0.00E+00
31	1.02E-01	2.53E-02	8.00E-04	7.84E+00	2.86E-05	2.25E-01	8.21E-01	5.02E-01	9.4	0.00E+00
32	8.33E-02	2.86E-03	1.95E-04	7.78E+00	6.99E-06	2.24E-01	8.20E-01	5.01E-01	7.6	0.00E+00
33	4.81E-02	5.44E+01	1.36E+01	1.05E+01	4.78E+00	5.81E-01	9.12E-01	1.03E+00	56.6	0.00E+00
34	5.78E-02	5.94E+01	1.64E+01	1.09E+01	5.08E+00	5.36E-01	9.23E-01	1.03E+00	63.4	0.00E+00
35	8.30E-02	5.96E+01	1.68E+01	1.33E+01	6.31E+00	5.49E-01	9.24E-01	1.03E+00	66.1	0.00E+00
36	1.26E-01	5.86E+01	1.62E+01	1.83E+01	9.03E+00	5.86E-01	9.23E-01	1.03E+00	68.9	0.00E+00
37	1.91E-01	5.72E+01	1.53E+01	2.72E+01	1.44E+01	6.28E-01	9.22E-01	1.04E+00	73.0	0.00E+00
38	2.79E-01	5.60E+01	1.45E+01	3.08E+01	1.86E+01	5.04E-01	9.21E-01	1.04E+00	79.5	0.00E+00
39	2.88E-01	5.57E+01	1.43E+01	3.18E+01	1.95E+01	5.08E-01	9.21E-01	1.04E+00	79.9	0.00E+00
40	3.01E-01	5.56E+01	1.42E+01	3.31E+01	2.08E+01	5.06E-01	9.21E-01	1.04E+00	81.0	0.00E+00
41	3.30E-01	5.55E+01	1.41E+01	3.53E+01	2.38E+01	4.96E-01	9.22E-01	1.04E+00	83.5	0.00E+00
42	4.00E-01	5.52E+01	1.40E+01	1.46E+01	1.28E+01	1.75E-01	9.23E-01	1.04E+00	89.6	0.00E+00
43	8.50E-01	3.81E+00	1.11E+00	5.79E+01	5.05E+01	3.65E-01	8.47E-01	1.04E+00	81.4	0.00E+00
44	8.83E-01	6.59E-02	2.19E-02	6.20E+01	5.40E+01	3.79E-01	8.42E-01	1.04E+00	80.6	0.00E+00
45	8.82E-01	1.06E-03	4.06E-04	6.20E+01	5.39E+01	3.80E-01	8.42E-01	1.04E+00	80.5	0.00E+00
46	8.74E-01	1.71E-05	7.54E-06	6.19E+01	5.28E+01	3.83E-01	8.41E-01	1.03E+00	79.8	0.00E+00
47	8.33E-01	2.77E-07	1.43E-07	6.05E+01	4.74E+01	3.99E-01	8.40E-01	1.03E+00	76.0	0.00E+00
48	6.42E-01	4.52E-09	2.94E-09	4.65E+01	2.81E+01	4.39E-01	8.35E-01	1.03E+00	58.6	0.00E+00

Valid ranges:

0.0 to 5.0 M H+
0.0 to 200 gU/L
0.0 to 100 gPu/L
10 to 30% TBP
10 to 40°C

Run Time is from 11:14:17 to 14:13:24

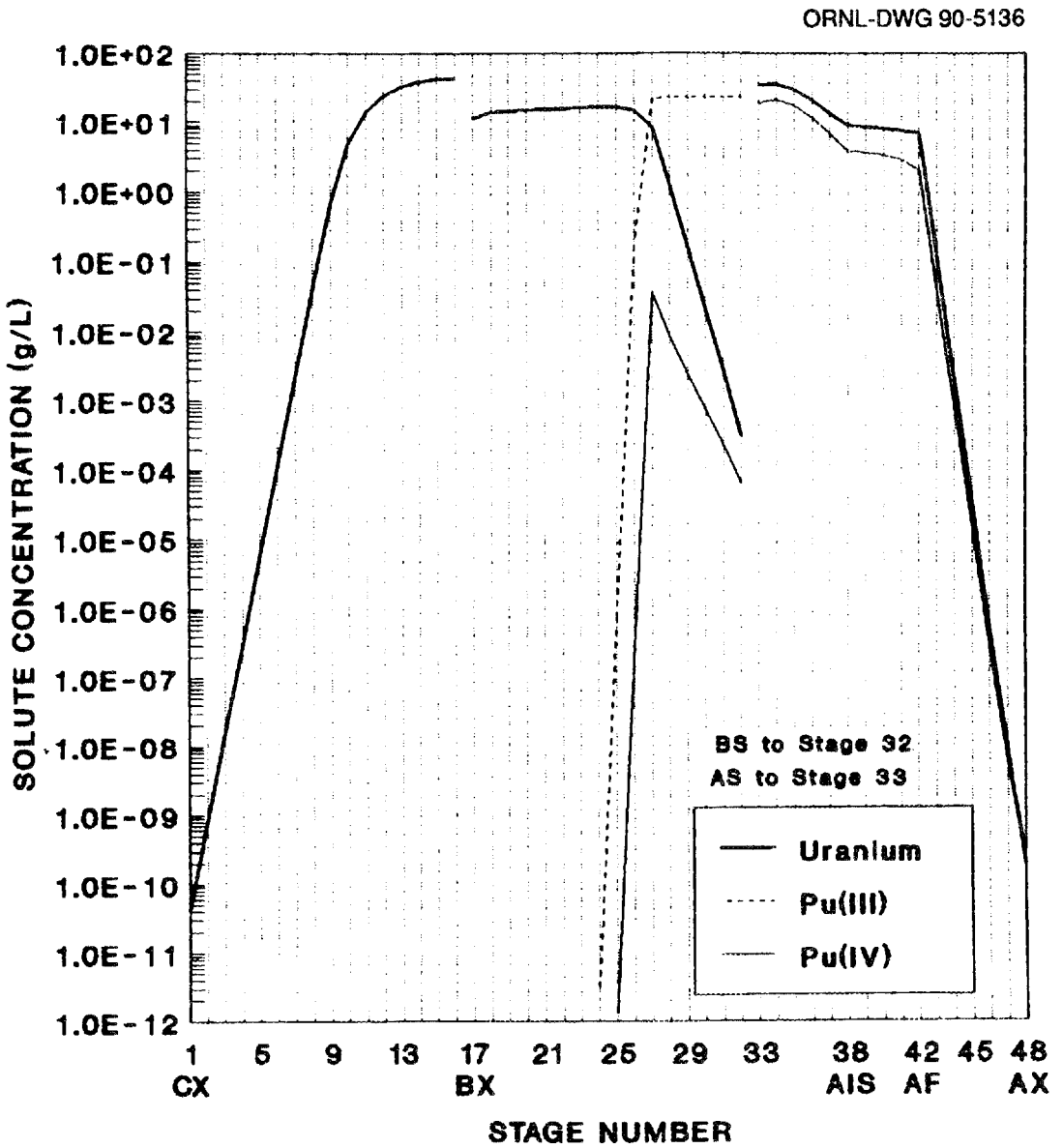


Fig. 13. Sample problem – Aqueous heavy-metal steady-state concentration profile.

4.3 DISCUSSION

The sample problem illustrates the point made in Sect. 2.2.1 regarding the plutonium reduction profile created when using the Fast integration technique. Steady-state heavy-metal concentration profiles for the B-Bank, shown in Figs. 17 and 18, compare results for Fast and Trapezoidal integration techniques. The lack of agreement is due to the different set of concentration values used by the two techniques for calculating the reduction rate. A determination of which profile is the most accurate must await a future study that uses actual extraction profile data for

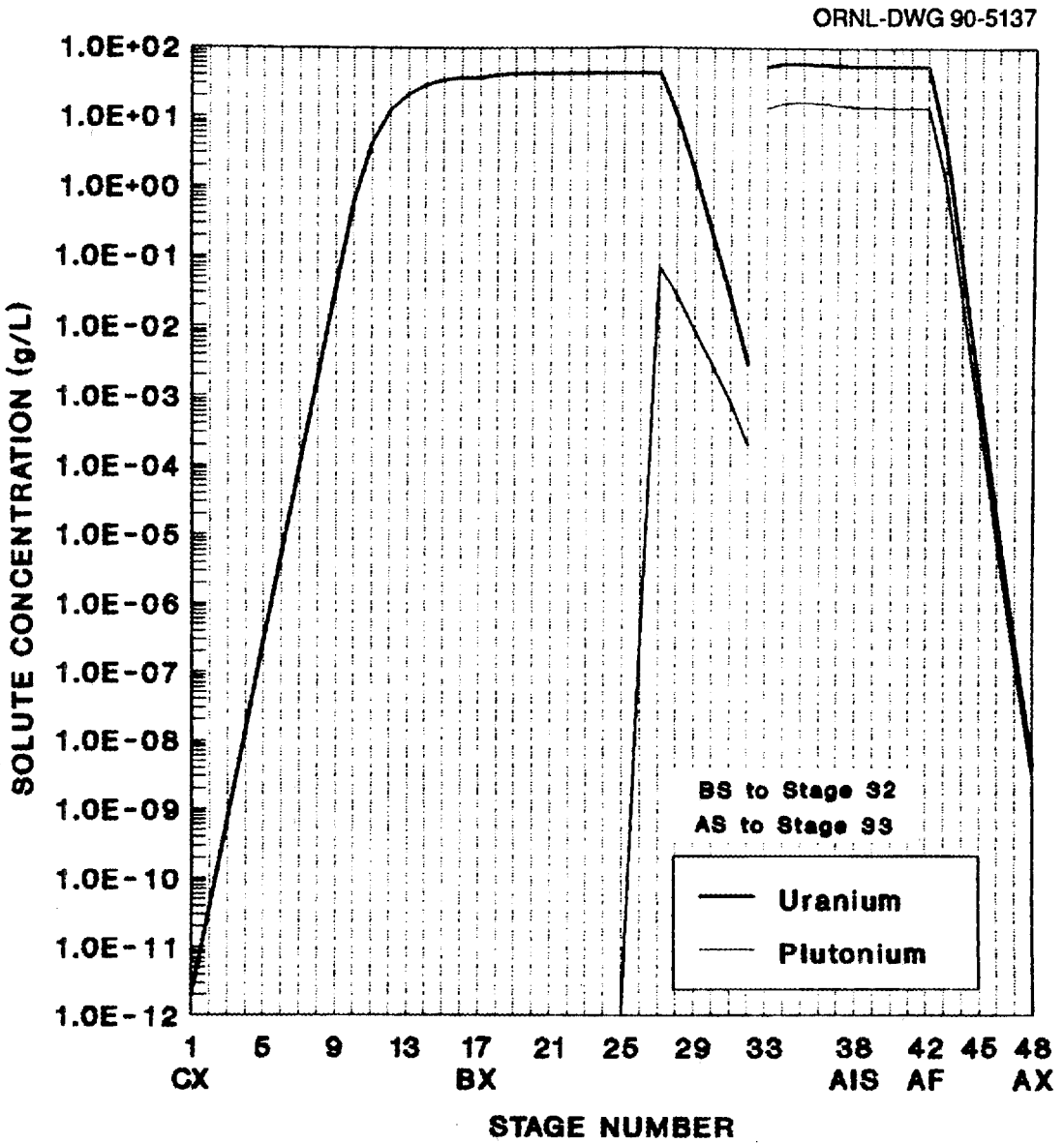


Fig. 14. Sample problem — Organic heavy-metal steady-state concentration profile.

verification, but it is believed that the Trapezoidal technique provides the best profile. The two techniques produce identical profiles for the A- and C-banks.

Figures 19 and 20 show the transient approach to steady-state for product stream concentrations and for overall material balances. Apparent steady-state, as noted from end-stream assays, occurs in ~350 min. However, an additional 1100 min is required to fully develop the internal concentration profile to the point that all solute inventories of all stages are constant to within 0.0001%/min.

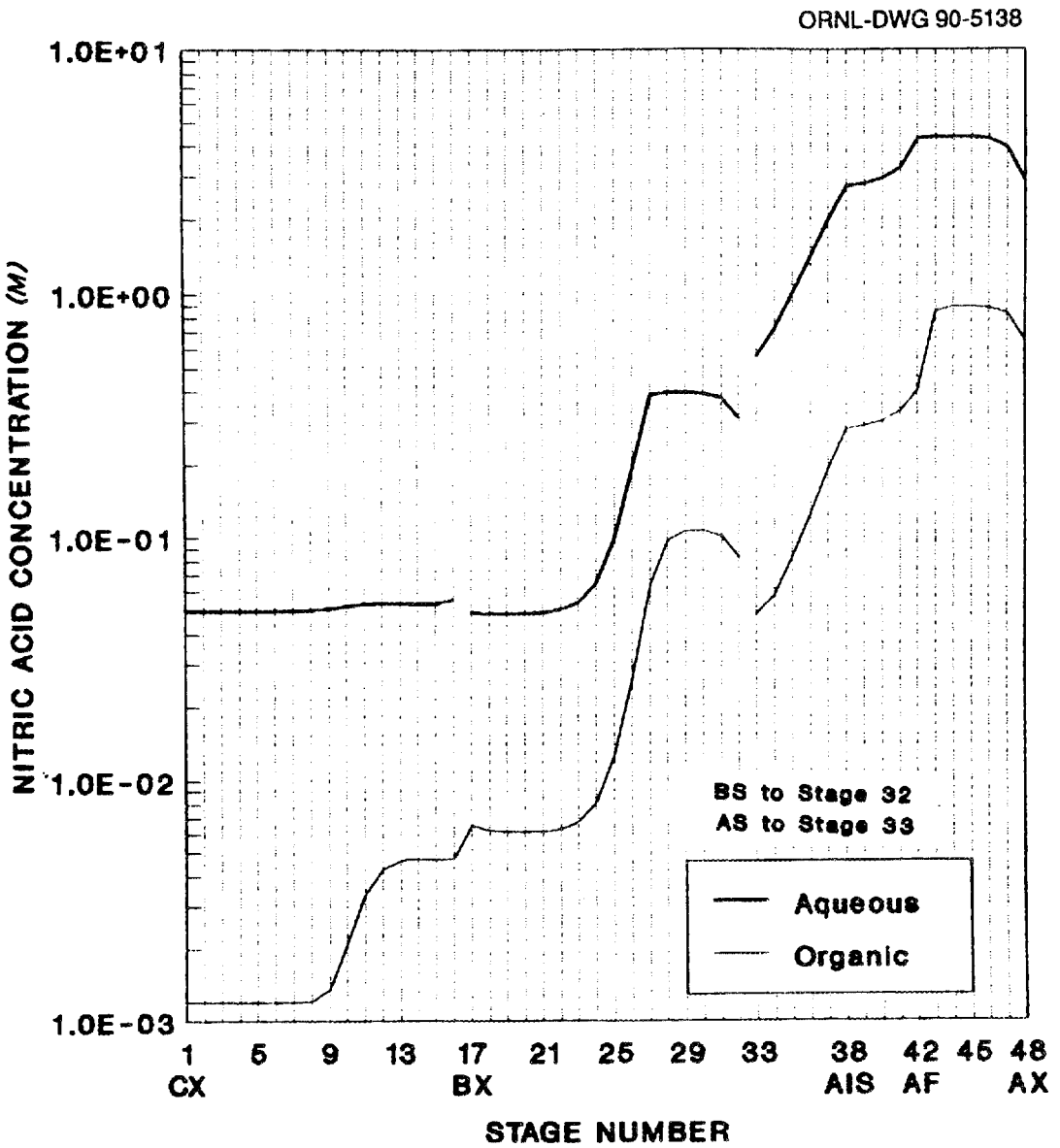


Fig. 15. Sample problem — Nitric acid steady-state concentration profile.

The steady-state values for this sample flow sheet show >99.99% recovery of uranium and plutonium [no losses to either the depleted aqueous (AW) or depleted organic (CW) streams]. The plutonium product stream (BP) assay is 99.999% Pu and 0.001% U. The uranium product stream (CP) assay is 100% U.

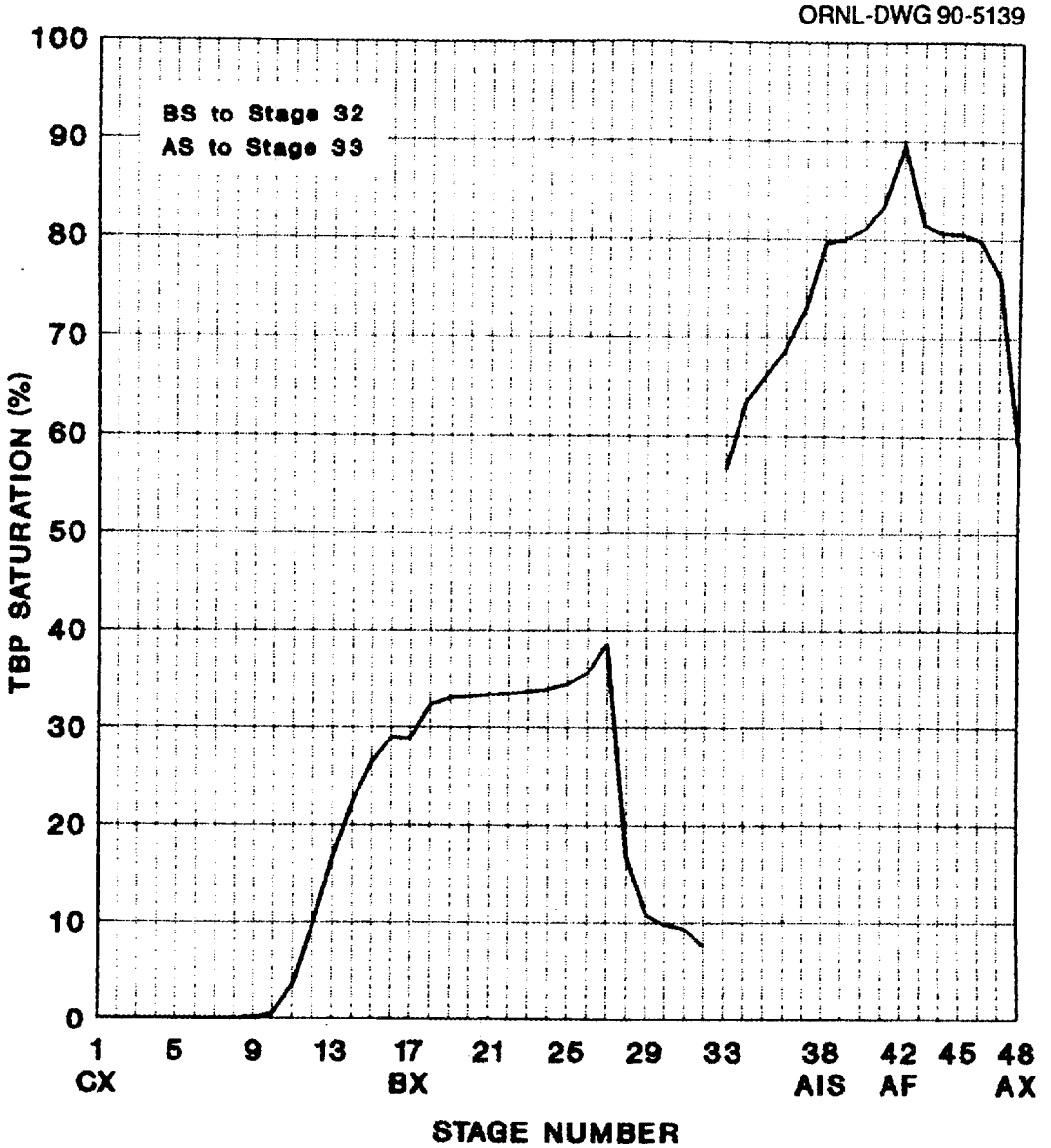


Fig. 16. Sample problem — TBP steady-state saturation profile.

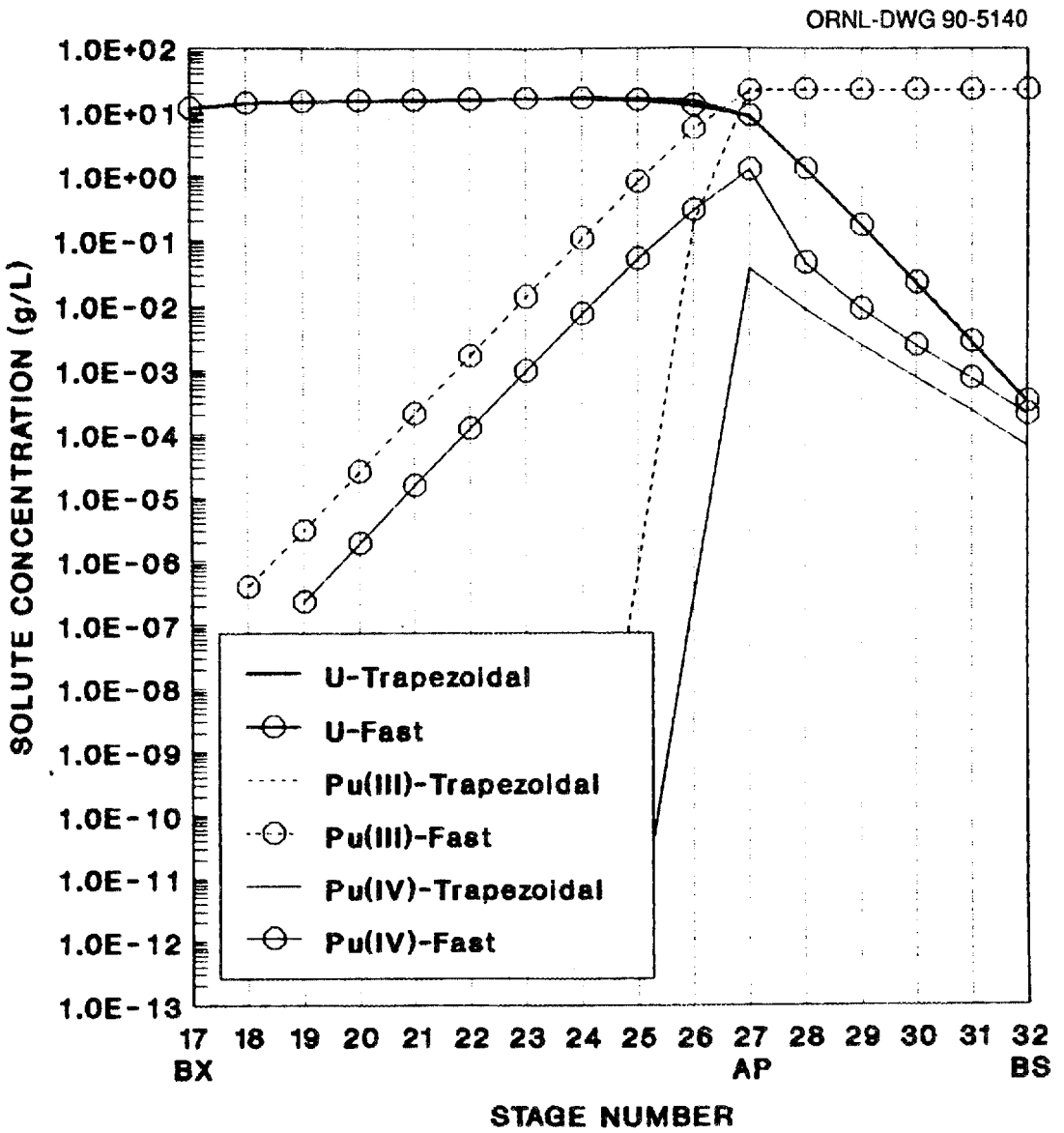


Fig. 17. Sample problem — Effect of integration technique on B-bank aqueous heavy-metal steady-state profile.

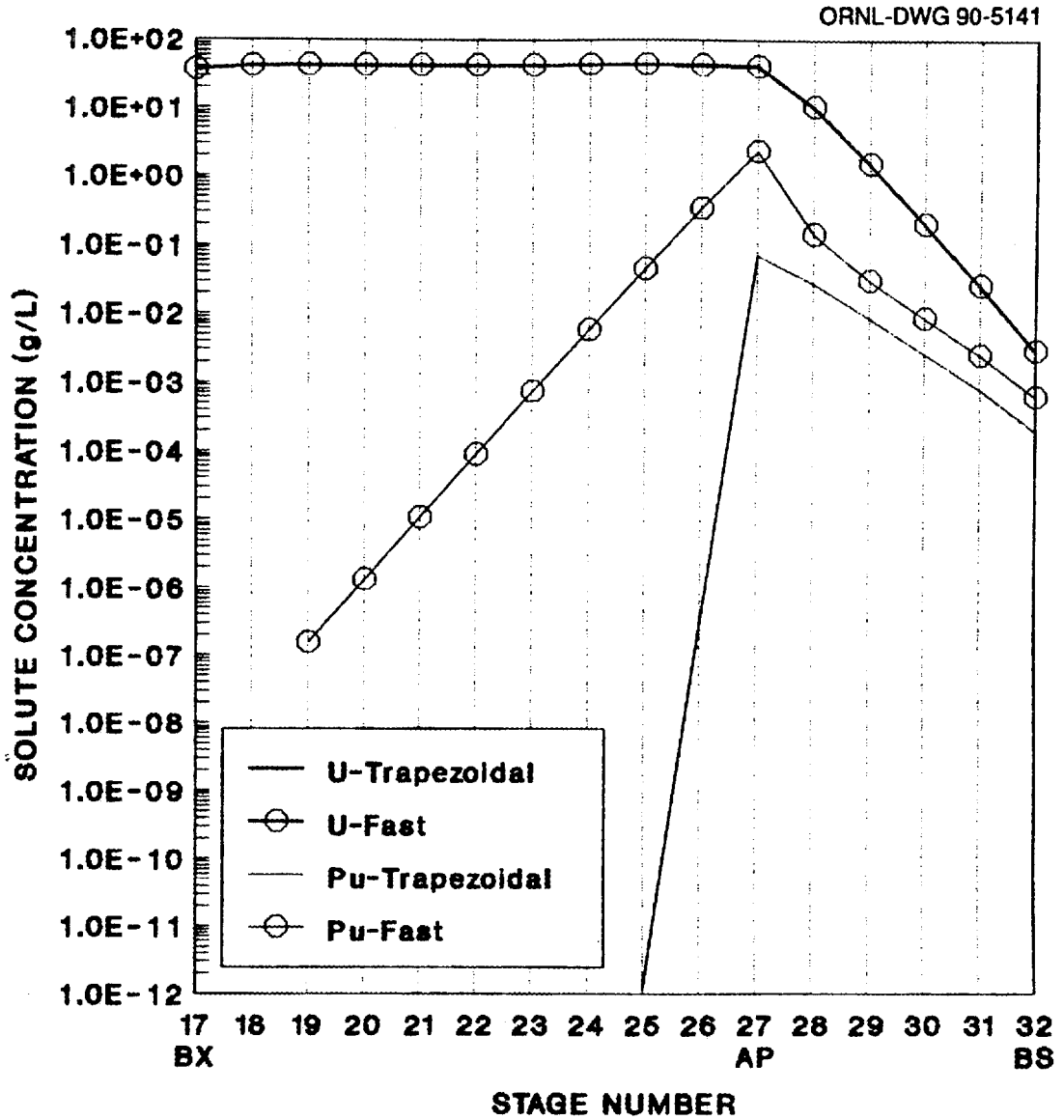


Fig. 18. Sample problem — Effect of integration technique on B-bank organic heavy-metal steady-state profile.

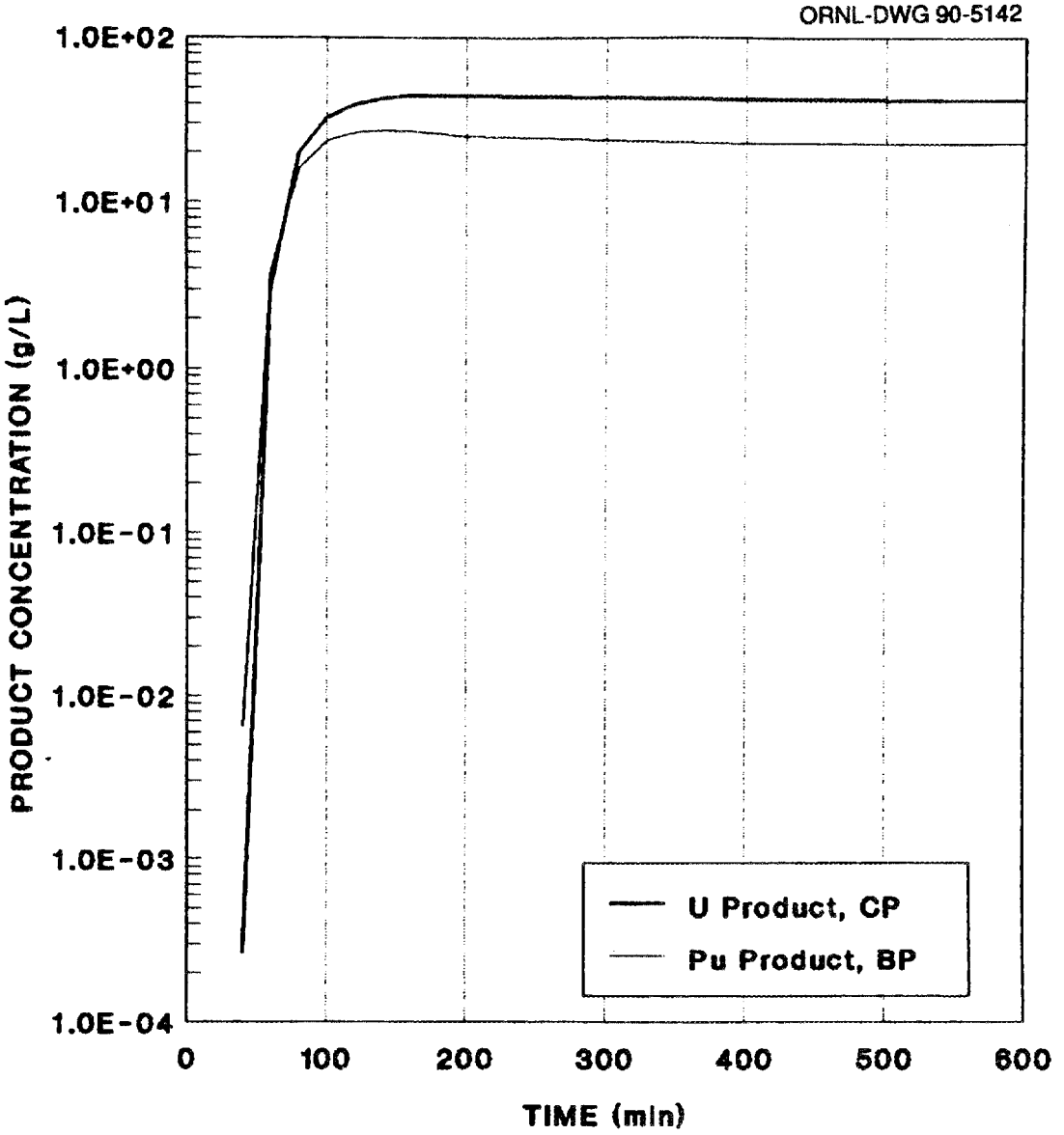


Fig. 19. Sample problem — Product concentrations vs time.

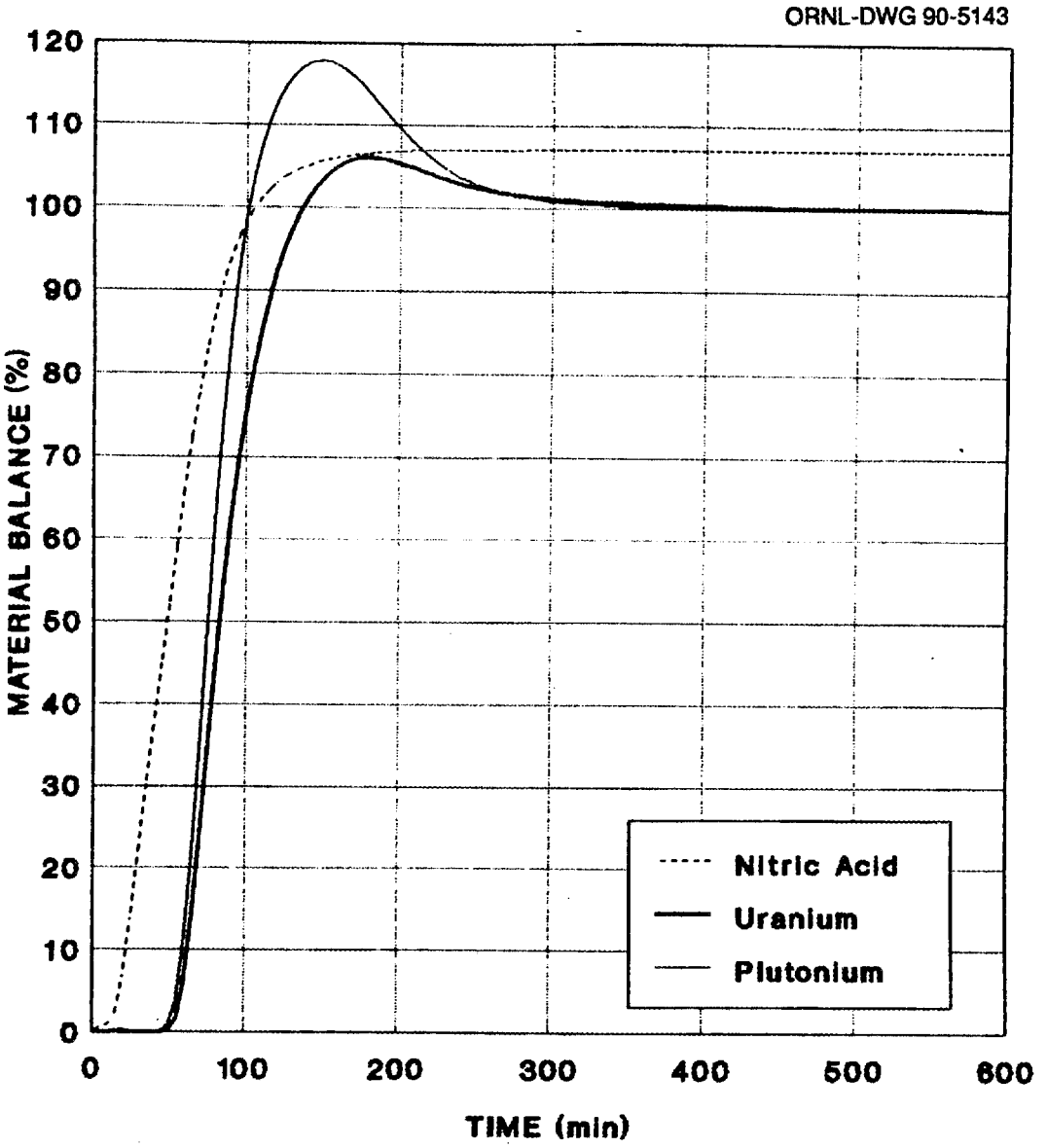


Fig. 20. Sample problem — Overall material balance vs time.

5. REFERENCES

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10. G. L. Richardson, *Effect of High Solvent Irradiation Exposures on TBP Processing of Spent LMFBR Fuels*, HEDL-TME 73-51, Hanford Engineering Development Laboratory, June 1973.

APPENDIX A
SEPHIS.BAS—THE MENU PROGRAM

```
10 REM PROGRAM SEPHIS -- Solvent Extraction Process Having Interacting
   Solutes -- MENU
20 WIDTH "scrn:", 80
30 SCREEN 0, 1, 0, 0
40 KEY OFF: CLS
50 R1% = 1: C1% = 1: R2% = 24: C2% = 79: GOSUB 410  'To draw double box
60 R1% = 10: C1% = 25: R2% = 14: C2% = 55: GOSUB 550  'To draw single box
70 FOR I% = 2 TO 24
80  LOCATE 10, I%: PRINT CHR$(196);
90 NEXT I%
100 FOR I% = 56 TO 78
110  LOCATE 10, I%: PRINT CHR$(196);
120 NEXT I%
130 LOCATE 10, 1: PRINT CHR$(199);
140 LOCATE 10, 25: PRINT CHR$(194);
150 LOCATE 10, 55: PRINT CHR$(194);
160 LOCATE 10, 79: PRINT CHR$(182); : COLOR 0, 7
170 LOCATE 3, 29: PRINT "PC - S E P H I S - MOD4"; : COLOR 7, 0
180 LOCATE 4, 31: PRINT "Version 2.11 (1990)";
190 LOCATE 6, 13: PRINT "A Solvent Extraction Process Having Interacting
    Solutes";
200 LOCATE 8, 17: PRINT "For Uranium, Plutonium, Thorium, and Nitric Acid";
210 LOCATE 9, 16: PRINT "Mass Transfer in Purex- or Thorex-type
    Flowsheets";
220 LOCATE 11, 34: PRINT "W.S. Groenier";
230 LOCATE 12, 30: PRINT "Fuel Recycle Division";
240 LOCATE 13, 26: PRINT "Oak Ridge National Laboratory"; : COLOR 0, 7
250 LOCATE 16, 34: PRINT "*** MENU ***";
260 LOCATE 18, 31: PRINT "1."; : COLOR 7, 0
270 LOCATE 18, 35: PRINT "Define a problem."; : COLOR 0, 7
280 LOCATE 20, 31: PRINT "2."; : COLOR 7, 0
290 LOCATE 20, 35: PRINT "Run a problem."; : COLOR 0, 7
300 LOCATE 22, 31: PRINT "3."; : COLOR 7, 0
310 LOCATE 22, 35: PRINT "Print a problem.";
320 LOCATE 25, 1: INPUT ; "Enter the number (1 to 3) of your choice (0 to
    quit). ", RUNNO%
330 CLS
340 IF RUNNO% < 0 OR RUNNO% > 3 THEN BEEP: GOTO 50
350 IF RUNNO% = 0 THEN 400
360 ON RUNNO% GOTO 370, 380, 390
370 RUN "seprep"
380 RUN "secalc"
390 RUN "seprnt"
400 END
410 REM Subroutine to draw a double box.
```

```
420  FOR I% = R1% + 1 TO R2% - 1
430   LOCATE I%, C1%: PRINT CHR$(186);
440   LOCATE I%, C2%: PRINT CHR$(186);
450  NEXT I%
460  FOR J% = C1% + 1 TO C2% - 1
470   LOCATE R1%, J%: PRINT CHR$(205);
480   LOCATE R2%, J%: PRINT CHR$(205);
490  NEXT J%
500  LOCATE R1%, C1%: PRINT CHR$(201);
510  LOCATE R1%, C2%: PRINT CHR$(187);
520  LOCATE R2%, C1%: PRINT CHR$(200);
530  LOCATE R2%, C2%: PRINT CHR$(188);
540 RETURN
550 REM Subroutine to draw a single box.
560  FOR I% = R1% + 1 TO R2% - 1
570   LOCATE I%, C1%: PRINT CHR$(179);
580   LOCATE I%, C2%: PRINT CHR$(179);
590  NEXT I%
600  FOR J% = C1% + 1 TO C2% - 1
610   LOCATE R1%, J%: PRINT CHR$(196);
620   LOCATE R2%, J%: PRINT CHR$(196);
630  NEXT J%
640  LOCATE R1%, C1%: PRINT CHR$(218);
650  LOCATE R1%, C2%: PRINT CHR$(191);
660  LOCATE R2%, C1%: PRINT CHR$(192);
670  LOCATE R2%, C2%: PRINT CHR$(217);
680 RETURN
```

APPENDIX B
SEPREP.BAS—THE PROBLEM DEFINITION PROGRAM

```
10 REM PROGRAM SEPREP -- Solvent Extraction Process Having Interacting
   Solutes -- Problem Definition
20 WIDTH "scrn:", 80
30 SCREEN 0, 1, 0, 0
40 KEY OFF: CLS
50 DIM CON(6), CN(9, 100), T(100)
60 R1% = 1: C1% = 1: R2% = 24: C2% = 79: GOSUB 4430  'To draw double box
70 R1% = 10: C1% = 25: R2% = 14: C2% = 55: GOSUB 4570  'To draw single box
80 FOR I% = 1 TO 24
90  LOCATE 10, I%: PRINT CHR$(196);
100 NEXT I%
110 FOR I% = 56 TO 78
120  LOCATE 10, I%: PRINT CHR$(196);
130 NEXT I%
140 LOCATE 10, 1: PRINT CHR$(199);
150 LOCATE 10, 25: PRINT CHR$(194);
160 LOCATE 10, 55: PRINT CHR$(194);
170 LOCATE 10, 79: PRINT CHR$(182); : COLOR 0, 7
180 LOCATE 3, 29: PRINT "PC - S E P H I S - MOD4"; : COLOR 7, 0
190 LOCATE 4, 31: PRINT "Version 2.11 (1990)";
200 LOCATE 6, 13: PRINT "A Solvent Extraction Process Having Interacting
    Solutes";
210 LOCATE 8, 17: PRINT "For Uranium, Plutonium, Thorium, and Nitric Acid";
220 LOCATE 9, 16: PRINT "Mass Transfer in Purex- or Thorex-type
    Flowsheets";
230 LOCATE 11, 34: PRINT "W.S. Groenier";
240 LOCATE 12, 30: PRINT "Fuel Recycle Division";
250 LOCATE 13, 26: PRINT "Oak Ridge National Laboratory"; : COLOR 0, 7
260 LOCATE 18, 25: PRINT "*** PROBLEM DEFINITION ONLY ***"; : COLOR 7, 0
265 LOCATE 21, 19: PRINT "A Problem Definition file is to be prepared";
266 LOCATE 22, 21: PRINT "Choose the location for this file below";
270 LOCATE 25, 1: INPUT ; "Do you want to continue (Y/N)? ", REPLY$
280 IF REPLY$ <> "Y" THEN CLS : GOTO 4410
290 LOCATE 25, 1: PRINT SPACE$(79); : LOCATE 25, 1
295 LOCATE 25, 1: INPUT ; "Will the file be on a diskette (Y/N)? ", REPLY$
296 IF REPLY$ <> "Y" THEN 320
297 LOCATE 25, 1: PRINT SPACE$(79); : LOCATE 25, 1
300 PRINT "Insert diskette -- Press any key to continue.";
310 K$ = INKEY$: IF K$ = "" THEN 310
320 CLS : P$ = "###.#": Q$ = "####.##": PP$ = "###.##": QQ$ = "###.###":
    PQ$ = "##.##^^^^": PPP$ = "###.####"
330 R1% = 1: C1% = 1: R2% = 20: C2% = 79: GOSUB 4570  'To draw single box
340 LOCATE 2, 32: PRINT "PROBLEM DEFINITION:";
350 LOCATE 21, 1: INPUT ; "Enter Problem Title. ", TITLE$
360 LOCATE 4, 2: PRINT "Problem Title:  "; TITLE$
```

```
370 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
380 INPUT ; "Enter `0' for Purex or `1' for Thorex Process. ", IPROCE%
390 IF IPROCE% < 0 OR IPROCE% > 1 THEN BEEP: GOTO 370
400 IF IPROCE% = 0 THEN 420
410 LOCATE 5, 2: PRINT "Process:  Thorex."; : GOTO 430
420 LOCATE 5, 2: PRINT "Process:  Purex.";
430 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
440 INPUT ; "Enter total number of stages (up to 100). ", NTOST%
450 IF NTOST% < 1 OR NTOST% > 100 THEN BEEP: GOTO 430
460 LOCATE 6, 2: PRINT "Total stages:  "; NTOST%
470 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
480 INPUT ; "Enter Volume % TBP in solvent. ", CTBP
490 LOCATE 6, 40: PRINT "Volume % TBP in solvent:  "; : PRINT USING P$;
    CTBP
500 CTBP = CTBP / 100!
510 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
520 INPUT ; "Enter initial or default temperature in degrees C. ", TEMPI
530 LOCATE 7, 2: PRINT "Initial or default temperature ("; CHR$(248); "C):
    "; : PRINT USING P$; TEMPI
540 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
550 INPUT ; "Enter `0' for no unusual stage connections or `1' for special
    routing. ", NSTR%
560 IF NSTR% < 0 OR NSTR% > 1 THEN BEEP: GOTO 540
570 IF NSTR% = 0 THEN 650
580 LOCATE 22, 1: INPUT ; "Enter stage no. from which organic is taken. ",
    ISTR%
590 IF ISTR% < 1 OR ISTR% > NTOST% THEN BEEP: LOCATE 22, 1: PRINT
    SPACE$(79); : GOTO 580
600 LOCATE 23, 1: INPUT ; "Enter stage no. to which organic is returned. ",
    JSTR%
610 IF JSTR% < 1 OR JSTR% > NTOST% THEN BEEP: LOCATE 23, 1: PRINT
    SPACE$(79); : GOTO 600
620 LOCATE 8, 2: PRINT "Organic taken from stage "; ISTR%; " feeds stage ";
    JSTR%; ".";
630 LOCATE 22, 1: PRINT SPACE$(79); : LOCATE 23, 1: PRINT SPACE$(79);
640 GOTO 670
650 LOCATE 8, 2: PRINT "No unusual stage connections.";
660 ISTR% = 0: JSTR% = 0
670 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
680 IF IPROCE% = 1 THEN IRXN% = 0: GOTO 810
690 PRINT "Enter `0` for no plutonium reaction.";
700 LOCATE 22, 1: PRINT "Enter `1` for instantaneous reduction of Pu(IV).";
710 LOCATE 23, 1: PRINT "Enter `2` for reduction of Pu(IV) by U(IV).";
720 LOCATE 24, 1: INPUT ; "Enter `3` for reduction of Pu(IV) by
    hydroxylamine nitrate. ", IRXN%
730 IF IRXN% < 0 OR IRXN% > 3 THEN BEEP: LOCATE 24, 1: PRINT SPACE$(79); :
    GOTO 630
740 ON (IRXN% + 1) GOTO 750, 760, 770, 780
750 LOCATE 9, 2: PRINT "No plutonium reaction."; : GOTO 790
760 LOCATE 9, 2: PRINT "Instantaneous reduction of Pu(IV)."; : GOTO 790
770 LOCATE 9, 2: PRINT "Reduction of Pu(IV) by U(IV)."; : GOTO 790
780 LOCATE 9, 2: PRINT "Reduction of Pu(IV) by hydroxylamine nitrate.";
790 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 23, 1: PRINT SPACE$(79);
800 LOCATE 22, 1: PRINT SPACE$(79); : LOCATE 21, 1: PRINT SPACE$(79);
```

```
810 LOCATE 21, 1: PRINT "Enter time increment (min.).  HINT - For accurate
    transient results use 1/4 of";
820 LOCATE 22, 1: PRINT "stage residence time.  See User's Manual.";
830 LOCATE 24, 1
840 INPUT ; "Make your entry here. ", DTHETA
850 IF DTHETA <= 0 THEN BEEP: GOTO 790
860 LOCATE 10, 2: PRINT "Time increment (min.):  "; : PRINT USING Q$;
    DTHETA
870 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 23, 1: PRINT SPACE$(79);
880 LOCATE 22, 1: PRINT SPACE$(79); : LOCATE 21, 1: PRINT SPACE$(79);
890 LOCATE 21, 1: INPUT ; "Enter time between printings of the
    concentration profile (min.). ", DPRINT%
900 IF DPRINT% < DTHETA THEN BEEP: GOTO 880
910 LOCATE 11, 2: PRINT "Time between printings of the concentration
    profile (min.):  "; : PRINT USING "####"; DPRINT%
920 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
930 INPUT ; "Enter time when calculations should stop (min.). ", TSTOP%
940 IF TSTOP% < DTHETA THEN BEEP: GOTO 920
950 LOCATE 12, 2: PRINT "Time when calculations will stop (min.):  "; :
    PRINT USING "####"; TSTOP%
960 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
970 INPUT ; "Tolerance for steady-state (%/min.). ", TOL
980 LOCATE 13, 2: PRINT "Tolerance for steady-state (%/min.):  "; : PRINT
    USING PPP$; TOL
990 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
1000 PRINT "Enter `1' if mixer volumes are to be defined for each phase.";
1010 LOCATE 22, 1: PRINT "Enter `2' if only total mixer volumes are to be
     defined.";
1020 LOCATE 23, 1: INPUT ; "Enter `3' if mixer volumes will be phase flow
     times unit time. ", IVOLM%
1030 IF IVOLM% < 1 OR IVOLM% > 3 THEN BEEP ELSE 1060
1040 LOCATE 23, 1: PRINT SPACE$(79);
1050 LOCATE 22, 1: PRINT SPACE$(79); : GOTO 990
1060 ON IVOLM% GOTO 1070, 1080, 1090
1070 LOCATE 14, 2: PRINT "Mixer volumes to be defined for each phase."; :
     GOTO 1100
1080 LOCATE 14, 2: PRINT "Total mixer volumes to be defined."; : GOTO 1100
1090 LOCATE 14, 2: PRINT "Mixer volumes = (phase flow)(unit time).";
1100 LOCATE 23, 1: PRINT SPACE$(79); : LOCATE 22, 1: PRINT SPACE$(79);
1110 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
1120 PRINT "Enter `1' if settler volumes are to be defined for each
     phase.";
1130 LOCATE 22, 1: PRINT "Enter `2' if only total settler volumes are to be
     defined.";
1140 LOCATE 23, 1: INPUT ; "Enter  3' if settler volumes will be phase flow
     times unit time. ", IVOLS%
1150 IF IVOLS% < 1 OR IVOLS% > 3 THEN BEEP ELSE 1180
1160 LOCATE 23, 1: PRINT SPACE$(79);
1170 LOCATE 22, 1: PRINT SPACE$(79); : GOTO 1110
1180 ON IVOLS% GOTO 1190, 1200, 1210
1190 LOCATE 15, 2: PRINT "Settler volumes to be defined for each phase."; :
     GOTO 1220
1200 LOCATE 15, 2: PRINT "Total settler volumes to be defined."; : GOTO
     1220
1210 LOCATE 15, 2: PRINT "Settler volumes = (phase flow)(unit time).";
```

```
1220 LOCATE 23, 1: PRINT SPACE$(79);
1230 LOCATE 22, 1: PRINT SPACE$(79);
1240 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
1250 PRINT "Enter `0' if the initial concentration profile is zero.";
1260 LOCATE 22, 1: PRINT "Enter `1' if the initial concentration profile is
     to be defined.";
1270 LOCATE 23, 1: INPUT ; "Enter `2' if the initial concentration profile
     is from a previous problem. ", IPRO%
1280 IF IPRO% < 0 OR IPRO% > 2 THEN BEEP ELSE 1310
1290 LOCATE 23, 1: PRINT SPACE$(79);
1300 LOCATE 22, 1: PRINT SPACE$(79); : GOTO 1240
1310 ON (IPRO% + 1) GOTO 1320, 1330, 1340
1320 LOCATE 16, 2: PRINT "Initial concentration profile = 0."; : GOTO 1350
1330 LOCATE 16, 2: PRINT "Initial concentration profile to be defined."; :
     GOTO 1350
1340 LOCATE 16, 2: PRINT "Initial concentration profile to be read from a
     previous problem.";
1350 LOCATE 23, 1: PRINT SPACE$(79);
1360 LOCATE 22, 1: PRINT SPACE$(79);
1370 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
1380 PRINT "Integration method:  Enter `0' for Runge-Kutta, `1' for
     Trapezoidal, or `2' for";
1390 LOCATE 22, 1: PRINT "Fast.  HINT - For accurate transient results use
     Fast.  See User's Manual.";
1400 LOCATE 23, 1: INPUT ; "Make your entry here. ", IFAST%
1410 IF IFAST% < 0 OR IFAST% > 2 THEN BEEP ELSE 1440
1420 LOCATE 23, 1: PRINT SPACE$(79);
1430 LOCATE 22, 1: PRINT SPACE$(79); : GOTO 1370
1440 ON (IFAST% + 1) GOTO 1450, 1460, 1470
1450 LOCATE 17, 2: PRINT "Runge-Kutta integration will be used."; : GOTO
     1480
1460 LOCATE 17, 2: PRINT "Trapezoidal integration will be used."; : GOTO
     1480
1470 LOCATE 17, 2: PRINT "Fast integration will be used.";
1480 LOCATE 23, 1: PRINT SPACE$(79);
1490 LOCATE 22, 1: PRINT SPACE$(79);
1500 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
1510 INPUT ; "Enter `1' to define extra product streams, `0' for none. ",
     NEWOUT%
1520 IF NEWOUT% < 0 OR NEWOUT% > 1 THEN BEEP: GOTO 1500
1530 IF NEWOUT% = 0 THEN 1550
1540 LOCATE 18, 2: PRINT "Extra product stream(s)."; : GOTO 1560
1550 LOCATE 18, 2: PRINT "No extra product streams.";
1560 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 21, 1
1570 PRINT "Enter Drive (Path) and FILENAME for this Problem Definition
     data file.";
1580 LOCATE 22, 1: INPUT ; "Examples are B:\xxxxxxxx or C:\Subdir\xxxxxxxx.
     ", DATFIL1$
1585 DATFIL1$ = DATFIL1$ + ".DAT"
1590 LOCATE 19, 2: PRINT "Problem Definition data are in:  "; DATFIL1$
1600 LOCATE 21, 1: PRINT SPACE$(79); : LOCATE 22, 1: PRINT SPACE$(79);
1610 LOCATE 25, 1: INPUT ; "Is the above information correct (Y/N)? ",
     REPLY$
1620 IF REPLY$ <> "Y" THEN CLS : GOTO 330
1630 ON ERROR GOTO 7400
```

```
1640 OPEN DATFIL1$ FOR OUTPUT AS #1
1650 CLS : WRITE #1, DATE$, LEFT$(TIME$, 5)
1660 WRITE #1, TITLE$, NTOST%, CTBP, TEMPI, NSTR%, ISTR%, JSTR%, IRXN%,
     IPROCE%, DTHETA, DPRINT%, TSTOP%, TOL, NEWOUT%, IVOLM%, IVOLS%, IPRO%,
     IFAST%
1670 R1% = 1: C1% = 1: R2% = 23: C2% = 79: GOSUB 4570  'To draw a single
     box
1680 LOCATE 2, 34: PRINT "FEED STREAMS:";
1690 LOCATE 24, 1: INPUT ; "Enter stage number for feed. ", NST%
1700 IF NST% < 1 OR NST% > NTOST% THEN BEEP: CLS : GOTO 1670
1710 LOCATE 4, 2: PRINT "Feed to Stage No.:  "; NST%
1720 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
1730 INPUT ; "Enter type of feed (`1' for aqueous, `0' for organic). ",
     JHAS%
1740 IF JHAS% = 1 THEN 1760
1750 IF JHAS% = 0 THEN 1770 ELSE BEEP: GOTO 1720
1760 LOCATE 6, 2: PRINT "Feed is Aqueous."; : GOTO 1780
1770 LOCATE 6, 2: PRINT "Feed is Organic.";
1780 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
1790 INPUT ; "Enter flow rate (Liters/min.). ", FDRT
1800 LOCATE 8, 2: PRINT "Feed flow rate (L/min.) is:  "; : PRINT USING QQ$;
     FDRT
1810 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
1820 INPUT ; "Enter Nitric Acid concentration (M). ", CON(1)
1830 LOCATE 10, 2: PRINT "Nitric Acid (M):  "; : PRINT USING QQ$; CON(1)
1840 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
1850 INPUT ; "Enter Uranium concentration (gU/L). ", CON(2)
1860 LOCATE 12, 2: PRINT "Uranium (g/L):  "; : PRINT USING QQ$; CON(2)
1870 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
1880 IF IPROCE% = 1 THEN 2060
1890 INPUT ; "Enter Plutonium (IV) concentration (gPu/L). ", CON(3)
1900 LOCATE 14, 2: PRINT "Plutonium (IV) (g/L):  "; : PRINT USING QQ$;
     CON(3)
1910 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
1920 IF JHAS% = 0 THEN 2020
1930 INPUT ; "Enter Plutonium (III) concentration (gPu/L). ", CON(4)
1940 LOCATE 16, 2: PRINT "Plutonium (III) (g/L):  "; : PRINT USING QQ$;
     CON(4)
1950 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
1960 INPUT ; "Enter Plutonium Reductant concentration (M). ", CON(5)
1970 LOCATE 18, 2: PRINT "Plutonium Reductant (M):  "; : PRINT USING QQ$;
     CON(5)
1980 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
1990 INPUT ; "Enter Inextractable Nitrate Ion concentration (M). ", CON(6)
2000 LOCATE 20, 2: PRINT "Inextractable Nitrate Ion (M):  "; : PRINT USING
     QQ$; CON(6)
2010 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
2020 INPUT ; "Enter feed temperature in degrees C (0 for default). ", TEMP
2030 IF ABS(TEMP) < .001 THEN TEMP = TEMPI
2040 LOCATE 22, 2: PRINT "Temperature ("; CHR$(248); "C):  "; : PRINT USING
     P$; TEMP
2050 GOTO 2130
2060 INPUT ; "Enter Thorium concentration (gTh/L). ", CON(3)
2070 LOCATE 14, 2: PRINT "Thorium (g/L):  "; : PRINT USING QQ$; CON(3)
2080 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
```

```
2090 IF JHAS% = 0 THEN 2020
2100 INPUT ; "Enter Inextractable Nitrate Ion concentration (M). ", CON(4)
2110 LOCATE 16, 2: PRINT "Inextractable Nitrate Ion (M):  "; : PRINT USING
     QQ$; CON(4)
2120 GOTO 2010
2130 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 25, 1
2140 INPUT ; "Is the above information correct (Y/N)? ", REPLY$
2150 IF REPLY$ <> "Y" THEN CLS : GOTO 1670
2160 LOCATE 25, 1: PRINT SPACE$(79); : LOCATE 25, 1
2170 INPUT ; "Another feed stream (Y/N)? ", REPLY$
2180 CLS : IF REPLY$ = "Y" THEN INDEX% = 1 ELSE INDEX% = 0
2190 WRITE #1, NST%, JHAS%, FDRT
2200 IF JHAS% = 0 THEN V% = 3 ELSE IF IPROCE% = 0 THEN V% = 6 ELSE V% = 4
2210 FOR J = 1 TO V%
2220  WRITE #1, CON(J)
2230 NEXT J
2240 WRITE #1, TEMP, INDEX%
2250 IF REPLY$ = "Y" THEN 1670
2260 IF NEWOUT% = 0 THEN 2500
2270 R1% = 1: C1% = 1: R2% = 10: C2% = 79: GOSUB 4570  'To draw single box
2280 LOCATE 2, 33: PRINT "PRODUCT STREAMS:";
2290 LOCATE 3, 23: PRINT "(in addition to usual end streams)";
2300 LOCATE 11, 1: INPUT ; "Enter stage no. for product. ", NST%
2310 IF NST% < 1 OR NST% > NTOST% THEN BEEP: CLS : GOTO 2270
2320 LOCATE 5, 2: PRINT "Product from Stage No.:  "; NST%
2330 LOCATE 11, 1: PRINT SPACE$(79); : LOCATE 11, 1
2340 INPUT ; "Enter type of product (`1' for aqueous, `0' for organic). ",
     JHAS%
2350 IF JHAS% = 1 THEN 2370
2360 IF JHAS% = 0 THEN 2380 ELSE BEEP: GOTO 2330
2370 LOCATE 7, 2: PRINT "Product is Aqueous."; : GOTO 2390
2380 LOCATE 7, 2: PRINT "Product is Organic.";
2390 LOCATE 11, 1: PRINT SPACE$(79); : LOCATE 11, 1
2400 INPUT ; "Enter flow rate (Liters/min.). ", OTRT
2410 LOCATE 9, 2: PRINT "Product flow rate (L/min.):  "; : PRINT USING QQ$;
     OTRT
2420 LOCATE 11, 1: PRINT SPACE$(79); : LOCATE 25, 1
2430 INPUT ; "Is the above information correct (Y/N)? ", REPLY$
2440 IF REPLY$ <> "Y" THEN CLS : GOTO 2270
2450 LOCATE 25, 1: PRINT SPACE$(79); : LOCATE 25, 1
2460 INPUT ; "Another product stream (Y/N)? ", REPLY$
2470 CLS : IF REPLY$ = "Y" THEN INDEX% = 1 ELSE INDEX% = 0
2480 WRITE #1, NST%, JHAS%, OTRT, INDEX%
2490 IF REPLY$ = "Y" THEN 2270
2500 IF IPRO% <> 1 THEN 3340
2510 IF IPROCE% = 1 THEN 2530
2520 GOSUB 4710: GOTO 2540  'To prepare screen for Purex aqueous profile
     data
2530 GOSUB 4870  'To prepare screen for Thorex aqueous profile data
2540 M% = 0
2550 FOR I% = 1 TO NTOST%
2560  M% = M% + 1
2570  LOCATE 25, 1: PRINT "Stage "; I%;
2580  LOCATE 25, 13: INPUT ; "Enter Aqueous Nitric Acid (M). ", CON(1)
2590  LOCATE 6 + M%, 3: PRINT USING "###"; I%;
```

```
2600  LOCATE 6 + M%, 8: PRINT USING PQ$; CON(1);
2610  LOCATE 25, 13: PRINT SPACE$(65);
2620  LOCATE 25, 13: INPUT ; "Enter Aqueous Uranium (g/L). ", CON(2)
2630  LOCATE 6 + M%, 18: PRINT USING PQ$; CON(2);
2640  LOCATE 25, 13: PRINT SPACE$(65);
2650  IF IPROCE% = 0 THEN 2720
2660  LOCATE 25, 13: INPUT ; "Enter Aqueous Thorium (g/L). ", CON(3)
2670  LOCATE 6 + M%, 28: PRINT USING PQ$; CON(3);
2680  LOCATE 25, 13: PRINT SPACE$(65);
2690  LOCATE 25, 13: INPUT ; "Enter Aqueous Nitrate (M). ", CON(4)
2700  LOCATE 6 + M%, 38: PRINT USING PQ$; CON(4);
2710  GOTO 2830
2720  LOCATE 25, 13: INPUT ; "Enter Aqueous Pu(IV) (g/L). ", CON(3)
2730  LOCATE 6 + M%, 28: PRINT USING PQ$; CON(3);
2740  LOCATE 25, 13: PRINT SPACE$(65);
2750  LOCATE 25, 13: INPUT ; "Enter Aqueous Pu(III) (g/L). ", CON(4)
2760  LOCATE 6 + M%, 38: PRINT USING PQ$; CON(4);
2770  LOCATE 25, 13: PRINT SPACE$(65);
2780  LOCATE 25, 13: INPUT ; "Enter Aqueous Reductant (M). ", CON(5)
2790  LOCATE 6 + M%, 48: PRINT USING PQ$; CON(5);
2800  LOCATE 25, 13: PRINT SPACE$(65);
2810  LOCATE 25, 13: INPUT ; "Enter Aqueous Nitrate (M). ", CON(6)
2820  LOCATE 6 + M%, 58: PRINT USING PQ$; CON(6);
2830  LOCATE 25, 13: PRINT SPACE$(65);
2840  LOCATE 25, 13: INPUT ; "Enter Temperature in degrees C (0 for
      default). ", TEMP
2850  IF ABS(TEMP) < .001 THEN TEMP = TEMPI
2860  LOCATE 6 + M%, 70: PRINT USING PP$; TEMP
2870  LOCATE 25, 1: PRINT SPACE$(79); : LOCATE 25, 1
2880  INPUT ; "Are the entries for the last stage correct (Y/N)? ", REPLY$
2890  LOCATE 25, 1: PRINT SPACE$(79);
2900  IF REPLY$ <> "Y" THEN 2570
2910  IF IPROCE% = 0 THEN V% = 6 ELSE V% = 4
2920  FOR J% = 1 TO V%
2930   WRITE #1, CON(J%)
2940  NEXT J%
2950  WRITE #1, TEMP
2960  IF M% MOD 17 = 0 THEN CLS : M% = 0 ELSE 3000
2970  IF IPROCE% = 1 THEN 2990
2980  GOSUB 4710: GOTO 3000  'To prepare screen for Purex aqueous profile
      data
2990  GOSUB 4870  'To prepare screen for Thorex aqueous profile data
3000 NEXT I%
3010 CLS : M% = 0
3020 IF IPROCE% = 1 THEN 3040
3030 GOSUB 4790: GOTO 3050  'To prepare screen for Purex organic profile
     data
3040 GOSUB 4950  'To prepare screen for Thorex organic profile data
3050 FOR I% = 1 TO NTOST%
3060  M% = M% + 1
3070  LOCATE 25, 1: PRINT "Stage "; I%;
3080  LOCATE 25, 13: INPUT ; "Enter Organic Nitric Acid (M). ", CON(1)
3090  LOCATE 6 + M%, 3: PRINT USING "###"; I%;
3100  LOCATE 6 + M%, 8: PRINT USING PQ$; CON(1);
3110  LOCATE 25, 13: PRINT SPACE$(65);
```

```
3120  LOCATE 25, 13: INPUT ; "Enter Organic Uranium (g/L). ", CON(2)
3130  LOCATE 6 + M%, 18: PRINT USING PQ$; CON(2);
3140  LOCATE 25, 13: PRINT SPACE$(65);
3150  IF IPROCE% = 0 THEN 3190
3160  LOCATE 25, 13: INPUT ; "Enter Organic Thorium (g/L). ", CON(3)
3170  LOCATE 6 + M%, 28: PRINT USING PQ$; CON(3);
3180  GOTO 3210
3190  LOCATE 25, 13: INPUT ; "Enter Organic Pu(IV) (g/L). ", CON(3)
3200  LOCATE 6 + M%, 28: PRINT USING PQ$; CON(3);
3210  LOCATE 25, 1: PRINT SPACE$(79); : LOCATE 25, 1
3220  INPUT ; "Are the entries for the last stage correct (Y/N)? ", REPLY$
3230  LOCATE 25, 1: PRINT SPACE$(79);
3240  IF REPLY$ <> "Y" THEN 3070
3250  FOR J% = 1 TO 3
3260   WRITE #1, CON(J%)
3270  NEXT J%
3280  IF M% MOD 17 = 0 THEN CLS : M% = 0 ELSE 3320
3290  IF IPROCE% = 1 THEN 3310
3300  GOSUB 4790: GOTO 3320  'To prepare screen for Purex organic profile
      data
3310  GOSUB 4950  'To prepare screen for Thorex organic profile data
3320 NEXT I%
3330 CLS : GOTO 3750
3340 IF IPRO% <> 2 THEN 3750
3350 CLS : LOCATE 10, 1: PRINT "Enter Drive (Path) and FILENAME for
     Previous Problem Results data file.";
3360 LOCATE 11, 1: INPUT ; "Examples are B:\xxxxxxxx or C:\Subdir\xxxxxxxx.
     ", DATFIL2$
3365 DATFIL2$ = DATFIL2$ + ".DAT"
3370 CLS : LOCATE 10, 1: PRINT "Ensure that the previous Problem Results
     data file is in place.  If necessary,";
3380 LOCATE 12, 1: PRINT "remove any diskette that occupies the same drive
     as that specified.";
3390 LOCATE 14, 1: INPUT ; "Was it necessary to remove a diskette (Y/N)? ",
     REPLY$
3400 CLS : IF REPLY$ = "N" THEN DSK% = 1
3410 ON ERROR GOTO 7550
3480 COLOR 0, 7: LOCATE 15, 34: PRINT "PLEASE WAIT": COLOR 7, 0
3485 OPEN DATFIL2$ FOR INPUT AS #2
3486 IF IPROCE% = 0 THEN V% = 6 ELSE V% = 4
3487 INPUT #2, TL$: INPUT #2, DA$, TI$, TS
3490 FOR I% = 1 TO NTOST%
3500  IF V% = 6 THEN INPUT #2, J%, CN(1, I%), CN(2, I%), CN(3, I%), Y1, Y2,
      Y3, CN(4, I%), CN(5, I%), CN(6, I%), A1, A2, T(I%), A3, A4, A5, A6,
      A7, A8, A9
3510  IF V% = 4 THEN INPUT #2, J%, CN(1, I%), CN(2, I%), CN(3, I%), Y1, Y2,
      Y3, CN(4, I%), X5, X6, A1, A2, T(I%), A3, A4, A5, A6, A7, A8, A9
3520 NEXT I%
3530 CLOSE #2: OPEN DATFIL2$ FOR INPUT AS #2
3540 INPUT #2, TL$: INPUT #2, DA$, TI$, TS
3550 FOR I% = 1 TO NTOST%
3560  INPUT #2, J%, X1, X2, X3, CN(7, I%), CN(8, I%), CN(9, I%), X4, X5,
      X6, A1, A2, TEMP, A3, A4, A5, A6, A7, A8, A9
3570 NEXT I%
3580 CLOSE #2 : CLS : IF DSK% = 1 THEN 3620
```

```
3590 LOCATE 10, 1: PRINT "Replace diskette that you previously removed.";
3600 LOCATE 14, 1: PRINT "Press any key to continue.";
3610 K$ = INKEY$: IF K$ = "" THEN 3610
3620 CLS : COLOR 0, 7: LOCATE 15, 34: PRINT "PLEASE WAIT": COLOR 7, 0
3630 FOR I% = 1 TO NTOST%
3640  FOR K% = 1 TO V%
3650   WRITE #1, CN(K%, I%)
3660  NEXT K%
3670  WRITE #1, T(I%)
3680 NEXT I%
3690 FOR I% = 1 TO NTOST%
3700  FOR K% = 7 TO 9
3710   WRITE #1, CN(K%, I%)
3720  NEXT K%
3730 NEXT I%
3740 CLS
3750 IF IVOLM% = 3 THEN 4060
3760 V% = 1
3770 GOSUB 5030  'To prepare screen for mixer volumes
3780 MM% = 0: M% = 0: N% = 0
3790 LOCATE 25, 1: INPUT ; "Enter Stage. ", NST%
3800 IF V% <> 1 THEN 3850
3810 IF NST% = 1 THEN V% = 0: GOTO 3850
3820 BEEP: LOCATE 25, 1: PRINT SPACE$(79);
3830 INPUT ; "You must enter Stage 1 first -- Enter Stage. ", NST%
3840 GOTO 3800
3850 MM% = MM% + 1: M% = M% + 1: IF M% MOD 18 = 0 THEN N% = 42: M% = 1
3860 LOCATE 6 + M%, 3 + N%: PRINT USING "###"; NST%;
3870 LOCATE 25, 1: PRINT SPACE$(79);
3880 ON IVOLM% GOTO 3890, 3950
3890 LOCATE 25, 1: INPUT ; "Enter Aqueous Mixer Volume (L). ", VOLA
3900 LOCATE 6 + M%, 9 + N%: PRINT USING PQ$; VOLA;
3910 LOCATE 25, 1: PRINT SPACE$(79);
3920 LOCATE 25, 1: INPUT ; "Enter Organic Mixer Volume (L). ", VOLO
3930 LOCATE 6 + M%, 19 + N%: PRINT USING PQ$; VOLO;
3940 GOTO 3980
3950 LOCATE 25, 1: INPUT ; "Enter Total Mixer Volume (L). ", VOLA
3960 LOCATE 6 + M%, 29 + N%: PRINT USING PQ$; VOLA;
3970 VOLO = 0
3980 LOCATE 25, 1: PRINT SPACE$(79);
3990 LOCATE 25, 1: INPUT ; "More Mixer Volume Data (Y/N)? ", REPLY$
4000 IF REPLY$ = "Y" THEN INDEX% = 1 ELSE INDEX% = 0
4010 WRITE #1, NST%, VOLA, VOLO, INDEX%
4020 IF REPLY$ <> "Y" THEN 4050
4030 IF MM% MOD 34 = 0 THEN CLS : GOTO 3770
4040 LOCATE 25, 1: PRINT SPACE$(79); : GOTO 3790
4050 CLS
4060 IF IVOLS% = 3 THEN 4370
4070 V% = 1
4080 GOSUB 5110  'To prepare screen for settler volumes
4090 MM% = 0: M% = 0: N% = 0
4100 LOCATE 25, 1: INPUT ; "Enter Stage. ", NST%
4110 IF V% <> 1 THEN 4160
4120 IF NST% = 1 THEN V% = 0: GOTO 4160
4130 BEEP: LOCATE 25, 1: PRINT SPACE$(79);
```

```
4140 INPUT ; "You must enter Stage 1 first -- Enter Stage. ", NST%
4150 GOTO 4110
4160 MM% = MM% + 1: M% = M% + 1: IF M% MOD 18 = 0 THEN N% = 42: M% = 1
4170 LOCATE 6 + M%, 3 + N%: PRINT USING "###"; NST%;
4180 LOCATE 25, 1: PRINT SPACE$(79);
4190 ON IVOLS% GOTO 4200, 4260
4200 LOCATE 25, 1: INPUT ; "Enter Aqueous Settler Volume (L). ", VOLA
4210 LOCATE 6 + M%, 9 + N%: PRINT USING PQ$; VOLA;
4220 LOCATE 25, 1: PRINT SPACE$(79);
4230 LOCATE 25, 1: INPUT ; "Enter Organic Settler Volume (L). ", VOLO
4240 LOCATE 6 + M%, 19 + N%: PRINT USING PQ$; VOLO;
4250 GOTO 4290
4260 LOCATE 25, 1: INPUT ; "Enter Total Settler Volume (L). ", VOLA
4270 LOCATE 6 + M%, 29 + N%: PRINT USING PQ$; VOLA;
4280 VOLO = 0
4290 LOCATE 25, 1: PRINT SPACE$(79);
4300 LOCATE 25, 1: INPUT ; "More Settler Volume Data (Y/N)? ", REPLY$
4310 IF REPLY$ = "Y" THEN INDEX% = 1 ELSE INDEX% = 0
4320 WRITE #1, NST%, VOLA, VOLO, INDEX%
4330 IF REPLY$ <> "Y" THEN 4360
4340 IF MM% MOD 34 = 0 THEN CLS : GOTO 4080
4350 LOCATE 25, 1: PRINT SPACE$(79); : GOTO 4100
4360 CLS
4370 CLOSE #1
4380 LOCATE 10, 1: INPUT ; "Do you want a printout of this problem
     definition data (Y/N)? ", REPLY$
4390 IF REPLY$ = "Y" THEN 5190  'To obtain the printout
4400 CLS
4410 RUN "sephis"
4420 END
4430 REM Subroutine to draw a double box.
4440  FOR I% = R1% + 1 TO R2% - 1
4450   LOCATE I%, C1%: PRINT CHR$(186);
4460   LOCATE I%, C2%: PRINT CHR$(186);
4470  NEXT I%
4480  FOR J% = C1% + 1 TO C2% - 1
4490   LOCATE R1%, J%: PRINT CHR$(205);
4500   LOCATE R2%, J%: PRINT CHR$(205);
4510  NEXT J%
4520  LOCATE R1%, C1%: PRINT CHR$(201);
4530  LOCATE R1%, C2%: PRINT CHR$(187);
4540  LOCATE R2%, C1%: PRINT CHR$(200);
4550  LOCATE R2%, C2%: PRINT CHR$(188);
4560 RETURN
4570 REM Subroutine to draw a single box.
4580  FOR I% = R1% + 1 TO R2% - 1
4590   LOCATE I%, C1%: PRINT CHR$(179);
4600   LOCATE I%, C2%: PRINT CHR$(179);
4610  NEXT I%
4620  FOR J% = C1% + 1 TO C2% - 1
4630   LOCATE R1%, J%: PRINT CHR$(196);
4640   LOCATE R2%, J%: PRINT CHR$(196);
4650  NEXT J%
4660  LOCATE R1%, C1%: PRINT CHR$(218);
4670  LOCATE R1%, C2%: PRINT CHR$(191);
```

```
4680  LOCATE R2%, C1%: PRINT CHR$(192);
4690  LOCATE R2%, C2%: PRINT CHR$(217);
4700 RETURN
4710 REM Subroutine to prepare screen for Purex aqueous profile data.
4720  R1% = 1: C1% = 1: R2% = 24: C2% = 79: GOSUB 4570  'To draw single box
4730  LOCATE 2, 26: PRINT "INITIAL CONCENTRATION PROFILE:";
4740  LOCATE 3, 36: PRINT "(Aqueous)";
4750  LOCATE 4, 2: PRINT "Stage    HNO3       U        Pu(IV)    Pu(III)
      REDUCTANT  NITRATE    TEMP";
4760  LOCATE 5, 3: PRINT "No.     (M)       (g/L)     (g/L)      (g/L)
      (M)        (M)        (C)";
4770  LOCATE 6, 2: PRINT "----- --------- --------- --------- --------- ---
      ------ ---------   -----";
4780 RETURN
4790 REM Subroutine to prepare screen for Purex organic profile data.
4800  R1% = 1: C1% = 1: R2% = 24: C2% = 79: GOSUB 4570  'To draw single box
4810  LOCATE 2, 26: PRINT "INITIAL CONCENTRATION PROFILE:";
4820  LOCATE 3, 36: PRINT "(Organic)";
4830  LOCATE 4, 2: PRINT "Stage    HNO3       U        Pu(IV)";
4840  LOCATE 5, 3: PRINT "No.     (M)       (g/L)     (g/L)";
4850  LOCATE 6, 2: PRINT "----- --------- --------- ---------";
4860 RETURN
4870 REM Subroutine to prepare screen for Thorex aqueous profile data.
4880  R1% = 1: C1% = 1: R2% = 24: C2% = 79: GOSUB 4570  'To draw single box
4890  LOCATE 2, 26: PRINT "INITIAL CONCENTRATION PROFILE:";
4900  LOCATE 3, 36: PRINT "(Aqueous)";
4910  LOCATE 4, 2: PRINT "Stage    HNO3       U         Th       NITRATE
      TEMP";
4920  LOCATE 5, 3: PRINT "No.     (M)       (g/L)     (g/L)       (M)
      (C)";
4930  LOCATE 6, 2: PRINT "----- --------- --------- --------- ---------
      -----";
4940 RETURN
4950 REM Subroutine to prepare screen for Thorex organic profile data.
4960  R1% = 1: C1% = 1: R2% = 24: C2% = 79: GOSUB 4570  'To draw single box
4970  LOCATE 2, 26: PRINT "INITIAL CONCENTRATION PROFILE:";
4980  LOCATE 3, 36: PRINT "(Organic)";
4990  LOCATE 4, 2: PRINT "Stage    HNO3       U         Th";
5000  LOCATE 5, 3: PRINT "No.     (M)       (g/L)     (g/L)";
5010  LOCATE 6, 2: PRINT "----- --------- --------- ---------";
5020 RETURN
5030 REM Subroutine to prepare screen for mixer volumes.
5040  R1% = 1: C1% = 1: R2% = 24: C2% = 79: GOSUB 4570  'To draw single box
5050  LOCATE 2, 34: PRINT "MIXER VOLUMES:";
5060  LOCATE 3, 7: PRINT "(Provide data only for first stage and stages
      where volume changes)";
5070  LOCATE 4, 2: PRINT "Stage       Mixer Volume (L)              Stage
      Mixer Volume (L)";
5080  LOCATE 5, 3: PRINT "No.   Aqueous   Organic    Total          No.
      Aqueous   Organic    Total";
5090  LOCATE 6, 2: PRINT "-----  -------   -------   -------        -----
      -------   -------   -------";
5100 RETURN
5110 REM Subroutine to prepare screen for settler volumes.
5120  R1% = 1: C1% = 1: R2% = 24: C2% = 79: GOSUB 4570  'To draw single box
```

```
5130  LOCATE 2, 33: PRINT "SETTLER VOLUMES:";
5140  LOCATE 3, 7: PRINT "(Provide data only for first stage and stages
      where volume changes)";
5150  LOCATE 4, 2: PRINT "Stage      Settler Volume (L)              Stage
      Settler Volume (L)";
5160  LOCATE 5, 3: PRINT "No.   Aqueous   Organic    Total          No.
      Aqueous   Organic    Total";
5170  LOCATE 6, 2: PRINT "-----  -------   -------   -------        -----
      -------   -------   -------";
5180 RETURN
5190 REM The following routine provides a printout of problem definition
     data.
5200 ON ERROR GOTO 7680
5210 OPEN DATFIL1$ FOR INPUT AS #1
5220 LOCATE 12, 1: PRINT "Have printer ON and READY -- Then press any
     key.";
5230 K$ = INKEY$: IF K$ = "" THEN 5230
5240 LOCATE 12, 1: PRINT SPACE$(79);
5250 COLOR 0, 7: LOCATE 15, 34: PRINT "PLEASE WAIT": COLOR 7, 0
5260 LPRINT CHR$(15);
5270 WIDTH "lpt1:", 135
5280 INPUT #1, DAT$, TIM$
5290 INPUT #1, TITLE$, NTOST%, CTBP, TEMPI, NSTR%, ISTR%, JSTR%, IRXN%,
     IPROCE%, DTHETA, DPRINT%, TSTOP%, TOL, NEWOUT%, IVOLM%, IVOLS%, IPRO%,
     IFAST%
5300 LPRINT "PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11:";
     SPACE$(63); DAT$; " "; TIM$
5310 LPRINT : LPRINT "     Problem:  "; TITLE$
5320 LPRINT
5330 IF IPROCE% = 0 THEN LPRINT SPACE$(10); "PUREX PROCESS."
5340 IF IPROCE% = 1 THEN LPRINT SPACE$(10); "THOREX PROCESS."
5350 PQ$ = "     ##.##^^^^": R$ = "     ###.#"
5360 LPRINT SPACE$(10); "Total stages:  "; NTOST%
5370 LPRINT SPACE$(10); "Volume % TBP in solvent:  "; : LPRINT USING P$;
     CTBP * 100!
5380 LPRINT SPACE$(10); "Initial or default temperature ("; CHR$(248); "C):
     ";
5390 LPRINT USING P$; TEMPI
5400 IF NSTR% = 0 THEN LPRINT SPACE$(10); "No unusual stage connections"
5410 IF NSTR% = 1 THEN LPRINT SPACE$(10); "Organic taken from stage ";
     ISTR%; " feeds stage "; JSTR%; "."
5420 IF IPROCE% = 1 THEN 5480
5430 ON (IRXN% + 1) GOTO 5440, 5450, 5460, 5470
5440 LPRINT SPACE$(10); "No Plutonium reaction.": GOTO 5480
5450 LPRINT SPACE$(10); "Instantaneous reduction of Pu(IV).": GOTO 5480
5460 LPRINT SPACE$(10); "Reduction of Pu(IV) by U(IV).": GOTO 5480
5470 LPRINT SPACE$(10); "Reduction of Pu(IV) by hydroxylamine nitrate."
5480 LPRINT SPACE$(10); "Minutes per time increment:  "; : LPRINT USING Q$;
     DTHETA
5490 LPRINT SPACE$(10); "Minutes between printing of the concentration
     profile:  "; : LPRINT USING "####"; DPRINT%
5500 LPRINT SPACE$(10); "Calculations will stop after ";
5510 LPRINT USING "####"; TSTOP%;
5520 LPRINT " minutes or when a tolerance of ";
5530 LPRINT USING PPP$; TOL;
```

```
5540 LPRINT " % per minute is reached."
5550 ON IVOLM% GOTO 5560, 5570, 5580
5560 LPRINT SPACE$(10); "Mixer volumes are defined for each phase.": GOTO
     5590
5570 LPRINT SPACE$(10); "Total mixer volumes are defined (phase ratios =
     flow ratios).": GOTO 5590
5580 LPRINT SPACE$(10); "Mixer volumes = (phase flow)(unit time)."
5590 ON IVOLS% GOTO 5600, 5610, 5620
5600 LPRINT SPACE$(10); "Settler volumes are defined for each phase.": GOTO
     5630
5610 LPRINT SPACE$(10); "Total settler volumes are defined (phase ratios =
     flow ratios).": GOTO 5630
5620 LPRINT SPACE$(10); "Settler volumes = (phase flow)(unit time)."
5630 ON (IPRO% + 1) GOTO 5640, 5650, 5660
5640 LPRINT SPACE$(10); "Initial concentration profile is zero.": GOTO 5670
5650 LPRINT SPACE$(10); "Initial concentration profile is defined.": GOTO
     5670
5660 LPRINT SPACE$(10); "Initial concentration profile is from a previous
     problem."
5670 ON (IFAST% + 1) GOTO 5680, 5690, 5700
5680 LPRINT SPACE$(10); "Runge-Kutta integration will be used.": GOTO 5710
5690 LPRINT SPACE$(10); "Trapezoidal integration will be used.": GOTO 5710
5700 LPRINT SPACE$(10); "Fast integration will be used."
5710 IF NEWOUT% = 0 THEN LPRINT SPACE$(10); "No extra product streams."
5720 IF NEWOUT% = 1 THEN LPRINT SPACE$(10); "Extra product stream(s)."
5730 LPRINT : LPRINT SPACE$(10); "The FILESPEC for this Problem Definition
     data file is:  "; DATFIL1$: LPRINT
5740 LPRINT "FEED AND PRODUCT STREAM DATA:"
5750 LN% = 22
5760 IF IPROCE% = 0 THEN GOSUB 6980  'To set up Purex feed & product chart
5770 IF IPROCE% = 1 THEN GOSUB 7040  'To set up Thorex feed & product chart
5780 INPUT #1, NST%, JHAS%, FDRT
5790 IF JHAS% = 0 THEN V% = 3 ELSE IF IPROCE% = 0 THEN V% = 6 ELSE V% = 4
5800 FOR I = 1 TO V%
5810  INPUT #1, CON(I)
5820 NEXT I
5830 INPUT #1, TEMP, INDEX%
5840 IF JHAS% = 1 THEN LPRINT SPACE$(8); "AQUEOUS ";
5850 IF JHAS% = 0 THEN LPRINT SPACE$(4); : LPRINT USING P$; CTBP * 100!; :
     LPRINT " % TBP ";
5860 LPRINT USING "###"; NST%;
5870 FOR I = 1 TO V%
5880  LPRINT USING PQ$; CON(I);
5890 NEXT I
5900 IF V% = 3 THEN LPRINT SPACE$(42);
5910 IF V% = 4 THEN LPRINT SPACE$(28);
5920 LPRINT USING PQ$; FDRT;
5930 LPRINT USING R$; TEMP
5940 LN% = LN% + 1
5950 IF INDEX% <> 1 THEN 5980
5960 IF LN% < 55 THEN 5780
5970 LPRINT CHR$(12); : LN% = 0: GOTO 5760
5980 IF NEWOUT% = 0 THEN 6120
5990 IF LN% < 55 THEN 6030
6000 LPRINT CHR$(12); : LN% = 0
```

```
6010 IF IPROCE% = 0 THEN GOSUB 6980  'To set up Purex feed & product chart
6020 IF IPROCE% = 1 THEN GOSUB 7040  'To set up Thorex feed & product chart
6030 INPUT #1, NST%, JHAS%, OTRT, INDEX%
6040 IF JHAS% = 1 THEN LPRINT SPACE$(8); "AQUEOUS ";
6050 IF JHAS% = 0 THEN LPRINT SPACE$(8); "ORGANIC ";
6060 LPRINT USING "###"; NST%;
6070 LPRINT "      Product stream removed (actual flow rate to be
     computed)";
6080 LPRINT SPACE$(22); : LPRINT USING PQ$; OTRT
6090 LN% = LN% + 1
6100 IF INDEX% <> 1 THEN 6120
6110 IF LN% >= 55 THEN 6000 ELSE 6030
6120 IF IPRO% = 0 THEN 6530
6130 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 6150
6140 LPRINT CHR$(12); : LN% = 0
6150 LPRINT "INITIAL AQUEOUS PROFILE DATA:": LN% = LN% + 1
6160 IF IPROCE% = 0 THEN GOSUB 7100: V% = 6  'To set up Purex aqueous
     profile chart
6170 IF IPROCE% = 1 THEN GOSUB 7160: V% = 4  'To set up Thorex aqueous
     profile chart
6180 FOR I% = 1 TO NTOST%
6190  IF LN% < 55 THEN 6230
6200  LPRINT CHR$(12); : LN% = 0
6210  IF IPROCE% = 0 THEN GOSUB 7100  'To set up Purex aqueous profile
      chart
6220  IF IPROCE% = 1 THEN GOSUB 7160  'To set up Thorex aqueous profile
      chart
6230  FOR J% = 1 TO V%
6240   INPUT #1, CON(J%)
6250  NEXT J%
6260  INPUT #1, TEMP
6270  LPRINT SPACE$(16); : LPRINT USING "###"; I%;
6280  FOR J% = 1 TO V%
6290   LPRINT USING PQ$; CON(J%);
6300  NEXT J%
6310  IF V% = 6 THEN LPRINT SPACE$(14);
6320  IF V% = 4 THEN LPRINT SPACE$(42);
6330  LPRINT USING R$; TEMP
6340  LN% = LN% + 1
6350 NEXT I%
6360 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 6380
6370 LPRINT CHR$(12); : LN% = 0
6380 LPRINT "INITIAL ORGANIC PROFILE DATA:": LN% = LN% + 1
6390 IF IPROCE% = 0 THEN GOSUB 7280  'To set up Purex organic profile chart
6400 IF IPROCE% = 1 THEN GOSUB 7340  'To set up Thorex organic profile
     chart
6410 FOR I% = 1 TO NTOST%
6420  IF LN% < 55 THEN 6460
6430  LPRINT CHR$(12); : LN% = 0
6440  IF IPROCE% = 0 THEN GOSUB 7280  'To set up Purex organic profile
      chart

6450  IF IPROCE% = 1 THEN GOSUB 7340  'To set up Thorex organic profile
      chart
6460  FOR J% = 1 TO 3
```

```
6470   INPUT #1, CON(J%)
6480  NEXT J%
6490  LPRINT SPACE$(16); : LPRINT USING "###"; I%;
6500  LPRINT USING PQ$; CON(1); CON(2); CON(3)
6510  LN% = LN% + 1
6520 NEXT I%
6530 IF IVOLM% = 3 THEN 6740
6540 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 6560
6550 LPRINT CHR$(12); : LN% = 0
6560 LPRINT "MIXER VOLUME DATA (L):": LN% = LN% + 1
6570 GOSUB 7220  'To set up volume chart
6580 PX% = 0
6590 INPUT #1, NST%, VOLA, VOLO, INDEX%
6600 NS% = NST%: VLA = VOLA: VLO = VOLO: IDEX% = INDEX%
6610 IF IVOLM% <> 1 THEN 6640
6620 LPRINT SPACE$(16); : LPRINT USING "###"; NS%;
6630 LPRINT USING PQ$; VLA; VLO: GOTO 6660
6640 LPRINT SPACE$(16); : LPRINT USING "###"; NS%;
6650 LPRINT SPACE$(28); : LPRINT USING PQ$; VLA
6660 LN% = LN% + 1
6670 IF LN% < 55 THEN 6690
6680 IF NS% = NTOST% THEN 6740 ELSE LPRINT CHR$(12); : LN% = 0: GOSUB 7220
6690 IF PX% = 1 THEN 6720
6700 IF IDEX% <> 1 THEN 6730
6710 INPUT #1, NST%, VOLA, VOLO, INDEX%
6720 IF NST% = NS% + 1 THEN PX% = 0: GOTO 6600 ELSE NS% = NS% + 1: PX% = 1:
     GOTO 6610
6730 IF NS% <> NTOST% THEN NS% = NS% + 1: GOTO 6610
6740 IF IVOLS% = 3 THEN 6950
6750 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 6770
6760 LPRINT CHR$(12); : LN% = 0
6770 LPRINT "SETTLER VOLUME DATA (L):": LN% = LN% + 1
6780 GOSUB 7220  'To set up volume chart
6790 PX% = 0
6800 INPUT #1, NST%, VOLA, VOLO, INDEX%
6810 NS% = NST%: VLA = VOLA: VLO = VOLO: IDEX% = INDEX%
6820 IF IVOLS% <> 1 THEN 6850
6830 LPRINT SPACE$(16); : LPRINT USING "###"; NS%;
6840 LPRINT USING PQ$; VLA; VLO: GOTO 6870
6850 LPRINT SPACE$(16); : LPRINT USING "###"; NS%;
6860 LPRINT SPACE$(28); : LPRINT USING PQ$; VLA
6870 LN% = LN% + 1
6880 IF LN% < 55 THEN 6900
6890 IF NS% = NTOST% THEN 6950 ELSE LPRINT CHR$(12); : LN% = 0: GOSUB 7220
6900 IF PX% = 1 THEN 6930
6910 IF IDEX% <> 1 THEN 6940
6920 INPUT #1, NST%, VOLA, VOLO, INDEX%
6930 IF NST% = NS% + 1 THEN PX% = 0: GOTO 6810 ELSE NS% = NS% + 1: PX% = 1:
     GOTO 6820
6940 IF NS% <> NTOST% THEN NS% = NS% + 1: GOTO 6820
6950 LPRINT CHR$(12);
6960 LPRINT CHR$(18);
6970 GOTO 4400
6980 REM Subroutine to set up chart for Purex feed & product stream data.
```

```
6990  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        PU (IV)
      PU (III)       REDUCTANT    NITRATE ION    FLOW RATE      TEMP"
7000  LPRINT SPACE$(17); "NO.       (M)           (g/L)          (g/L)
      (g/L)            (M)          (M)          (L/min)        (C)"
7010  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------   -----------   -----------   -----------    ------"
7020  LN% = LN% + 3
7030 RETURN
7040 REM Subroutine to set up chart for Thorex feed & product stream data.
7050  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        THORIUM
      NITRATE ION                                FLOW RATE       TEMP"
7060  LPRINT SPACE$(17); "NO.       (M)           (g/L)          (g/L)
      (M)                                       (L/min)        (C)"
7070  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------                               -----------    ------"
7080  LN% = LN% + 3
7090 RETURN
7100 REM Subroutine to set up Purex aqueous profile chart.
7110  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        PU (IV)
      PU (III)       REDUCTANT    NITRATE ION                   TEMP"
7120  LPRINT SPACE$(17); "NO.       (M)           (g/L)          (g/L)
      (g/L)            (M)          (M)                        (C)"
7130  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------   -----------   -----------                  ------"
7140  LN% = LN% + 3
7150 RETURN
7160 REM Subroutine to set up Thorex aqueous profile chart.
7170  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        THORIUM
      NITRATE ION                                               TEMP"
7180  LPRINT SPACE$(17); "NO.       (M)           (g/L)          (g/L)
      (M)                                                     (C)"
7190  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------                                              ------"
7200  LN% = LN% + 3
7210 RETURN
7220 REM Subroutine to set up volume chart.
7230  LPRINT SPACE$(16); "STAGE    AQUEOUS       ORGANIC        TOTAL"
7240  LPRINT SPACE$(17); "NO.     VOLUME        VOLUME        VOLUME"
7250  LPRINT SPACE$(16); "-----  -----------   -----------   -----------"
7260  LN% = LN% + 3
7270 RETURN
7280 REM Subroutine to set up Purex organic profile chart.
7290  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        PU (IV)"
7300  LPRINT SPACE$(17); "NO.       (M)           (g/L)          (g/L)"
7310  LPRINT SPACE$(16); "-----  -----------   -----------   -----------"
7320  LN% = LN% + 3
7330 RETURN
7340 REM Subroutine to set up Thorex organic profile chart.
7350  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        THORIUM"
7360  LPRINT SPACE$(17); "NO.       (M)           (g/L)          (g/L)"
7370  LPRINT SPACE$(16); "-----  -----------   -----------   -----------"
7380  LN% = LN% + 3
7390 RETURN
7400 REM Error trapping routine.
7410  LOCATE 25, 1: PRINT SPACE$(79);
```

```
7420  IF ERR = 64 THEN LOCATE 25, 1: PRINT "Bad file name"; : GOTO 7460
7430  IF ERR = 61 THEN LOCATE 25, 1: PRINT "Disk full"; : GOTO 7500
7440  IF ERR = 71 THEN LOCATE 25, 1: PRINT "Disk not ready"; : GOTO 7540
7450  ON ERROR GOTO 0
7460  PRINT " - Press any key to continue";
7470  K$ = INKEY$: IF K$ = "" THEN 7470
7480  LOCATE 25, 1: PRINT SPACE$(79);
7490  RESUME 1560
7500  PRINT " - Replace with new disk and press any key";
7510  K$ = INKEY$: IF K$ = "" THEN 7510
7520  LOCATE 25, 1: PRINT SPACE$(79);
7530  RESUME 1640
7540  PRINT " - Insert data disk in correct drive and press any key"; :
      GOTO 7510
7550 REM Error trapping routine.
7560  LOCATE 15, 34: PRINT SPACE$(12);
7570  IF ERR = 64 THEN LOCATE 25, 1: PRINT "Bad file name"; : GOTO 7610
7580  IF ERR = 71 THEN LOCATE 25, 1: PRINT "Disk not ready"; : GOTO 7640
7590  IF ERR = 53 THEN LOCATE 25, 1: PRINT "File not found"; : GOTO 7610
7600  ON ERROR GOTO 0
7610  PRINT " - Press any key to continue";
7620  K$ = INKEY$: IF K$ = "" THEN 7620
7630  RESUME 3350
7640  PRINT " - Insert data disk in correct drive and press any key";
7650  K$ = INKEY$: IF K$ = "" THEN 7650
7660  LOCATE 25, 1: PRINT SPACE$(79);
7670  RESUME 3480
7680 REM Error trapping routine.
7690  LOCATE 15, 34: PRINT SPACE$(12);
7700  IF ERR = 24 THEN LOCATE 25, 1: PRINT "Your printer is not ready"; :
      GOTO 7720
7710  ON ERROR GOTO 0
7720  PRINT " - Check it and press any key";
7730  K$ = INKEY$: IF K$ = "" THEN 7730
7740  LOCATE 25, 1: PRINT SPACE$(79);
7750  COLOR 0, 7: LOCATE 15, 34: PRINT "PLEASE WAIT"; : COLOR 7, 0
7760  RESUME
```

APPENDIX C
SECALC.BAS—THE MAIN MODULE

The Main Module of the calculational program (SECALC.BAS) includes 7 routines (STARTS, CONVPU1, CONVPU2, CONVPU3, CONVTH1, CONVTH2, and CONVTH3). The main program is described in Sect. C.1 with a listing in Sect. C2. The STARTS routine is described in C.3 and listed in C.4. The CONV routines are described and listed in C.5 and C.6 respectively.

C.1 Main Program (SECALC)

Statements	Description
10- 400	Introductory material that produces the initial title screen, notes the need for a previously prepared Problem Definition file (and provides a means to exit if such is not available), and requests the Filespecs for the available Problem Definition file and for the Problem Results file that is to be produced. Filespecs must include drive (path) designation (e.g., B:\FILENAME or C:\Subdir\FILENAME) but no extension (B:\FILENAME.DAT is incorrect).
410- 500	Defines format for printing of results, opens the Problem Definition file for input, opens the Problem Results file for output, and opens a scratch file for temporary data storage. The user is reminded to have the printer on and ready. (Note: The printer should be adjusted to use the IBM character set.)
510- 650	General information from the Problem Definition file is read and array variables are dimensioned.
660- 790	Stage calculations will be made by sweeping through the cascade in both directions. The direction for the first set of calculations (made in the direction of aqueous phase flow) is defined in statement 660 as NDIREC% = 1. Statement 670 calculates the specific heat of the organic phase (SPH) and the molar concentration of TBP (T) as follows:

$$SPH = 0.321 + 0.078\ CTBP \tag{C.1}$$

$$T = 3.65145\ CTBP \tag{C.2}$$

where CTBP = volume fraction of TBP in the organic phase,
SPH = specific heat of the organic phase, cal./g°C, and
T = molarity of TBP.

The above is based on a TBP density of 0.9725 g/mL and a TBP

Statements	Description
	molecular weight of 266.3. The maximum inventory change of any component in any stage (CODUM) is initiated at a value of 200%. Stage and feed stream temperatures are initially set at the default value (TEMPI) provided by the Problem Definition file.
800	A subroutine in statements 7670-7970 is used to set up a status screen by which cascade calculations can be monitored.
810-1240	General information from the Problem Definition file is printed out and a "Problem is defined." statement appears on the screen.
1250	The STARTS routine begins here. It contains general input functions and sets the system hydraulics. The routine ends with statement 3070 that places a "Cascade flows are established." statement on the screen. For details of the STARTS routine, see Sect. C.3.
3080-3130 3700-3740 4240-4250	The initial aqueous and organic concentration profiles are converted to a solute-free basis through the use of routines CONVPU2 and CONVPU3, respectively, or alternately, CONVTH2 and CONVTH3. For details of these routines, see Sect. C.5.
4260-4700	Stage volumes are read from the Problem Definition file, if supplied. If no volume data are supplied, the volumes are assumed to be numerically equal to the flow rate per unit time; i.e., one stage throughput per minute. When volume data are supplied, only data for the first stage are necessary unless volumes change in other stages. If no data are found for a given stage, the volumes for the previous stage are assumed to apply. All mixer and settler phase volumes are established based on supplied phase volume data, calculated from supplied total stage volume data, or set numerically equal to the phase flow. These data are sent to the printer.
4710-5050	The phases in each stage are equilibrated for an initial concentration profile if not previously equilibrated, defined as zero concentration, or provided from a previous problem result. The equilibration routine is by-passed if IPRO% = 0 or if EQCKDG% = 1. The equilibration routine calls Subprogram UCORPU or UCORTH to obtain distribution coefficients for the equilibrations. For details of these Subprograms, see Sect. D.3. Calculations are made from an overall material balance and the definition of the distribution coefficient.

$$A\ X_1 + O\ Y_1 = A\ X_2 + O\ Y_2 \tag{C.3}$$

$$D = Y_1 / X_1 \tag{C.4}$$

$$X1 = (A\ X_2 + O\ Y_2) / (A + D\ O) \tag{C.5}$$

$$Y_1 = Y_2 + (X_2 - X_1)\ A / O \tag{C.6}$$

Statements	Description
	where D = Distribution coefficient from UCORPU or UCORTH, X = Aqueous phase concentration in mixer, Y = Organic phase concentration in mixer, A = Aqueous phase volume, and O = Organic phase volume. Subscripts 1 and 2 refer to the equilibrium condition and the condition prior to equilibrium respectively. Several (up to 3) equilibrations are made until the aqueous phase concentration changes by <1% upon re-equilibration as denoted by the index ICK%. If the change is <1%, ICK% = 1, otherwise ICK% = 0. Concentrations in the settlers are set equal to mixer concentrations. Mixer temperatures are set equal to the temperature profile provided from the Problem Definition file or, if none is provided, set to the default temperature. (Note: All discussion to follow will use condition 1 and condition 2 to refer to the beginning and end, respectively, of a time increment over which stage calculations are made.)
5060-5310	The printout for problem results is begun, total time and print time are set to zero, and the total solute fed to the system (SOIN) is calculated from feed rates and feed concentrations. Statements are placed on the screen denoting the type of integration used and if plutonium undergoes reduction. Routing indices NSTOP%, NBORT%, NPRNT%, and NMAXT% are set to 1, the time increment counter (NSTG%) is set to 0, and control is transferred to statement 6210 where the total time is compared with time to print. Since they are both zero at this point, control is transferred to statement 6230 where the print index (NPRNT%) is set to 0. Print time is advanced for the subsequent printout and the appropriate print Subprogram (PRTPU or PRTTH) is called. For details of these Subprograms, see Sect. D.7. The print Subprogram prints out all stage concentrations for zero time. Since no other routing index was changed to 0, mixer concentrations for condition 2 are reset to those for condition 1, as the print Subprogram converted condition-2 values to molar units. Control then transfers to statement 5320 where the first time increment is shown on the screen.
5320-5330	The STAGES Subprogram is now called for the current time increment. Details of this Subprogram are shown in Sect. D.5. The STAGES Subprogram is entered with concentrations at the beginning of the time increment, designated as condition 1. STAGES performs stage-wise calculations and returns concentrations for the end of the time increment, designated as condition 2. STAGES also returns values of the array CODUM, the maximum inventory change of any component in a stage per minute.
5340-5400	The direction for calculations (NDIREC%) is reversed for the next time increment, routing index NSTOP% is set to 0 pending a

Statements	Description
	check on steady-state attainment, the counter NSTG% is incremented, time is advanced, and the maximum inventory change in a stage (COMAX) is calculated and shown on the screen. COMAX is the largest value in the array CODUM, each element of which represents the maximum inventory change of any component in a stage. Note that the total process time is represented exactly by TOTIME; integer values are represented by TOME%.
5410-5710	Settler concentrations are converted to molar units and the total solute leaving the system (SOT) is calculated from settler concentrations and exit stream flow rates.
5720-5930	A bar graph is drawn on the screen to show, for each solute, the overall material balance at this time.
5940-6180	If the integer (truncated) value of process time (TOME%) is equal to the exact value (TOTIME), the overall material balance for each solute is logged into the scratch file. A steady-state operation check is made by comparing values of CODUM with the specified tolerance (TOL). If any value of CODUM is larger than TOL, steady-state has not been attained and the index NSTOP% is reset to 1. Concentrations for condition 1 are made equal to those for condition 2 for use in a subsequent stage calculation.
6190-6430	These statements consider program control based on several options. 1. If steady-state operation was attained (NSTOP% = 0), the appropriate print Subprogram (PRTPU or PRTTH) is called and control advances to statement 6440 en route to the end of the program. 2. If a key on the keyboard was pressed to prematurely stop calculations, the index NBORT% is set to 0 and the appropriate print Subprogram is called; control then advances to statement 6690 en route to requesting the user's desire to continue or stop. 3. If process time equals the time that was requested for printing results, the index NPRNT% is set to 0, print time is advanced for the subsequent printout, and the appropriate print Subprogram is called. Control then advances to statement 6350 where mixer concentrations for condition 2 are reset to those for condition 1, as the print Subprogram converted condition-2 values to molar units. Control then transfers to statement 5320 where the next time increment is shown on the screen. 4. If none of the above occurred and process time is less than the maximum specified time (TSTOP%), control transfers to statement 5320 where the next time increment is shown on

Statements	Description
	the screen. However, if process time equals or exceeds TSTOP%, the index NMAXT% is set to 0 and the appropriate print Subprogram is called; control then advances to statement 6730 en route to requesting the user's desire to continue or stop.
6440-6680	The Problem Results file is prepared by writing the problem title, time and date, and stage concentrations (including densities, extraction factors, flow rates, and degree of solvent saturation). The printout for problem results is completed by printing valid ranges for the distribution data incorporated in Subprograms UCORPU or UCORTH. Computer run time is also printed. If steady-state operation was attained, the statement "Steady-state condition is met ---" is placed on the screen. Control then transfers to statement 6840.
6690-6720	The statement "Calculations stopped ----" is placed on the screen and control transfers to statement 6760.
6730-6750	The statement "Maximum time reached ----" is placed on the screen and control transfers to statement 6760.
6760-6830	The user is asked if calculations should continue. If the reply is not in the affirmative, control transfers to statement 6440. If calculations are to continue, control transfers to statement 6350 (after first doubling the value of TSTOP% if NMAXT% = 0) where mixer concentrations for condition 2 are reset to those for condition 1, as the print Subprogram converted condition-2 values to molar units. Control then transfers to statement 5320 where the next time increment is shown on the screen.
6840-6940	Final wrapup of the program occurs by transferring the overall material balance values for each component from the scratch file to the Problem Results file. Up to 1000 sets of data will be transferred. If the calculations went on for more than 1000 minutes, only the final 1000 sets will be transferred. The scratch file is then erased and the program terminates.

C.2 Listing of Program SECALC (The Main Module)

```
10 REM PROGRAM SECALC -- Solvent Extraction Process Having Interacting
   Solutes -- Problem Calculations -- MAIN MODULE
20 REM This module contains the MAIN program; STARTS routine; CONVPU1, 2,
   and 3 routines; and CONVTH1, 2, and 3 routines.
30 REM $DYNAMIC
40 REM $INCLUDE: 'A:SECOM.BI'
50 WIDTH "scrn:", 80
60 SCREEN 0, 1, 0, 0
```

```
70 KEY OFF: CLS
80 R1% = 1: C1% = 1: R2% = 23: C2% = 79: GOSUB 6950  'To draw double box
90 R1% = 10: C1% = 25: R2% = 14: C2% = 55: GOSUB 7090  'To draw single box
100 FOR I% = 1 TO 24
110  LOCATE 10, I%: PRINT CHR$(196);
120 NEXT I%
130 FOR I% = 56 TO 78
140  LOCATE 10, I%: PRINT CHR$(196);
150 NEXT I%
160 LOCATE 10, 1: PRINT CHR$(199);
170 LOCATE 10, 25: PRINT CHR$(194);
180 LOCATE 10, 55: PRINT CHR$(194);
190 LOCATE 10, 79: PRINT CHR$(182); : COLOR 0, 7
200 LOCATE 3, 29: PRINT "PC - S E P H I S - MOD4"; : COLOR 7, 0
210 LOCATE 4, 31: PRINT "Version 2.11 (1990)";
220 LOCATE 6, 13: PRINT "A Solvent Extraction Process Having Interacting
    Solutes";
230 LOCATE 8, 17: PRINT "For Uranium, Plutonium, Thorium, and Nitric Acid";
240 LOCATE 9, 16: PRINT "Mass Transfer in Purex- or Thorex-type
    Flowsheets";
250 LOCATE 11, 34: PRINT "W.S. Groenier";
260 LOCATE 12, 30: PRINT "Fuel Recycle Division";
270 LOCATE 13, 26: PRINT "Oak Ridge National Laboratory"; : COLOR 0, 7
280 LOCATE 17, 24: PRINT "*** PROBLEM CALCULATION ONLY ***"; : COLOR 7, 0
290 LOCATE 19, 20: PRINT "Problem Definition file must be available";
295 LOCATE 20, 21: PRINT "Choose the location for this file below";
300 LOCATE 21, 14: PRINT "If not prepared, return to MENU and run Option
    No. 1.";
310 LOCATE 24, 1: INPUT ; "Do you want to continue (Y/N)? ", REPLY$
320 IF REPLY$ <> "Y" THEN CLS : GOTO 6930
330 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
335 INPUT ; "Will the file be on a diskette (Y/N)? ", REPLY$
336 IF REPLY$ <> "Y" THEN 370
337 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
340 PRINT "Insert diskette -- Press any key to continue.";
360 K$ = INKEY$: IF K$ = "" THEN 360
370 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 25, 1: PRINT SPACE$(79); :
    LOCATE 24, 1
380 PRINT "Enter Drive (Path) and FILENAME of Problem Definition data file.
    ";
385 LOCATE 25, 1: INPUT ; "Make your entry here. ", DATFIL1$
390 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 25, 1: PRINT SPACE$(79); :
    LOCATE 24, 1
400 PRINT "Enter Drive (Path) and FILENAME for Problem Results data file.";
404 LOCATE 25, 1: INPUT ; "Make your entry here. ", DATFIL2$
405 DATFIL1$ = DATFIL1$ + ".DAT"
406 DATFIL2$ = DATFIL2$ + ".DAT"
410 CLS : P$ = "###.#": Q$ = "####.##": PP$ = "###.##": PQ$ = "
    ##.##^^^^": R$ = "     ###.#": RR$ = "    ###.#": QQ$ = "    ##.##^^^^":
    PPP$ = "###.####"
420 ON ERROR GOTO 7980
430 OPEN DATFIL1$ FOR INPUT AS #1
440 OPEN DATFIL2$ FOR OUTPUT AS #2
441 DATFIL3$ = DATFIL2$
442 IF RIGHT$(DATFIL3$, 1) = "\" THEN 445
```

```
443 DATFIL3$ = LEFT$(DATFIL3$, LEN(DATFIL3$) - 1)
444 GOTO 442
445 DATFIL3$ = DATFIL3$ + "scratch"
450 OPEN DATFIL3$ FOR RANDOM AS #3 LEN = 40
460 FIELD 3, 10 AS F1$, 10 AS F2$, 10 AS F3$, 10 AS F4$
470 ON ERROR GOTO 8070
480 LOCATE 10, 1: PRINT "Output will be directed to the PRINTER.";
490 LOCATE 15, 1: PRINT "Have printer ON and READY -- Then press any key.";
500 K$ = INKEY$: IF K$ = "" THEN 500
510 LPRINT CHR$(15);
520 WIDTH "lpt1:", 135
530 INPUT #1, DAT1$, TIM1$
540 INPUT #1, TITLE$, NTOST%, CTBP, TEMPI, NSTR%, ISTR%, JSTR%, IRXN%,
    IPROCE%, DTHETA, DPRINT%, TSTOP%, TOL, NEWOUT%, IVOLM%, IVOLS%, IPRO%,
    IFAST%
550 DIM CODUM(NTOST%), CODUMM(6, NTOST%), X(6, NTOST%, 2), Y(3, NTOST%, 2)
560 DIM XS(NTOST%, 3, 6, 2), YS(NTOST%, 3, 3, 2), ANET(NTOST%),
    ONET(NTOST%), AT(NTOST%), OT(NTOST%)
570 DIM XFD(6, NTOST%), YFD(3, NTOST%), AFDRT(NTOST%), OFDRT(NTOST%)
580 DIM AFDTEM(NTOST%), OFDTEM(NTOST%), ALVRT(NTOST%), OLVRT(NTOST%)
590 DIM TPROF(NTOST%, 2), ATS(NTOST%, 3, 2), OTS(NTOST%, 3, 2)
600 DIM AVOL(NTOST%), OVOL(NTOST%), ASVOL(NTOST%), OSVOL(NTOST%)
610 DIM CON(6)
620 DIM AOUT(NTOST%), OOUT(NTOST%), AAOUT(NTOST%), OOOUT(NTOST%)
630 DIM ARY(6), DTRY(3), AQ(6), ORG(3), EXT1(NTOST%), EXT2(NTOST%),
    EXT3(NTOST%)
640 DIM RXNTRM(6, NTOST%), AIN(6), OIN(3), MB(3), SOIN(4), SOT(4)
650 DIM ADEN(NTOST%), ODEN(NTOST%), TSAT(NTOST%)
660 NDIREC% = 1
670 SPH = .321 + .078 * CTBP: T = 3.65145 * CTBP
680 FOR I% = 1 TO NTOST%
690  CODUM(I%) = 200!
700  AFDTEM(I%) = TEMPI: OFDTEM(I%) = TEMPI
710 NEXT I%
720 FOR I% = 1 TO 2
730  FOR J% = 1 TO NTOST%
740   TPROF(J%, I%) = TEMPI
750   FOR K% = 1 TO 3
760    ATS(J%, K%, I%) = TEMPI: OTS(J%, K%, I%) = TEMPI
770   NEXT K%
780  NEXT J%
790 NEXT I%
800 GOSUB 7670  'To set up status screen
810 LPRINT "PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11:";
    SPACE$(63); DAT1$; " "; TIM1$
820 LPRINT : LPRINT "     Problem:  "; TITLE$: LPRINT
830 IF IPROCE% = 0 THEN LPRINT SPACE$(10); "PUREX PROCESS"
840 IF IPROCE% = 1 THEN LPRINT SPACE$(10); "THOREX PROCESS"
850 LPRINT SPACE$(10); "Total stages:  "; NTOST%
860 LPRINT SPACE$(10); "Volume % TBP in solvent:  "; : LPRINT USING P$;
    CTBP * 100!
870 LPRINT SPACE$(10); "Initial or default temperature ("; CHR$(248); "C):
    ";
880 LPRINT USING P$; TEMPI
890 IF NSTR% = 0 THEN LPRINT SPACE$(10); "No unusual stage connections"
```

```
900 IF NSTR% = 1 THEN LPRINT SPACE$(10); "Organic taken from stage ";
    ISTR%; " feeds stage "; JSTR%; "."
910 IF IPROCE% = 1 THEN 970
920 ON (IRXN% + 1) GOTO 930, 940, 950, 960
930 LPRINT SPACE$(10); "No Plutonium reaction.": GOTO 970
940 LPRINT SPACE$(10); "Instantaneous reduction of Pu(IV).": GOTO 970
950 LPRINT SPACE$(10); "Reduction of Pu(IV) by U(IV).": GOTO 970
960 LPRINT SPACE$(10); "Reduction of Pu(IV) by hydroxylamine nitrate."
970 LPRINT SPACE$(10); "Minutes per time increment:  "; : LPRINT USING Q$;
    DTHETA

980 LPRINT SPACE$(10); "Minutes between printing of the concentration
    profile:  "; : LPRINT USING "####"; DPRINT%
990 LPRINT SPACE$(10); "Calculations will stop after ";
1000 LPRINT USING "####"; TSTOP%;
1010 LPRINT " minutes or when a tolerance of ";
1020 LPRINT USING PPP$; TOL;
1030 LPRINT " % per minute is reached."
1040 ON IVOLM% GOTO 1050, 1060, 1070
1050 LPRINT SPACE$(10); "Mixer volumes are defined for each phase.": GOTO
     1080
1060 LPRINT SPACE$(10); "Total mixer volumes are defined (phase ratios =
     flow ratios).": GOTO 1080
1070 LPRINT SPACE$(10); "Mixer volumes = (phase flow)(unit time)."
1080 ON IVOLS% GOTO 1090, 1100, 1110
1090 LPRINT SPACE$(10); "Settler volumes are defined for each phase.": GOTO
     1120
1100 LPRINT SPACE$(10); "Total settler volumes are defined (phase ratios =
     flow ratios).": GOTO 1120
1110 LPRINT SPACE$(10); "Settler volumes = (phase flow)(unit time)."
1120 ON (IPRO% + 1) GOTO 1130, 1140, 1150
1130 LPRINT SPACE$(10); "Initial concentration profile is zero.": GOTO 1160
1140 LPRINT SPACE$(10); "Initial concentration profile is defined.": GOTO
     1160
1150 LPRINT SPACE$(10); "Initial concentration profile is from a previous
     problem."
1160 ON (IFAST% + 1) GOTO 1170, 1180, 1190
1170 LPRINT SPACE$(10); "Runge-Kutta integration will be used.": GOTO 1200
1180 LPRINT SPACE$(10); "Trapezoidal integration will be used.": GOTO 1200
1190 LPRINT SPACE$(10); "Fast integration will be used."
1200 IF NEWOUT% = 0 THEN LPRINT SPACE$(10); "No extra product streams."
1210 IF NEWOUT% = 1 THEN LPRINT SPACE$(10); "Extra product stream(s)."
1220 LPRINT : LPRINT SPACE$(10); "The FILESPEC for this Problem Definition
     data file is:  "; DATFIL1$
1230 LPRINT SPACE$(10); "The FILESPEC for this Problem Results data file
     is:  "; DATFIL2$
1240 LOCATE 6, 1: PRINT "Problem is defined.";
1250 REM The STARTS routine - General input functions, sets system
     hydraulics.
```

```
3080 IF IPRO% = 0 THEN 4240
3090 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 3110
3100 LPRINT CHR$(12); : LN% = 0
3110 LPRINT "INITIAL AQUEOUS PROFILE DATA:": LN% = LN% + 1
3120 IF IPROCE% = 0 THEN 3140  'CONVPU2 routine
```

```
3130 IF IPROCE% = 1 THEN 3430  'CONVTH2 routine
```

```
3700 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 3720
3710 LPRINT CHR$(12); : LN% = 0
3720 LPRINT "INITIAL ORGANIC PROFILE DATA:": LN% = LN% + 1
3730 IF IPROCE% = 0 THEN 3750  'CONVPU3 routine
3740 IF IPROCE% = 1 THEN 4000  'CONVTH3 routine
```

```
4240 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 4260
4250 LPRINT CHR$(12); : LN% = 0
4260 LPRINT "STAGE VOLUME AND FLOW RATE DATA (Molal basis):": LN% = LN% + 1
4270 GOSUB 7230  'To set up volume and flow rate chart
4280 IF IVOLM% = 3 THEN 4380
4290 PX% = 0
4300 INPUT #1, NST%, VOLA, VOLO, INDEX%
4310 NS% = NST%: VLA = VOLA: VLO = VOLO: IDEX% = INDEX%
4320 AVOL(NS%) = VLA: OVOL(NS%) = VLO
4330 IF PX% = 1 THEN 4360
4340 IF IDEX% <> 1 THEN 4370
4350 INPUT #1, NST%, VOLA, VOLO, INDEX%
4360 IF NST% = NS% + 1 THEN PX% = 0: GOTO 4310 ELSE NS% = NS% + 1: PX% = 1:
     GOTO 4320
4370 IF NS% <> NTOST% THEN NS% = NS% + 1: GOTO 4320
4380 IF IVOLS% = 3 THEN 4480
4390 PX% = 0
4400 INPUT #1, NST%, VOLA, VOLO, INDEX%
4410 NS% = NST%: VLA = VOLA: VLO = VOLO: IDEX% = INDEX%
4420 ASVOL(NS%) = VLA: OSVOL(NS%) = VLO
4430 IF PX% = 1 THEN 4460
4440 IF IDEX% <> 1 THEN 4470
4450 INPUT #1, NST%, VOLA, VOLO, INDEX%
4460 IF NST% = NS% + 1 THEN PX% = 0: GOTO 4410 ELSE NS% = NS% + 1: PX% = 1:
     GOTO 4420
4470 IF NS% <> NTOST% THEN NS% = NS% + 1: GOTO 4420
4480 FOR I% = 1 TO NTOST%
4490  ON IVOLM% GOTO 4540, 4500, 4530
4500  OVOL(I%) = AVOL(I%) * OT(I%) / (AT(I%) + OT(I%))
4510  AVOL(I%) = AVOL(I%) - OVOL(I%)
4520  GOTO 4540
4530  AVOL(I%) = AT(I%): OVOL(I%) = OT(I%)
4540  ON IVOLS% GOTO 4590, 4550, 4580
4550  OSVOL(I%) = ASVOL(I%) * OT(I%) / (AT(I%) + OT(I%))
4560  ASVOL(I%) = ASVOL(I%) - OSVOL(I%)
4570  GOTO 4590
4580  ASVOL(I%) = AT(I%): OSVOL(I%) = OT(I%)
4590  IF AVOL(I%) < .0001 THEN AVOL(I%) = 0!
4600  IF OVOL(I%) < .0001 THEN OVOL(I%) = 0!
4610  IF ASVOL(I%) < .0001 THEN ASVOL(I%) = 0!
4620  IF OSVOL(I%) < .0001 THEN OSVOL(I%) = 0!
4630 NEXT I%
4640 LOCATE 10, 1: PRINT "Stage volumes and flows are defined.";
4650 FOR I% = 1 TO NTOST%
4660  IF LN% >= 55 THEN LPRINT CHR$(12); : LN% = 0: GOSUB 7230
4670  LPRINT SPACE$(5); : LPRINT USING "### "; I%;
```

```
4680  LPRINT USING PQ$; AVOL(I%); OVOL(I%); ASVOL(I%); OSVOL(I%); AT(I%);
      OT(I%); ANET(I%); ONET(I%)
4690  LN% = LN% + 1
4700 NEXT I%
4710 IF IPRO% = 0 OR EQCKDG% = 1 THEN 5060
4720 FOR I% = 1 TO NTOST%
4730  AV = AVOL(I%) + ASVOL(I%): OV = OVOL(I%) + OSVOL(I%)
4740  FOR J% = 1 TO 3
4750   FOR K% = 1 TO 6
4760    ARY(K%) = X(K%, I%, 2)
4770   NEXT K%
4780   ICK% = 0: TEMPC = TPROF(I%, 2)
4790   IF IPROCE% <> 0 THEN 4820
4800   CALL UCORPU  'The UCORPU Subprogram is called here.
4810   GOTO 4830
4820   CALL UCORTH  'The UCORTH Subprogram is called here.
4830   FOR K% = 1 TO 3
4840    X(K%, I%, 1) = (OV * Y(K%, I%, 2) + AV * X(K%, I%, 2)) / (AV + OV *
        DTRY(K%))
4850    Y(K%, I%, 1) = Y(K%, I%, 2) + (X(K%, I%, 2) - X(K%, I%, 1)) * AV /
        OV
4860    IF ABS(X(K%, I%, 1) - X(K%, I%, 2)) > (.01 * X(K%, I%, 1)) THEN
        ICK% = 1
4870    X(K%, I%, 2) = X(K%, I%, 1): Y(K%, I%, 2) = Y(K%, I%, 1)
4880   NEXT K%
4890   FOR K% = 4 TO V%
4900    X(K%, I%, 1) = X(K%, I%, 2)
4910   NEXT K%
4920   IF ICK% = 0 THEN 4940
4930  NEXT J%
4940  FOR J% = 1 TO 3
4950   FOR K% = 1 TO 2
4960    ATS(I%, J%, K%) = TPROF(I%, 1): OTS(I%, J%, K%) = TPROF(I%, 1)
4970    FOR L% = 1 TO V%
4980     XS(I%, J%, L%, K%) = X(L%, I%, 1)
4990    NEXT L%
5000    FOR L% = 1 TO 3
5010     YS(I%, J%, L%, K%) = Y(L%, I%, 1)
5020    NEXT L%
5030   NEXT K%
5040  NEXT J%
5050 NEXT I%
5060 LPRINT CHR$(12); : TIM2$ = TIME$: DAT2$ = DATE$
5070 LPRINT "PROBLEM RESULTS FOR SEPHIS MOD4, Ver. 2.11:"; SPACE$(71);
     DAT2$; " "; LEFT$(TIM2$, 5)
5080 LPRINT : LPRINT "     Problem:  "; TITLE$: LPRINT "     (mixer
     concentrations shown)": LPRINT
5090 TOTIME = 0!: PRTIME% = 0: LN% = 5: TOME% = 0
5100 FOR I% = 1 TO NTOST%
5110  FOR J% = 1 TO 4
5120   SOIN(J%) = SOIN(J%) + AFDRT(I%) * XFD(J%, I%)
5130  NEXT J%
5140 NEXT I%
5150 FOR I% = 1 TO NTOST%
5160  FOR J% = 1 TO 3
```

```
5170   SOIN(J%) = SOIN(J%) + OFDRT(I%) * YFD(J%, I%)
5180  NEXT J%
5190 NEXT I%
5200 IF IPROCE% = 0 THEN SOIN(3) = SOIN(3) + SOIN(4)
5210 ON (IFAST% + 1) GOTO 5220, 5230, 5240
5220 LOCATE 11, 1: PRINT "Using Runge-Kutta integration."; : GOTO 5250
5230 LOCATE 11, 1: PRINT "Using trapezoidal integration."; : GOTO 5250
5240 LOCATE 11, 1: PRINT "Using `fast' integration.";
5250 IF IPROCE% = 1 THEN 5301
5260 ON (IRXN% + 1) GOTO 5270, 5280, 5290, 5300
5270 LOCATE 12, 1: PRINT "No plutonium reaction."; : GOTO 5301
5280 LOCATE 12, 1: PRINT "Pu(IV) reduced instantaneously."; : GOTO 5301
5290 LOCATE 12, 1: PRINT "Pu(IV) reduced by U(IV)."; : GOTO 5301
5300 LOCATE 12, 1: PRINT "Pu(IV) reduced by hydroxylamine nitrate.";
5301 LOCATE 13, 1: PRINT "Print time =        min.";
5302 LOCATE 14, 1: PRINT "Maximum time =      min.";
5303 LOCATE 13, 16: PRINT USING "####"; PRTIME%;
5304 LOCATE 14, 16: PRINT USING "####"; TSTOP%;
5305 LOCATE 10, 58: PRINT USING PPP$; TOL;
5310 NSTOP% = 1: NBORT% = 1: NPRNT% = 1: NMAXT% = 1: NSTG% = 0: GOTO 6210
5320 LOCATE 6, 57: PRINT USING "####.##"; TOTIME + DTHETA;
5330 CALL STAGES(NDIREC%)  'The STAGES Subprogram is called here.
5340 NDIREC% = -NDIREC%: NSTOP% = 0: NSTG% = NSTG% + 1: TOTIME = DTHETA *
     NSTG%
5350 NBORT% = 1: NPRNT% = 1: NMAXT% = 1: TOME% = FIX(TOTIME): COMAX = 0!
5360 FOR I% = 1 TO NTOST%
5365  FOR J% = 1 TO V%
5370   IF CODUMM(J%, I%) > COMAX THEN COMAX = CODUMM(J%, I%): ICO% = J%:
       IST% = I%
5375  NEXT J%
5380 NEXT I%
5390 IF COMAX > 100! THEN COMAX = 100!
5395 LOCATE 9, 76: PRINT USING "###"; IST%;
5397 LOCATE 10, 77: PRINT USING "##"; ICO%;
5400 LOCATE 9, 58: PRINT USING PPP$; COMAX;
5420 FOR I% = 1 TO NTOST%
5540  IF I% = 1 THEN OOOUT(1) = OT(1): AAOUT(1) = ALVRT(1): GOTO 5570
5550  IF I% = NTOST% THEN AAOUT(NTOST%) = AT(NTOST%): OOOUT(NTOST%) =
      OLVRT(NTOST%): GOTO 5570
5560  AAOUT(I%) = ALVRT(I%): OOOUT(I%) = OLVRT(I%)
5570 NEXT I%
5580 FOR I% = 1 TO 4
5590  SOT(I%) = 0!
5600 NEXT I%
5610 FOR I% = 1 TO 4
5620  FOR J% = 1 TO NTOST%
5630   SOT(I%) = SOT(I%) + AAOUT(J%) * XS(J%, 3, I%, 2)
5640  NEXT J%
5650 NEXT I%
5660 FOR I% = 1 TO 3
5670  FOR J% = 1 TO NTOST%
5680   SOT(I%) = SOT(I%) + OOOUT(J%) * YS(J%, 3, I%, 2)
5690  NEXT J%
5700 NEXT I%
5710 IF IPROCE% = 0 THEN SOT(3) = SOT(3) + SOT(4)
```

```
5720 FOR I% = 1 TO 3
5730  R1% = 15 + 2 * I%
5740  IF SOIN(I%) < .000001 THEN MB(I%) = 0!: GOTO 5930
5750  LOCATE R1%, 2: PRINT SPACE$(78);
5760  MB(I%) = 100! * SOT(I%) / SOIN(I%)
5770  LOCATE 12 + I%, 69: PRINT USING PP$; MB(I%);
5780  IF MB(I%) < 90! THEN 5930
5790  IF MB(I%) > 100! THEN MMB% = 79: GOTO 5870
5800  IF MB(I%) > 99! THEN 5860
5810  MMB% = CINT(3! • CINT(MB(I%) - 90!) + 2!)
5820  FOR J% = 2 TO MMB%
5830   LOCATE R1%, J%: PRINT CHR$(176);
5840  NEXT J%
5850  GOTO 5930
5860  MMB% = CINT(5! * (10! * MB(I%) - 990!) + 29!)
5870  FOR J% = 2 TO 29
5880   LOCATE R1%, J%: PRINT CHR$(176);
5890  NEXT J%
5900  FOR J% = 30 TO MMB%
5910   LOCATE R1%, J%: PRINT CHR$(178);
5920  NEXT J%
5930 NEXT I%
5940 ON ERROR GOTO 8140
5950 IF TOME% = 0 THEN 6000
5960 IF ABS(TOME% - TOTIME) > .001 THEN 6000
5970 LSET F1$ = MKI$(TOME%): LSET F2$ = MKS$(MB(1))
5980 LSET F3$ = MKS$(MB(2)): LSET F4$ = MKS$(MB(3))
5990 PUT #3, TOME%
6000 FOR I% = 1 TO NTOST%
6010  IF CODUM(I%) > TOL THEN NSTOP% = 1
6020  TPROF(I%, 1) = TPROF(I%, 2)
6030  FOR J% = 1 TO 3
6040   ATS(I%, J%, 1) = ATS(I%, J%, 2): OTS(I%, J%, 1) = OTS(I%, J%, 2)
6050  NEXT J%
6060  FOR J% = 1 TO 3
6070   X(J%, I%, 1) = X(J%, I%, 2): Y(J%, I%, 1) = Y(J%, I%, 2)
6080   FOR K% = 1 TO 3
6090    XS(I%, K%, J%, 1) = XS(I%, K%, J%, 2): YS(I%, K%, J%, 1) = YS(I%,
        K%, J%, 2)
6100   NEXT K%
6110  NEXT J%
6120  FOR J% = 4 TO V%
6130   X(J%, I%, 1) = X(J%, I%, 2)
6140   FOR K% = 1 TO 3
6150    XS(I%, K%, J%, 1) = XS(I%, K%, J%, 2)
6160   NEXT K%
6170  NEXT J%
6180 NEXT I%
6190 IF NSTOP% = 0 THEN 6250
6200 K$ = INKEY$: IF LEN(K$) <> 0 THEN NBORT% = 0: GOTO 6250
6210 IF TOTIME >= TSTOP% THEN NMAXT% = 0: GOTO 6250
6220 IF ABS(TOTIME - PRTIME%) > .001 THEN 5320
6230 NPRNT% = 0
6240 PRTIME% = PRTIME% + DPRINT%
6245 LOCATE 13, 16: PRINT USING "####"; PRTIME%;
```

```
6250 LPRINT "TIME = "; : LPRINT USING Q$; TOTIME; : LPRINT " MINUTES":
     LPRINT
6260 LN% = LN% + 2
6270 IF IPROCE% <> 0 THEN 6300
6280 CALL PRTPU  'The PRTPU Subprogram is called here.
6290 GOTO 6310
6300 CALL PRTTH  'The PRTTH Subprogram is called here.
6310 IF NSTOP% = 0 THEN 6440
6320 IF NBORT% = 0 THEN 6690
6330 IF NPRNT% = 0 THEN 6350
6340 IF NMAXT% = 0 THEN 6730
6350 FOR I% = 1 TO NTOST%
6360  FOR J% = 1 TO 3
6370   X(J%, I%, 2) = X(J%, I%, 1): Y(J%, I%, 2) = Y(J%, I%, 1)
6380  NEXT J%
6390  FOR J% = 4 TO V%
6400   X(J%, I%, 2) = X(J%, I%, 1)
6410  NEXT J%
6420 NEXT I%
6430 GOTO 5320
6440 ON ERROR GOTO 8140
6450 WRITE #2, TITLE$
6460 WRITE #2, DAT2$, LEFT$(TIM2$, 5), TOTIME
6470 TIM3$ = TIME$
6480 REM TIM2$ was when calculations began, TIM3$ is when calculations
     stopped.
6490 E$ = ""
6500 FOR I% = 1 TO NTOST%
6510  IF IPROCE% <> 0 THEN 6540
6520  WRITE #2, I%, X(1, I%, 2), X(2, I%, 2), X(3, I%, 2), Y(1, I%, 2),
      Y(2, I%, 2), Y(3, I%, 2), X(4, I%, 2), X(5, I%, 2), X(6, I%, 2),
      ADEN(I%), AOUT(I%), TPROF(I%, 2), EXT2(I%), EXT3(I%), EXT1(I%),
      ODEN(I%), OOUT(I%), TSAT(I%), CODUM(I%)
6530  GOTO 6550
6540  WRITE #2, I%, X(1, I%, 2), X(2, I%, 2), X(3, I%, 2), Y(1, I%, 2),
      Y(2, I%, 2), Y(3, I%, 2), X(4, I%, 2), E$, E$, E$, AOUT(I%),
      TPROF(I%, 2), EXT2(I%), EXT3(I%), EXT1(I%), E$, OOUT(I%), TSAT(I%),
      CODUM(I%)
6550 NEXT I%
6560 WRITE #2, TIM2$, TIM3$
6570 IF LN% < 50 THEN LPRINT : GOTO 6590
6580 LPRINT CHR$(12);
6590 IF IPROCE% <> 0 THEN 6620
6600 LPRINT "Valid ranges:": LPRINT "     0.0 to 5.0 M H+": LPRINT "
     0.0 to 200 gU/L": LPRINT "     0.0 to 100 gPu/L": LPRINT "     10 to
     30% TBP": LPRINT "     10 to 40"; CHR$(248); "C"
6610 GOTO 6630
6620 LPRINT "Valid ranges:": LPRINT "     0.0 to 3.0 M H+": LPRINT "
     0.0 to 20.0 gU/L": LPRINT "     0.0 to 150 gTh/L": LPRINT "     30%
     TBP": LPRINT "     15 to 70"; CHR$(248); "C"
6630 LPRINT : LPRINT "Run Time is from "; TIM2$; " to "; TIM3$
6640 LPRINT CHR$(12); : IF NBORT% = 0 OR NMAXT% = 0 THEN 6840
6650 LOCATE 3, 1: PRINT SPACE$(35); : LOCATE 4, 1: PRINT SPACE$(35);
6660 COLOR 0, 7: LOCATE 3, 1: PRINT "Steady-state condition is met ---"; :
     LOCATE 4, 1: PRINT "    Press any key to continue    "; : COLOR 7, 0
```

```
6670 K$ = INKEY$: IF K$ = "" THEN 6670
6680 GOTO 6840
6690 LOCATE 3, 1: PRINT SPACE$(35); : LOCATE 4, 1: PRINT SPACE$(35);
6700 COLOR 0, 7: LOCATE 3, 1: PRINT "Calculations stopped ----"; : LOCATE
     4, 1: PRINT "Press any key to continue"; : COLOR 7, 0
6710 K$ = INKEY$: IF K$ = "" THEN 6710
6720 GOTO 6760
6730 LOCATE 3, 1: PRINT SPACE$(35); : LOCATE 4, 1: PRINT SPACE$(35);
6740 COLOR 0, 7: LOCATE 3, 1: PRINT "Maximum time reached ----"; : LOCATE
     4, 1: PRINT "Press any key to continue"; : COLOR 7, 0
6750 K$ = INKEY$: IF K$ = "" THEN 6750
6760 LOCATE 3, 1: PRINT SPACE$(35); : LOCATE 4, 1: PRINT SPACE$(35);
6770 COLOR 0, 7: LOCATE 3, 1: INPUT ; "Do you want to continue for more
     time (Y/N)? ", REPLY$: COLOR 7, 0
6780 IF REPLY$ <> "Y" THEN 6440
6790 IF NMAXT% = 0 THEN TSTOP% = 2 * TSTOP%
6795 LOCATE 14, 16: PRINT USING "####"; TSTOP%;
6800 LOCATE 3, 1: PRINT SPACE$(50);
6810 COLOR 0, 7: LOCATE 3, 1: PRINT "   CALCULATING --- PLEASE WAIT   ";
6820 LOCATE 4, 1: PRINT "      Press any key to quit      "; : COLOR 7, 0
6830 GOTO 6350
6840 FOR I% = 1 TO TOME%
6850  GET #3, I%
6860  TME% = CVI(F1$)
6870  IF TME% <= (TOTIME - 1000!) THEN 6900
6880  MB(1) = CVS(F2$): MB(2) = CVS(F3$): MB(3) = CVS(F4$)
6890  WRITE #2, TME%, MB(1), MB(2), MB(3)
6900 NEXT I%
6910 LPRINT CHR$(18); : CLOSE #1: CLOSE #2: CLOSE #3: CLS
6920 KILL DATFIL3$
6930 RUN "sephis"
6940 END
6950 REM Subroutine to draw a double box.
6960  FOR I% = R1% + 1 TO R2% - 1
6970   LOCATE I%, C1%: PRINT CHR$(186);
6980   LOCATE I%, C2%: PRINT CHR$(186);
6990  NEXT I%
7000  FOR J% = C1% + 1 TO C2% - 1
7010   LOCATE R1%, J%: PRINT CHR$(205);
7020   LOCATE R2%, J%: PRINT CHR$(205);
7030  NEXT J%
7040  LOCATE R1%, C1%: PRINT CHR$(201);
7050  LOCATE R1%, C2%: PRINT CHR$(187);
7060  LOCATE R2%, C1%: PRINT CHR$(200);
7070  LOCATE R2%, C2%: PRINT CHR$(188);
7080 RETURN
7090 REM Subroutine to draw a single box.
7100  FOR I% = R1% + 1 TO R2% - 1
7110   LOCATE I%, C1%: PRINT CHR$(179);
7120   LOCATE I%, C2%: PRINT CHR$(179);
7130  NEXT I%
7140  FOR J% = C1% + 1 TO C2% - 1
7150   LOCATE R1%, J%: PRINT CHR$(196);
7160   LOCATE R2%, J%: PRINT CHR$(196);
7170  NEXT J%
```

```
7180  LOCATE R1%, C1%: PRINT CHR$(218);
7190  LOCATE R1%, C2%: PRINT CHR$(191);
7200  LOCATE R2%, C1%: PRINT CHR$(192);
7210  LOCATE R2%, C2%: PRINT CHR$(217);
7220 RETURN
7230 REM Subroutine to set up volume and flow rate chart.
7240  LPRINT SPACE$(15); "MIXER VOLUME BY PHASE"; SPACE$(6); "SETTLER
      VOLUME BY PHASE";
7250  LPRINT SPACE$(9); "MIXER FLOW RATE"; SPACE$(10); "INTERSTAGE FLOW
      RATE"
7260  LPRINT SPACE$(5); "STAGE   -------------------------   --------------
      -----------   -------------------------   -------------------------"
7270  LPRINT SPACE$(6); "NO.      AQUEOUS       ORGANIC       AQUEOUS       AQUEOUS
      ORGANIC       AQUEOUS       ORGANIC       AQUEOUS       ORGANIC"
7280  LPRINT SPACE$(5); "-----   -----------   -----------   -----------   -----------
      -----------   -----------   -----------   -----------   -----------"
7290  LN% = LN% + 4
7300 RETURN
7310 REM Subroutine to set up chart for Purex feed & product stream data.
7320  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM       PU (IV)
      PU (III)      REDUCTANT    NITRATE ION    FLOW RATE     TEMP"
7330  LPRINT SPACE$(17); "NO.       (M)          (g/L)         (g/L)
      (g/L)          (M)          (M)          (L/min)       (C)"
7340  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------   -----------   -----------   -----------   ------"
7350  LN% = LN% + 3
7360 RETURN
7370 REM Subroutine to set up chart for Thorex feed & product stream data.
7380  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM       THORIUM
      NITRATE ION                               FLOW RATE     TEMP"
7390  LPRINT SPACE$(17); "NO.       (M)          (g/L)         (g/L)
      (M)                                      (L/min)       (C)"
7400  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------                               -----------   ------"
7410  LN% = LN% + 3
7420 RETURN
7430 REM Subroutine to set up Purex aqueous profile chart.
7440  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM       PU (IV)
      PU(III)       REDUCTANT    NITRATE ION                  TEMP"
7450  LPRINT SPACE$(17); "NO.       (M)          (g/L)         (g/L)
      (g/L)          (M)          (M)                        (C)"
7460  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------   -----------   -----------                 ------"
7470  LN% = LN% + 3
7480 RETURN
7490 REM Subroutine to set up Thorex aqueous profile chart.
7500  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM       THORIUM
      NITRATE ION                                              TEMP"
7510  LPRINT SPACE$(17); "NO.       (M)          (g/L)         (g/L)
      (M)                                                     (C)"
7520  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------                                             ------"
7530  LN% = LN% + 3
7540 RETURN
7550 REM Subroutine to set up Purex organic profile chart.
```

```
7560  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        PU (IV)"
7570  LPRINT SPACE$(17); "NO.       (M)          (g/L)          (g/L)"
7580  LPRINT SPACE$(16); "-----  -----------   -----------   -----------"
7590  LN% = LN% + 3
7600 RETURN
7610 REM Subroutine to set up Thorex organic profile chart.
7620  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        THORIUM"
7630  LPRINT SPACE$(17); "NO.       (M)          (g/L)          (g/L)"
7640  LPRINT SPACE$(16); "-----  -----------   -----------   -----------"
7650  LN% = LN% + 3
7660 RETURN
7670 REM Subroutine to set up status screen.
7680  CLS : LOCATE 1, 1: PRINT "SEPHIS MOD4 Ver. 2.11";
7690  COLOR 0, 7: LOCATE 1, 30: PRINT "*** STATUS SCREEN ***";
7700  LOCATE 3, 1: PRINT "   CALCULATING --- PLEASE WAIT   ";
7710  LOCATE 4, 1: PRINT "Press any key to quit prematurely"; : COLOR 7, 0
7720  LOCATE 3, 59: PRINT "TIME   STAGE";
7730  LOCATE 4, 58: PRINT "(min.)   NO.";
7740  LOCATE 5, 58: PRINT "------  -----";
7750  LOCATE 8, 50: PRINT "INVENTORY CHANGE (%/min.):";
7751  LOCATE 9, 52: PRINT "Max.:";
7752  LOCATE 9, 68: PRINT ">Stage:";
7753  LOCATE 10, 52: PRINT "Tol.:";
7754  LOCATE 10, 68: PRINT ">Comp.:";
7760  LOCATE 12, 50: PRINT "OVERALL MATERIAL BALANCE (%):";
7770  LOCATE 13, 54: PRINT "Nitric Acid:";
7780  LOCATE 14, 54: PRINT "Uranium:";
7790  IF IPROCE% = 0 THEN LOCATE 15, 54: PRINT "Plutonium:";
7800  IF IPROCE% = 1 THEN LOCATE 15, 54: PRINT "Thorium:";
7801  FOR I% = 57 TO 71
7802   LOCATE 2, I%: PRINT CHR$(196);
7803  NEXT I%
7804  FOR I% = 50 TO 78
7805   LOCATE 7, I%: PRINT CHR$(196);
7806   LOCATE 11, I%: PRINT CHR$(196);
7807   LOCATE 16, I%: PRINT CHR$(196);
7808  NEXT I%
7809  FOR I% = 3 TO 6
7810   LOCATE I%, 56: PRINT CHR$(179);
7811   LOCATE I%, 72: PRINT CHR$(179);
7812  NEXT I%
7813  FOR I% = 8 TO 15
7814   LOCATE I%, 49: PRINT CHR$(179);
7815   LOCATE I%, 79: PRINT CHR$(179);
7816  NEXT I%
7817  LOCATE 2, 56: PRINT CHR$(218);
7818  LOCATE 2, 72: PRINT CHR$(191);
7819  LOCATE 7, 49: PRINT CHR$(218);
7820  LOCATE 7, 56: PRINT CHR$(193);
7821  LOCATE 7, 72: PRINT CHR$(193);
7822  LOCATE 7, 79: PRINT CHR$(191);
7823  LOCATE 11, 49: PRINT CHR$(195);
7824  LOCATE 11, 79: PRINT CHR$(180);
7825  LOCATE 16, 49: PRINT CHR$(192);
7826  LOCATE 16, 79: PRINT CHR$(217);
```

```
7827  FOR I% = 3 TO 78
7828   LOCATE 22, I%: PRINT CHR$(196);
7830  NEXT I%
7840  FOR I% = 2 TO 29 STEP 3
7850   LOCATE 22, I%: PRINT CHR$(197);
7860  NEXT I%
7870  FOR I% = 34 TO 79 STEP 5
7880   LOCATE 22, I%: PRINT CHR$(197);
7890  NEXT I%
7900  LOCATE 23, 1: PRINT "90 91 92 93 94 95 96 97 98 99";
7910  LOCATE 23, 32: PRINT "99.1 99.2 99.3 99.4 99.5 99.6 99.7 99.8 99.9
      100";
7920  LOCATE 24, 27: PRINT "Overall Material Balance (%)";
7930  LOCATE 18, 1: PRINT "URANIUM:";
7940  IF IPROCE% = 0 THEN LOCATE 20, 1: PRINT "PLUTONIUM:";
7950  IF IPROCE% = 1 THEN LOCATE 20, 1: PRINT "THORIUM:";
7960  LOCATE 16, 1: PRINT "NITRIC ACID:";
7970 RETURN
7980 REM Error trapping routine.
7990  IF ERR = 64 THEN LOCATE 25, 1: PRINT "Bad file name"; : GOTO 8030
8000  IF ERR = 71 THEN LOCATE 25, 1: PRINT "Disk not ready"; : GOTO 8030
8010  IF ERR = 53 THEN LOCATE 25, 1: PRINT "File not found"; : GOTO 8030
8020  ON ERROR GOTO 0
8030  PRINT " - Press any key to continue";
8040  K$ = INKEY$: IF K$ = "" THEN 8040
8050  LOCATE 25, 1: PRINT SPACE$(79);
8060  RESUME 330
8070 REM Error trapping routine.
8080  IF ERR = 24 THEN LOCATE 25, 1: PRINT "Your printer is not ready"; :
      GOTO 8100
8090  ON ERROR GOTO 0
8100  PRINT " - Check it and press any key";
8110  K$ = INKEY$: IF K$ = "" THEN 8110
8120  LOCATE 25, 1: PRINT SPACE$(79);
8130  RESUME
8140 REM Error trapping routine.
8150  IF ERR = 61 THEN LOCATE 25, 1: PRINT "Disk full"; : GOTO 8170
8160  ON ERROR GOTO 0
8170  PRINT " - You will have to re-run this problem - Press any
8180  K$ = INKEY$: IF K$ = "" THEN 8180
8190  LOCATE 25, 1: PRINT SPACE$(79);
8200  RESUME 6910
```

C.3 STARTS Routine

Statements	Description
1250-1540	The STARTS routine contains general inpu the system hydraulics. The indicator EQCK at 0 denoting that the phases at the initia be equilibrated. The index TCONC% is set at - molar concentrations will be passed to conversi

Statements	Description
	provide the appropriate solute-free units. Feed stream flow rates and concentrations are read from the Problem Definition file. The flow rate of any extra product stream (in addition to the normal product streams from the ends of the cascade) are also read. The statement "Feed and product streams are identified." is placed on the screen.
1550-1800	The initial concentration and temperature profiles are read from the Problem Definition file, if supplied. The statement "Initial concentration profile is established." is placed on the screen. If the profile was from a previous problem result, the index EQCKDG% is set to 1 denoting that the phases are in equilibrium.
1810-1820	The CONVPU1 or the CONVTH1 routine is called to convert feed stream molar units to solute-free units. These routines also send feed stream data to the printer. Control then transfers to statement 2700.
2700-2920	Data for any extra product streams are sent to the printer. Note that actual product stream flow rates will be computed considering solute content and temperature. The flow rate data supplied from the Problem Definition file need only be approximate. The approximate values are printed here.
2930-3070	Flow rates are established for the cascade and the statement "Cascade flows are established." is placed on the screen. The flows are adjusted such that a hydraulic balance is achieved (i.e., no more fluid can leave a stage than enters). ANET and ONET values are the phase flow rates between stages; AT and OT values are the maximum phase flow rates within a stage.

C.4 Listing of the STARTS Routine

```
1250 REM The STARTS routine - General input functions, sets s
     hydraulics.
1260 LPRINT : LPRINT "FEED AND PRODUCT STREAM DATA:"
1270 LN% = 23
1280 EQCKDG% = 0: TCONC% = -1
1290 INPUT #1, NST%, JHAS%, FDRT
1300 IF JHAS% = 0 THEN V% = 3 ELSE IF IPROCE% = 0 "
1310 FOR I% = 1 TO V%
1320  INPUT #1, CON(I%)
1330 NEXT I%
1340 INPUT #1, TEMP, INDEX%
1350 IF JHAS% = 1 THEN 1420
1360 OFDRT(NST%) = FDRT
1370 IF ABS(TEMP) > .001 THEN OFDTEM(NST%) = TEMP
1380 FOR I% = 1 TO 3
```

```
1390  YFD(I%, NST%) = CON(I%)
1400 NEXT I%
1410 GOTO 1480
1420 AFDRT(NST%) = FDRT
1430 IF ABS(TEMP) > .001 THEN AFDTEM(NST%) = TEMP
1440 FOR I% = 1 TO V%
1450  XFD(I%, NST%) = CON(I%)
1460 NEXT I%
1470 IF CON(5) > .000001 THEN ISOL5% = 1
1480 IF INDEX% = 1 THEN 1290
1490 IF NEWOUT% = 0 THEN 1540
1500 INPUT #1, NST%, JHAS%, OTRT, INDEX%
1510 IF JHAS% = 1 THEN ALVRT(NST%) = OTRT
1520 IF JHAS% = 0 THEN OLVRT(NST%) = OTRT
1530 IF INDEX% = 1 THEN 1500
1540 LOCATE 7, 1: PRINT "Feed and product streams are identified.";
1550 IF IPROCE% = 0 THEN V% = 6 ELSE V% = 4
1560 IF IPRO% = 0 THEN 1800
1570 IF IPRO% = 2 THEN EQCKDG% = 1
1580 FOR I% = 1 TO NTOST%
1590  FOR J% = 1 TO V%
1600   INPUT #1, X(J%, I%, 2)
1610  NEXT J%
1620  INPUT #1, TPROF(I%, 2)
1630  IF ABS(TPROF(I%, 2)) < .001 THEN TPROF(I%, 2) = TEMP
1640  TPROF(I%, 1) = TPROF(I%, 2)
1650  FOR J% = 1 TO 6
1660   RXNTRM(J%, I%) = 0!
1670  NEXT J%
1680  IF X(5, I%, 2) > .000001 THEN ISOL5% = 1
1690  FOR J% = 1 TO 3
1700   FOR K% = 1 TO 2
1710    ATS(I%, J%, K%) = TPROF(I%, 1): OTS(I%, J%, K%) = TPROF(I%, 1)
1720   NEXT K%
1730  NEXT J%
1740 NEXT I%
1750 FOR I% = 1 TO NTOST%
1760  FOR J% = 1 TO 3
1770   INPUT #1, Y(J%, I%, 2)
1780  NEXT J%
1790 NEXT I%
1800 LOCATE 8, 1: PRINT "Initial concentration profile is established.";
1810 IF IPROCE% = 0 THEN 1830  'CONVPU1 routine
1820 IF IPROCE% = 1 THEN 2270  'CONVTH1 routine
```

```
2700 IF NEWOUT% = 0 THEN 2930
2710 FOR I% = 1 TO NTOST%
2720  IF ABS(ALVRT(I%)) < .000001 THEN 2820
2730  LPRINT SPACE$(8); "AQUEOUS ";
2740  LPRINT USING "###"; I%;
2750  LPRINT "      Product stream removed (actual flow rate to be
      computed)";
2760  LPRINT SPACE$(22); : LPRINT USING PQ$; ALVRT(I%)
2770  LN% = LN% + 1
2780  IF LN% < 55 THEN 2820
```

```
2790  LPRINT CHR$(12); : LN% = 0
2800  IF IPROCE% = 0 THEN GOSUB 7310  'To set up Purex feed and product
      chart
2810  IF IPROCE% = 1 THEN GOSUB 7370  'To set up Thorex feed and product
      chart
2820  IF ABS(OLVRT(I%)) < .000001 THEN 2920
2830  LPRINT SPACE$(8); "ORGANIC";
2840  LPRINT USING "###"; I%;
2850  LPRINT "      Product stream removed (actual flow rate to be
      computed);"
2860  LPRINT SPACE$(22); : LPRINT USING PQ$; OLVRT(I%)
2870  LN% = LN% + 1
2880  IF LN% < 55 THEN 2920
2890  LPRINT CHR$(12); : LN% = 0
2900  IF IPROCE% = 0 THEN GOSUB 7310  'To set up Purex feed and product
      chart
2910  IF IPROCE% = 1 THEN GOSUB 7370  'To set up Thorex feed and product
      chart
2920 NEXT I%
2930 IF ALVRT(1) > AFDRT(1) THEN ALVRT(1) = AFDRT(1)
2940 ANET(1) = AFDRT(1) - ALVRT(1): AT(1) = AFDRT(1)
2950 IF OLVRT(NTOST%) > OFDRT(NTOST%) THEN OLVRT(NTOST%) = OFDRT(NTOST%)
2960 ONET(NTOST%) = OFDRT(NTOST%) - OLVRT(NTOST%): OT(NTOST%) =
     OFDRT(NTOST%)
2970 FOR I% = 2 TO NTOST%
2980  IF ALVRT(I%) >= (ANET(I% - 1) + AFDRT(I%)) THEN ALVRT(I%) = ANET(I% -
      1) + AFDRT(I%)
2990  ANET(I%) = ANET(I% - 1) + AFDRT(I%) - ALVRT(I%): AT(I%) = ANET(I%) +
      ALVRT(I%)
3000  NST% = NTOST% + 1 - I%
3010  IF OLVRT(NST%) >= (ONET(NST% + 1) + OFDRT(NST%)) THEN OLVRT(NST%) =
      ONET(NST% + 1) + OFDRT(NST%)
3020  ONET(NST%) = ONET(NST% + 1) + OFDRT(NST%) - OLVRT(NST%)
3030  IF NSTR% = 1 AND NST% = (ISTR% - 1) THEN ONET(NST%) = OFDRT(NST%) -
      OLVRT(NST%)
3040  IF NSTR% = 1 AND NST% = JSTR% THEN ONET(NST%) = ONET(ISTR%) +
      OFDRT(NST%) - OLVRT(NST%) + ONET(NST% + 1)
3050  OT(NST%) = ONET(NST%) + OLVRT(NST%)
3060 NEXT I%
3070 LOCATE 9, 1: PRINT "Cascade flows are established.";
```

C.5 Unit Conversion Routines (CONVPU1, CONVPU2, CONVPU3, CONVTH1, CONVTH2, and CONVTH3)

Statements	Description
CONVPU1:	
1830-2260	Feed stream flow, temperature, and concentration data are sent to the printer. Concentrations are then converted to molarity and the MOLALP Subprogram is called to obtain the conversion factors CONVA and CONVO that are used to convert concentrations to solute-free units.

Statements	Description
CONVTH1:	
2270-2690	Feed stream flow, temperature, and concentration data are sent to the printer. Concentrations are then converted to molarity and the MOLALT Subprogram is called to obtain the conversion factors CONVA and CONVO that are used to convert concentrations to solute-free units.
CONVPU2:	
3140-3420	Initial aqueous concentration profile data (and stage temperatures) are sent to the printer. Concentrations are then converted to molarity and the MOLALP Subprogram is called to obtain the conversion factors CONVA that are used to convert concentrations to solute-free units.
CONVTH2:	
3430-3690	Initial aqueous concentration profile data (and stage temperatures) are sent to the printer. Concentrations are then converted to molarity and the MOLALT Subprogram is called to obtain the conversion factors CONVA that are used to convert concentrations to solute-free units.
CONVPU3:	
3750-3990	Initial organic concentration profile data are sent to the printer. Concentrations are then converted to molarity and the MOLALP Subprogram is called to obtain the conversion factors CONVO that are used to convert concentrations to solute-free units.
CONVTH3:	
4000-4230	Initial organic concentration profile data are sent to the printer. Concentrations are then converted to molarity and the MOLALT Subprogram is called to obtain the conversion factors CONVO that are used to convert concentrations to solute-free units.

Note: For details of the MOLALP and MOLALT Subprograms, see Sect. D.5.

C.6 Listing of Unit Conversion Factor Routines (CONVPU1, CONVPU2, CONVPU3, CONVTH1, CONVTH2, and CONVTH3)

```
1830 REM CONVPU1 routine - Converts feed stream data (molar/molal).
1840 GOSUB 7310  'To set up Purex feed and product chart
1850 FOR I% = 1 TO NTOST%
1860  IF ABS(AFDRT(I%) + OFDRT(I%)) < .000001 THEN 2250
1870  IF ABS(AFDRT(I%)) < .000001 THEN 1970
1880  LPRINT SPACE$(8); "AQUEOUS ";
1890  LPRINT USING "###"; I%;
1900  FOR J% = 1 TO 6
1910   LPRINT USING PQ$; XFD(J%, I%);
1920  NEXT J%
```

```
1930  LPRINT USING PQ$; AFDRT(I%);
1940  LPRINT USING R$; AFDTEM(I%)
1950  LN% = LN% + 1: TEMP = AFDTEM(I%)
1960  IF LN% >= 55 THEN LPRINT CHR$(12); : LN% = 0: GOSUB 7310
1970  IF ABS(OFDRT(I%)) < .000001 THEN 2080
1980  LPRINT SPACE$(4); : LPRINT USING P$; CTBP * 100!; : LPRINT " % TBP ";
1990  LPRINT USING "###"; I%;
2000  FOR J% = 1 TO 3
2010   LPRINT USING PQ$; YFD(J%, I%);
2020  NEXT J%
2030  LPRINT SPACE$(42);
2040  LPRINT USING PQ$; OFDRT(I%);
2050  LPRINT USING R$; OFDTEM(I%)
2060  LN% = LN% + 1: TEMP = OFDTEM(I%)
2070  IF LN% >= 55 THEN LPRINT CHR$(12); : LN% = 0: GOSUB 7310
2080  XFD(2, I%) = XFD(2, I%) / 238!: YFD(2, I%) = YFD(2, I%) / 238!
2090  XFD(3, I%) = XFD(3, I%) / 239!: YFD(3, I%) = YFD(3, I%) / 239!
2100  XFD(4, I%) = XFD(4, I%) / 239!
2110  FOR J% = 1 TO 6
2120   AQ(J%) = XFD(J%, I%)
2130  NEXT J%
2140  FOR J% = 1 TO 3
2150   ORG(J%) = YFD(J%, I%)
2160  NEXT J%
2170  CALL MOLALP  'The MOLALP Subprogram is called here.
2180  AFDRT(I%) = AFDRT(I%) / CONVA: OFDRT(I%) = OFDRT(I%) / CONVO
2190  FOR J% = 1 TO 3
2200   YFD(J%, I%) = YFD(J%, I%) * CONVO
2210  NEXT J%
2220  FOR J% = 1 TO V%
2230   XFD(J%, I%) = XFD(J%, I%) * CONVA
2240  NEXT J%
2250 NEXT I%
2260 GOTO 2700
```

```
2270 REM CONVTH1 routine - Converts feed stream data (molar/molal).
2280 GOSUB 7370  'To set up Thorex feed and product chart
2290 FOR I% = 1 TO NTOST%
2300  IF ABS(AFDRT(I%) + OFDRT(I%)) < .000001 THEN 2690
2310  IF ABS(AFDRT(I%)) < .000001 THEN 2420
2320  LPRINT SPACE$(8); "AQUEOUS ";
2330  LPRINT USING "###"; I%;
2340  FOR J% = 1 TO 4
2350   LPRINT USING PQ$; XFD(J%, I%);
2360  NEXT J%
2370  LPRINT SPACE$(28);
2380  LPRINT USING PQ$; AFDRT(I%);
2390  LPRINT USING R$; AFDTEM(I%)
2400  LN% = LN% + 1: TEMP = AFDTEM(I%)
2410  IF LN% >= 55 THEN LPRINT CHR$(12); : LN% = 0: GOSUB 7370
2420  IF ABS(OFDRT(I%)) < .000001 THEN 2530
2430  LPRINT SPACE$(4); : LPRINT USING P$; CTBP * 100!; : LPRINT " % TBP ";
2440  LPRINT USING "###"; I%;
2450  FOR J% = 1 TO 3
2460   LPRINT USING PQ$; YFD(J%, I%);
```

```
2470  NEXT J%
2480  LPRINT SPACE$(42);
2490  LPRINT USING PQ$; OFDRT(I%);
2500  LPRINT USING R$; OFDTEM(I%)
2510  LN% = LN% + 1: TEMP = OFDTEM(I%)
2520  IF LN% >= 55 THEN LPRINT CHR$(12); : LN% = 0: GOSUB 7370
2530  XFD(2, I%) = XFD(2, I%) / 238!: YFD(2, I%) = YFD(2, I%) / 238!
2540  XFD(3, I%) = XFD(3, I%) / 232!: YFD(3, I%) = YFD(3, I%) / 232!
2550  FOR J% = 1 TO 4
2560   AQ(J%) = XFD(J%, I%)
2570  NEXT J%
2580  FOR J% = 1 TO 3
2590   ORG(J%) = YFD(J%, I%)
2600  NEXT J%
2610  CALL MOLALT  'The MOLALT Subprogram is called here.
2620  AFDRT(I%) = AFDRT(I%) / CONVA: OFDRT(I%) = OFDRT(I%) / CONVO
2630  FOR J% = 1 TO 3
2640   YFD(J%, I%) = YFD(J%, I%) * CONVO
2650  NEXT J%
2660  FOR J% = 1 TO V%
2670   XFD(J%, I%) = XFD(J%, I%) * CONVA
2680  NEXT J%
2690 NEXT I%
```

```
3140 REM CONVPU2 routine - Converts aqueous initial profile (molar/molal).
3150 GOSUB 7430  'To set up Purex aqueous profile chart
3160 FOR I% = 1 TO NTOST%
3170  IF LN% >= 55 THEN LPRINT CHR$(12); : LN% = 0: GOSUB 7430
3180  LPRINT SPACE$(16); : LPRINT USING "###"; I%;
3190  FOR J% = 1 TO 6
3200   LPRINT USING PQ$; X(J%, I%, 2);
3210  NEXT J%
3220  LPRINT SPACE$(14); : LPRINT USING R$; TPROF(I%, 2)
3230  LN% = LN% + 1
3240  X(2, I%, 2) = X(2, I%, 2) / 238!
3250  X(3, I%, 2) = X(3, I%, 2) / 239!
3260  X(4, I%, 2) = X(4, I%, 2) / 239!
3270  FOR J% = 1 TO V%
3280   AQ(J%) = X(J%, I%, 2)
3290  NEXT J%
3300  TEMP = TPROF(I%, 2)
3310  CALL MOLALP  'The MOLALP Subprogram is called here.
3320  FOR J% = 1 TO V%
3330   AQ(J%) = AQ(J%) * CONVA
3340   FOR K% = 1 TO 2
3350    X(J%, I%, K%) = AQ(J%)
3360    FOR L% = 1 TO 3
3370     XS(I%, L%, J%, K%) = AQ(J%)
3380    NEXT L%
3390   NEXT K%
3400  NEXT J%
3410 NEXT I%
3420 GOTO 3700
```

```
3430 REM CONVTH2 routine - Converts aqueous initial profile (molar/molal).
```

```
3440 GOSUB 7490  'To set up Thorex aqueous profile chart
3450 FOR I% = 1 TO NTOST%
3460  IF LN% >= 55 THEN LPRINT CHR$(12); : LN% = 0: GOSUB 7490
3470  LPRINT SPACE$(16); : LPRINT USING "###"; I%;
3480  FOR J% = 1 TO 4
3490   LPRINT USING PQ$; X(J%, I%, 2);
3500  NEXT J%
3510  LPRINT SPACE$(42); : LPRINT USING R$; TPROF(I%, 2)
3520  LN% = LN% + 1
3530  X(2, I%, 2) = X(2, I%, 2) / 238!
3540  X(3, I%, 2) = X(3, I%, 2) / 232!
3550  FOR J% = 1 TO V%
3560   AQ(J%) = X(J%, I%, 2)
3570  NEXT J%
3580  TEMP = TPROF(I%, 2)
3590  CALL MOLALT  'The MOLALT Subprogram is called here.
3600  FOR J% = 1 TO V%
3610   AQ(J%) = AQ(J%) * CONVA
3620   FOR K% = 1 TO 2
3630    X(J%, I%, K%) = AQ(J%)
3640    FOR L% = 1 TO 3
3650     XS(I%, L%, J%, K%) = AQ(J%)
3660    NEXT L%
3670   NEXT K%
3680  NEXT J%
3690 NEXT I%
```

```
3750 REM CONVPU3 routine - Converts organic initial profile (molar/molal).
3760 GOSUB 7550  'To set up Purex organic profile chart
3770 FOR I% = 1 TO NTOST%
3780  IF LN% >= 55 THEN LPRINT CHR$(12); : LN% = 0: GOSUB 7550
3790  LPRINT SPACE$(16); : LPRINT USING "###"; I%;
3800  LPRINT USING PQ$; Y(1, I%, 2); Y(2, I%, 2); Y(3, I%, 2)
3810  LN% = LN% + 1
3820  Y(2, I%, 2) = Y(2, I%, 2) / 238!
3830  Y(3, I%, 2) = Y(3, I%, 2) / 239!
3840  FOR J% = 1 TO 3
3850   ORG(J%) = Y(J%, I%, 2)
3860  NEXT J%
3870  TEMP = TPROF(I%, 2)
3880  CALL MOLALP  'The MOLALP Subprogram is called here.
3890  FOR J% = 1 TO 3
3900   ORG(J%) = ORG(J%) * CONVO
3910   FOR K% = 1 TO 2
3920    Y(J%, I%, K%) = ORG(J%)
3930    FOR L% = 1 TO 3
3940     YS(I%, L%, J%, K%) = ORG(J%)
3950    NEXT L%
3960   NEXT K%
3970  NEXT J%
3980 NEXT I%
3990 GOTO 4240
```

```
4000 REM CONVTH3 routine - Converts organic initial profile (molar/molal).
4010 GOSUB 7610  'To set up Thorex organic profile chart
```

```
4020 FOR I% = 1 TO NTOST%
4030  IF LN% >= 55 THEN LPRINT CHR$(12); : LN% = 0: GOSUB 7610
4040  LPRINT SPACE$(16); : LPRINT USING "###"; I%;
4050  LPRINT USING PQ$; Y(1, I%, 2); Y(2, I%, 2); Y(3, I%, 2)
4060  LN% = LN% + 1
4070  Y(2, I%, 2) = Y(2, I%, 2) / 238!
4080  Y(3, I%, 2) = Y(3, I%, 2) / 232!
4090  FOR J% = 1 TO 3
4100   ORG(J%) = Y(J%, I%, 2)
4110  NEXT J%
4120  TEMP = TPROF(I%, 2)
4130  CALL MOLALT  'The MOLALT Subprogram is called here.
4140  FOR J% = 1 TO 3
4150   ORG(J%) = ORG(J%) * CONVO
4160   FOR K% = 1 TO 2
4170    Y(J%, I%, K%) = ORG(J%)
4180    FOR L% = 1 TO 3
4190     YS(I%, L%, J%, K%) = ORG(J%)
4200    NEXT L%
4210   NEXT K%
4220  NEXT J%
4230 NEXT I%
```

APPENDIX D
SECAL1.BAS—THE SECONDARY MODULE

The Secondary Module of the calculational program (SECAL1.BAS) includes 9 Subprograms (UCORPU, UCORTH, STAGES, PRTPU, PRTTH, MOLALP, MOLALT, MCHEMP, and SCHEMP). The main program is described in Sect. D.1 and listed in Sect. D.2. The various Subprograms are described and listed as follows:

Subprogram(s)	Description Section	Listing Section
UCOR	D.3	D.4
STAGES	D.5	D.6
PRT	D.7	D.8
MOLAL	D.9	D.10
MCHEMP, SCHEMP	D.11	D.12

D.1 Main Program (SECAL1)

Statements	Description
10- 70	Data statements are provided here that contain the correlating coefficients used in calculating distribution coefficients for the Thorex process. The data are read by statements in the UCORTH Subprogram (Sect. D.3).

D.2 Listing of Program SECAL1 (The Secondary Module)

```
DECLARE SUB MOLALP ()
DECLARE SUB MOLALT ()
DECLARE SUB UCORPU ()
DECLARE SUB UCORTH ()
DECLARE SUB MCHEMP (J%, AQVOL!, ORVOL!)
DECLARE SUB SCHEMP (J%, AQSVOL!, ORSVOL!)
```

```
10 REM PROGRAM SECAL1 -- Solvent Extraction Process Having Interacting
   Solutes -- Problem Calculations -- SECONDARY MODULE
20 REM This module contains Subprograms MOLALP, STAGES, UCORPU, MCHEMP,
   SCHEMP, PRTPU, MOLALT, PRTTH, and UCORTH.
30 REM $DYNAMIC
40 REM $INCLUDE: 'A:SECOM.BI'
```

```
50 DATA 5.16764, 12.7385, -6.10939, 0.825665, 0.895314, -0.258242,
   0.0628435, 0.00145494, 0.480975, -0.222463, 0.0320684, -0.000857849
60 DATA 4.98513, 13.7875, -7.02178, 0.883583, 1.52821, -0.527579,
   0.0324897, 0.00416738, 0.538601, -0.207956, 0.0304384, -0.00118149
70 DATA 2.55963, -7.66961, 2.03295, 1.58978, 1.31060, -0.475194, 0.0370571,
   0.00577316, 0.398105, -0.158715, 0.0312364, -0.00164366
```

D.3 UCOR Subprograms (UCORPU and UCORTH)

Statements	Description

UCORPU:

3120-3230 This Subprogram provides distribution coefficients for the Purex process. Refer to Sect. 2.3.1 for a description of the distribution coefficient correlation. The total nitrate concentration (TNM) is calculated from aqueous phase concentrations passed to the Subprogram.

$$TNM = HAM + 2\ UAM + 2\ PUAM + SNITR + 2\ PUIII \qquad (D.1)$$

where HAM = nitric acid concentration,
UAM = uranium concentration,
PUAM = plutonium (IV) concentration,
PUIII = plutonium (III) concentration, and
SNITR = non-extractable nitrate salt concentration.

This relationship, although not rigorously correct according to generally recognized chemical reaction mechanisms, permits a better correlation of experimental distribution data.

3240 The term DRT is calculated as:

$$DRT = 1000 / T - 3.3539 \qquad (D.2)$$

where T = absolute temperature, °K.

This value of DRT will be used when adjusting the distribution coefficient to a temperature other than 25°C.

3250-3280 Empirical equilibrium constants are calculated for U, Pu, and HNO_3 as:

$$UK = \left[3.7\ TNM^{1.57} + 1.4\ TNM^{3.9} + 0.11\ TNM^{7.3}\right] \left[4\ CTBP^{-0.17} - 3\right] (1.13) \qquad (D.3)$$

$$PUK = \left[0.135 + 0.122113\ (CTBP / 0.3)^{0.746} - 3.91\ CTBP + 0.01\ TNM^{2}\right] (UK) \qquad (D.4)$$

$$HK1 = 0.135\ TNM^{0.82} + 0.0052\ TNM^{3.44} \qquad (D.5)$$

Statements	Description
	where CTBP = volume fraction of TBP in the solvent, UK = empirical uranium equilibrium constant, PUK = empirical plutonium equilibrium constant, and HK1 = empirical nitric acid equilibrium constant. For CTBP < 1, the term HK1 is multiplied by the factor $\left[1 - 0.54\ e^{-15\ CTBP}\right]$. These relationships have evolved from fitting experimental distribution data reported by many sources.
3290-3330	The equilibrium constants are further adjusted for temperatures other than 25°C as follows: $UK_T = UK\ e^{2.5\ DRT}$ (D.6) $PUK_T = PUK\ e^{-0.8\ DRT}$ (D.7) $HK1_T = HK1\ e^{0.34\ DRT}$ (D.8) $HK2 = HK1$ (D.9)
3340-3380	The distribution coefficients are a function of the free (uncomplexed) TBP that is calculated from equilibrium constants and aqueous phase concentrations. The solution to a quadratic equation is required; this is done using the following expressions to obtain the free TBP (TF): $A = 2\left[(UK)\ (UAM) + (PUK)\ (PUAM) + (HK2)\ (HAM)\right]$ (D.10) $B = (HK1)(HAM) + 1$ (D.11) $TF = T / B$ (if $A < 10^{-6}$) (D.12) $TF = \left[-B + (B^2 + 4\ A\ T)^{0.5}\right] / (2\ A)$ (if $A \geq 10^{-6}$) (D.13) where T = molar concentration of TBP in the solvent.
3390-3400	Finally, the distribution coefficients (DTRY) are calculated. For nitric acid: $DTRY = (HK1)\ (TF) + (HK2)\ (TF)^2$ (D.14) For uranium: $DTRY = (UK)\ (TF)^2$ (D.15) For plutonium: $DTRY = (PUK)\ (TF)^2$ (D.16)
<u>UCORTH</u>:	
6780-6910	This Subprogram provides distribution coefficients for the Thorex process. Refer to Sect. 2.3.2 for a description of the distribution coefficient correlation. Correlating coefficients (C) based on experimental data are read from data statements

Statements	Description
	for use in equations of the type:
	$K = C_1 + C_2\ U + C_3\ U^2 + C_4\ U^3$ (D.17)
6920-6930	The total ionic strength of the aqueous phase (U) is calculated from aqueous phase concentrations passed to the Subprogram.
	U = 3 ARY(2) + 10 ARY(3) + ARY(1) (D.18)
	where ARY(1) = nitric acid concentration, ARY(2) = uranium concentration, and ARY(3) = thorium concentration.
	The total nitrate concentration (NO3) is also calculated.
	NO3 = 2 ARY(2) + 4 ARY(3) + ARY(1) (D.19)
6940-6970	Empirical equilibrium constants for U, Th, and HNO_3 are calculated using equations of the type shown above [Eq. D.17].
	$KU = C_1 + C_2\ U + C_3\ U^2 + C_4\ U^3$ (D.20)
	$KTH = C_5 + C_6\ U + C_7\ U^2 + C_8\ U^3$ (D.21)
	$KH = C_9 + C_{10}\ U + C_{11}\ U^2 + C_{12}\ U^3$ (D.22)
	where KU = empirical uranium equilibrium constant, KTH = empirical thorium equilibrium constant, and KH = empirical nitric acid equilibrium constant.
	This is done three times, once for each of the three solutes, as somewhat different values of C are used to minimize errors for each solute.
6980-7130	The distribution coefficients are a function of the free (uncomplexed) TBP that is calculated from equilibrium constants and aqueous phase concentrations. The solution to a cubic equation of the form:
	$a\ x^3 + b\ x^2 + c\ x + d = 0$ (D.23)
	is required where x is the free TBP content. Here,
	$a = (3\ KTH)\ [ARY(3)]\ (NO3)^4$ (D.24)
	$b = (2\ KU)\ [ARY(2)]\ (NO3)^2$ (D.25)
	$c = 1 + (KH)\ [ARY(1)]\ (NO3)$ (D.26)
	$d = -T$ (D.27)
	where T is the molar concentration of TBP in the solvent. The

Statements	Description
	term YY is set equal to the smaller of T or T/C, but not less than 0. A finite difference method is used in statements 7010-7090 to solve the equation. The free TBP content (TBP) is then equal to the value of YY.
7140-7160	The distribution coefficients (DTRY) are calculated.
	For nitric acid: $DTRY = (KH)\ (NO3)\ (TBP)$ (D.28)
	For uranium: $DTRY = (KU)\ (NO3)^2\ (TBP)^2$ (D.29)
	For thorium: $DTRY = (KTH)\ (NO3)^4\ (TBP)^3$ (D.30)
7170-7230	Finally, the DTRY values are adjusted for temperatures other than 25°C using the term XTEMP.
	$XTEMP = 1000 / T - 3.3539$ (D.31)
	where T = absolute temperature, °K.
	For nitric acid: $DTRY_T = DTRY\ e^{-0.818802\ XTEMP}$ (D.32)
	For uranium: $DTRY_T = DTRY\ e^{2.5\ XTEMP}$ (D.33)
	For thorium: $DTRY_T = DTRY\ e^{(C)(XTEMP)}$ (D.34)
	where
	$C = 0.891664 + 0.879688\ ARY(3) - 1.47438\ [ARY(3)]^2$ (D.35)

D.4 Listing of UCOR Subprograms (UCORPU and UCORTH)

```
3120 SUB UCORPU  'Provides Purex distribution coefficients.
3130 SHARED NTOST%, CTBP, NEWOUT%, SPH, IFAST%, IRXN%, DTHETA, IVOLM%,
     IVOLS%, IPRO%, TEMPI, ISOL5%, NSTR%, ISTR%, JSTR%, IPROCE%, LN%, V%,
     PQ$, QQ$, R$, RR$, T, CODUM(), CODUMM()
3140 SHARED TEMPC, ARY(), DTRY()
3150 HAM = ARY(1): UAM = ARY(2): PUAM = ARY(3)
3160 PUIII = ARY(4): SNITR = ARY(6)
3170 IF UAM < 0! THEN UAM = 0!
3180 IF PUAM < 0! THEN PUAM = 0!
3190 IF HAM < 0! THEN HAM = 0!
3200 IF SNITR < 0! THEN SNITR = 0!
3210 IF PUIII < 0! THEN PUIII = 0!
3220 TNM = HAM + 2! * UAM + 2! * PUAM + SNITR + 2! * PUIII
3230 IF TNM < 1E-10 THEN TNM = 1E-10
3240 DRT = 1000! / (TEMPC + 273.16) - 3.3539
3250 UK = (3.7 * TNM ^ 1.57 + 1.4 * TNM ^ 3.9 + .011 * TNM ^ 7.3) * (4! *
     CTBP ^ (-.17) - 3!) * 1.13
```

```
3260 PUK = UK * (.135 + .122113 * (CTBP / .3) ^ (.746 - 3.91 * CTBP) + .01
     * TNM ^ 2!)
3270 HK1 = .135 * TNM ^ .82 + .0052 * TNM ^ 3.44
3280 IF CTBP < 1! THEN HK1 = HK1 * (1! - .54 * EXP(-15! * CTBP))
3290 IF TEMPC = 25! THEN 3330
3300 UK = UK * EXP(2.5 * DRT)
3310 PUK = PUK * EXP(-.8 * DRT)
3320 HK1 = HK1 * EXP(.34 * DRT)
3330 HK2 = HK1
3340 A = 2! * (UK * UAM + PUK * PUAM + HK2 * HAM): B = HK1 * HAM + 1!
3350 IF A >= .000001 THEN 3380
3360 TF = T / B
3370 GOTO 3390
3380 TF = (-B + SQR(B ^ 2! + 4! * A * T)) / (2! * A)
3390 DTRY(1) = HK1 * TF + HK2 * TF ^ 2!: DTRY(2) = UK * TF ^ 2!: DTRY(3) =
     PUK * TF ^ 2!
3400 END SUB
```

```
6780 SUB UCORTH  'Provides Thorex distribution coefficients.
6790 SHARED NTOST%, CTBP, NEWOUT%, SPH, IFAST%, IRXN%, DTHETA, IVOLM%,
     IVOLS%, IPRO%, TEMPI, ISOL5%, NSTR%, ISTR%, JSTR%, IPROCE%, LN%, V%,
     PQ$, QQ$, R$, RR$, T, CODUM(), CODUMM()
6800 SHARED TEMPC, ARY(), DTRY()
6810 DIM COEF(12, 3), KU(3), KH(3), KTH(3), AZA(4), TBP(3)
6820 FOR I% = 1 TO 12
6830  READ COEF(I%, 1)
6840 NEXT I%
6850 FOR I% = 1 TO 12
6860  READ COEF(I%, 2)
6870 NEXT I%
6880 FOR I% = 1 TO 12
6890  READ COEF(I%, 3)
6900 NEXT I%
6910 RESTORE
6920 U = 3! * ARY(2) + 10! * ARY(3) + ARY(1)
6930 NO3 = 2! * ARY(2) + 4! * ARY(3) + ARY(1)
6940 FOR I% = 1 TO 3
6950  KU(I%) = COEF(1, I%) + COEF(2, I%) * U + COEF(3, I%) * U ^ 2! +
      COEF(4, I%) * U ^ 3!
6960  KTH(I%) = COEF(5, I%) + COEF(6, I%) * U + COEF(7, I%) * U ^ 2! +
      COEF(8, I%) * U ^ 3!
6970  KH(I%) = COEF(9, I%) + COEF(10, I%) * U + COEF(11, I%) * U ^ 2! +
      COEF(12, I%) * U ^ 3!
6980  AZA(1) = -T: AZA(2) = 1! + KH(I%) * ARY(1) * NO3
6990  AZA(3) = 2! * KU(I%) * ARY(2) * NO3 ^ 2!: AZA(4) = 3! * KTH(I%) *
      ARY(3) * NO3 ^ 4!
7000  IF -AZA(1) < (-AZA(1) / AZA(2)) THEN YY = -AZA(1) ELSE YY = -AZA(1) /
      AZA(2)
7010  IF YY < 0 THEN YY = -AZA(1)
7020  FOR J% = 1 TO 20
7030   D = AZA(4): C = AZA(4)
7040   FOR II% = 1 TO 2
7050    K% = 4 - II%: D = AZA(K%) + YY * D: C = D + YY * C
7060   NEXT II%
7070   D = AZA(1) + YY * D: DELTY = D / C
```

```
7080   IF ABS(DELTY) < .00001 AND ABS(D) < .00001 THEN 7110
7090   YY = YY - DELTY
7100  NEXT J%
7110  TBP(I%) = YY
7120  IF TBP(I%) < 0! THEN TBP(I%) = 0!
7130 NEXT I%
7140 DTRY(1) = KH(3) * NO3 * TBP(3)
7150 DTRY(2) = KU(1) * NO3 ^ 2! * TBP(1) ^ 2!
7160 DTRY(3) = KTH(2) * NO3 ^ 4! * TBP(2) ^ 3!
7170 IF TEMPC = 25! THEN 7230
7180 IF TEMPC < 15! OR TEMPC > 70! THEN 7230
7190 XTEMP = 1000! / (273.16 + TEMPC) - 3.3539
7200 DTRY(1) = DTRY(1) * EXP(-.818802 * XTEMP)
7210 DTRY(2) = DTRY(2) * EXP(2.5 * XTEMP)
7220 DTRY(3) = DTRY(3) * EXP((.891664 + .879688 * ARY(3) - 1.47438 * ARY(3)
     ^ 2!) * XTEMP)
7230 END SUB
```

D.5 STAGES Subprogram

Statements	Description
200- 320	The STAGES Subprogram is entered with concentrations at the beginning of the time increment, designated as condition 1, and returns concentrations for the end of the time increment, designated as condition 2. The Subprogram is also entered with a value of NDIREC% of +1 or -1 denoting if stage calculations will proceed in the direction of aqueous flow or organic flow respectively. Integrations for the mixers will be performed using one of three available numerical methods as specified from the Problem Definition file (Runge-Kutta, Trapezoidal, or Fast). In this initial set of statements the tolerance of fit for an iterative search of distribution coefficients (CCD) is set at 0.001, and an index denoting the number of times that the cascade is calculated for each integration (MSCAN%) is initially set at 0. The index TCONC% is set at +1 denoting that solute-free units will be passed to conversion routines.
330- 690	As each stage in the cascade is calculated, the stage number is placed on the screen. For the present time increment and stage being considered, the inventory change of a solute (CODUM) and the change in solute entering a stage from an upstream settler in the aqueous or organic stream (DELTAX and DELTAY) are initiated at 0. The total solute entering the stage with either phase (AIN and OIN) is calculated from values of flow rates and concentrations of feed streams and/or upstream settlers present at the beginning of the time increment. The change in total solute entering a stage from an upstream settler during the time increment (DELTAX and DELTAY) is calculated from upstream settler concentrations and interstage flow rates. If the Fast integration technique was specified, AIN and OIN values are incremented by an additional 50% of the

Statements	Description
	change in solute content of an upstream settler during the time increment. These calculations are all further amended to account for any special routing of the organic phase in statements 490-550. A lower limit on AIN and OIN values is provided in statements 560-570. The variables TX, ARY, AQ, and ORG are set at mixer concentrations from the previous time increment (or initial condition) in statement 580 for use in later calculations. All of the above as pertains to non-extractable components in the aqueous phase is carried out in statements 600-690.
700- 760	The stage temperature (TEMP) is set at that from the previous time increment (or initial condition). The conversion factor Subprogram is called to obtain mixer and settler phase volumes in molar units at this temperature for use in heat balance calculations. The variables AQ and ORG are used within the conversion factor Subprogram.
770- 860	A simple heat balance is made considering the flow rates and temperatures of all streams affecting the stage being considered. For upstream settlers, the assumed temperature is incremented by 50% of the temperature change within that settler during the time increment. From this heat balance, a new stage temperature is calculated in statement 850. The variable TEMPC is set to this new temperature for use in later calculations.
870- 890	The index IMCHEM% is set at 0 denoting that no chemical reactions have yet been considered. Control transfers to statement 2300 if the Trapezoidal integration technique is to be used for the mixers, statement 1980 if the Fast technique is specified, or statement 900 for the Runge-Kutta method. The mixers are modeled assuming perfect mixing of the phases and equilibrium mass-transfer conditions.
900-1970	<u>Runge-Kutta integration technique for mixers</u>. A fourth-order classical Runge-Kutta numerical integration technique is employed in this section.
900- 950	The counter (MCK%) for the number of trials is set to 0 and the appropriate UCOR Subprogram is called to obtain distribution coefficients based on concentrations existing from the previous time increment. The variables ARY and TEMPC, calculated above, are used within the UCOR Subprogram.
960-1160	A variable F is calculated for each solute by material balance around the mixer that represents the change in solute content in the mixer for a unit of time, the first derivative. New values of ARY are calculated as the average of the initial and final solute contents for the time increment. This procedure assumes that flow rates, volumes, and feed streams are constant

Statements	Description
	and that mixer concentrations vary by only a small amount over the time increment. The counter MCK% is incremented, the appropriate UCOR Subprogram is recalled using the new values of ARY, and the index MDEX% is set to 0. This index will represent a good fit of trial to result (MDEX% = 0) or not (MDEX% = 1). The differences between the original mixer solute contents (TX) and the new values (ARY) are calculated as fractional changes and compared to the tolerance CCD. If any of these changes exceed the tolerance, MDEX% is set to 1 and TX is set equal to ARY. For up to 5 trials, if a good fit is not attained, control returns to statement 960 to repeat the above procedure; otherwise program flow continues to statement 1170 where a similar procedure is followed.
1170-1190	The mixer concentrations for the end of the time increment are set equal to ARY and the variable PHI, which accumulates values of F, is set equal to F.
1200-1400	The variable F (derivative) is now recalculated using the latest values of distribution coefficients and mixer concentrations, ARY values are again calculated as averages of solute contents, the counter MCK% is incremented, the UCOR Subprogram is called, and the fractional changes in mixer concentrations are compared to the tolerance CCD. For up to another 5 trials (total of 10), if a good fit is not attained, control returns to statement 1200; otherwise program flow continues to statement 1410.
1410-1430	Mixer concentrations for the end of the time increment are set equal to ARY and PHI is incremented by twice the value of F.
1440-1640	The variable F (derivative) is again recalculated using the latest values of distribution coefficients and mixer concentrations. Values of ARY are calculated based on the change in solute represented by F (not as an average, as before). The counter MCK% is incremented, the UCOR Subprogram is called, and the fractional changes in mixer concentrations are again compared to the tolerance CCD. For up to another 5 trials (total of 15), if a good fit is not attained, control returns to statement 1440; otherwise program flow continues to statement 1650.
1650-1670	Mixer concentrations for the end of the time increment are set equal to ARY and PHI is incremented by twice the value of F.
1680-1880	The variable F (derivative) is again recalculated using the latest values of distribution coefficients and mixer concentrations. Values of ARY are calculated based on (F+PHI)/6 as an increment. The counter MCK% is incremented, the UCOR Subprogram is called, and the fractional changes in mixer concentrations are again compared to the tolerance CCD. For up to another 5 trials (total of 20), if a good fit is not

Statements	Description
	attained, control returns to statement 1680; otherwise program flow continues to statement 1890.

Note that in the above procedure, a bias may result from the fact that the solute concentrations in one upstream settler result from a calculation in the present time increment while those from the other upstream settler exist from the previous time increment. This situation occurs as a result of calculations being made one stage at a time in a single direction. The bias should be minimized by sweeping the cascade in the opposite direction in the next time increment. Note also that the UCOR Subprogram is called two times for each of the first five calculations.

1890-1970 A lower limit is set on the ARY values and mixer concentrations are defined for the end of the time increment. This integration procedure ends as control transfers to statement 2580.

1980-2290 Fast integration technique for mixers. A newly developed numerical integration technique is employed in this section. Although called the Fast technique, in practice it generally consumes more computer time than the Trapezoidal technique for the same size time increment for integrations. It will, in most cases, perform with large time increments (10 min.) without failure and thereby attain steady-state results very quickly. It is less accurate than the Runge-Kutta method for following transient conditions but will provide equivalent values for steady-state results. It is the only recommended technique for transient results where plutonium reduction is occurring.

1980-2040 The counter (MCK%) for the number of trials and the index (MDEX%) that denotes a good fit of trial to result are set to 0. The appropriate UCOR Subprogram is called to obtain distribution coefficients based on concentrations existing from the previous time increment or previous trial. The variables ARY and TEMPC, calculated above, are used within the UCOR Subprogram in the first trial.

2050-2240 An exponential factor, or weighting coefficient (WGHT), is calculated in statement 2060 for use in statement 2070 where new values of ARY are calculated. The differences between aqueous-phase concentrations at the end of the time increment (will be the previous time increment if this is the first trial) and the new values of ARY are calculated as fractional changes and compared to the tolerance CCD. The aqueous-phase concentrations at the end of the time increment are set equal to ARY. The counter MCK% is incremented. For up to 15 trials, if a good fit is not attained, control returns to statement 2000 to repeat the above procedure; otherwise program flow continues to statement 2250.

2250-2290 Control transfers to statement 2630 if chemical reactions have

Statements	Description
	already been considered or are not to be considered (IMCHEM% = 1, IRXN% = 0, or IPROCE% = 1). Otherwise the index IMCHEM% is set to 1 and a test is made for the presence of a chemical reductant. If no reductant is present (ISOL5% = 0), control transfers to statement 1980 and the foregoing procedure is repeated. If reductant is present, the chemical reaction Subprogram for mixers (MCHEMP) is called and control transfers to statement 1980 to repeat the foregoing procedure using aqueous-phase concentrations following chemical reaction. For details of the MCHEMP Subprogram, see Sect. D.11. This integration procedure ends as control transfers to statement 2630 as noted above.
Note that the UCOR Subprogram is only called once for each trial calculation if chemical reactions are not considered. As will be seen in a later discussion below, the Fast integration technique calculations will sweep the cascade in both directions in each time increment.	
2300-2570	Trapezoidal integration technique for mixers. A classical trapezoidal or finite difference numerical integration technique is employed in this section. It is less accurate than the Runge-Kutta method for following transient conditions but will provide equivalent steady-state results.
2300-2360	The counter (MCK%) for the number of trials and the index (MDEX%) that denotes a good fit of trial to result are set to 0. The appropriate UCOR Subprogram is called to obtain distribution coefficients based on concentrations existing from the previous time increment or previous trial. The variables ARY and TEMPC, calculated above, are used within the UCOR Subprogram in the first trial.
2370-2570	Statements 2380 and 2390 employ a trapezoidal approximation for the determination of aqueous concentrations at the end of the time increment. Organic-phase concentrations at the end of the time increment are calculated in statement 2410. Differences between aqueous-phase concentrations at the end of the time increment and the ARY values are calculated as fractional changes and compared to the tolerance CCD. The ARY values are then set equal to the calculated aqueous-phase concentrations. The counter MCK% is incremented. For up to 21 trials, if a good fit is not attained, control returns to statement 2320 to repeat the above procedure; otherwise this integration procedure ends as program flow continues to statement 2580.
As with the Runge-Kutta technique, Trapezoidal integration technique calculations will alternately sweep the cascade in opposite directions in successive time increments. Note also that the UCOR Subprogram is called only once for each trial calculation.	

Statements	Description
2580-2620	Exponential factors (FACTA and FACTO) for temperature and concentration changes in the settlers are initially set to 0. If no chemical reactions are to be considered or no reductant is present (IRXN% = 0, IPROCE% = 1, or ISOL5% = 0), control transfers to statement 2630. Otherwise, the chemical reaction Subprogram for mixers (MCHEMP) is called and program flow continues to statement 2630.
2630-3060	Trapezoidal integration technique for settlers. A classical trapezoidal or finite difference numerical integration technique is employed for the settlers in this section. The settlers are modeled assuming no mass transfer between the phases and perfect mixing of the phases in each of three settler zones. The use of three perfectly mixed zones in succession is a compromise between plug-flow and perfectly mixed models. These zones serve as liquid holdup regions between the mixers of adjacent stages. Chemical reactions within a phase, however, are allowed to occur.
2630-2660	Exponential factors (FACTA and FACTO) for temperature and concentration changes in the settlers are set to 150 or to values as defined in statements 2650 and 2660 based on settler phase volumes.
2670-2680	Exit stream temperatures for zone 1 for the time increment are calculated assuming a well-mixed tank.
2690-2860	The inventory change in zone 1 (CNGINV) is initially set at 0 and then calculated using mixer exit stream concentrations (if significant) and expressed as a percentage. The variable CODUM, which represents maximum inventory change is set equal to CNGINV if CNGINV > CODUM. Exit stream concentrations for zone 1 for the time increment are calculated assuming a well-mixed tank.
2870-3010	A similar procedure is followed for settler zones 2 and 3 to produce exit stream temperatures and concentrations.
3020-3060	If no chemical reactions are to be considered or no reductant is present (IRXN% = 0, IPROCE% = 1, or ISOL5% = 0), control transfers to statement 3060. Otherwise, the chemical reaction Subprogram for settlers (SCHEMP) is called and program flow continues to statement 3060. For details of the SCHEMP Subprogram, see Sect. D.11. This integration procedure for settlers ends as program flow continues to statement 3070.
3070-3110	The sign of the index NDIREC%, which denotes if stage calculations proceed in the direction of aqueous flow or organic flow, is reversed and the index MSCAN%, denoting the number of times the cascade is calculated for each integration,

Statements	Description
	is incremented. If the Fast integration technique is specified for mixers and if MSCAN% < 2, control transfers to statement 330 where the cascade integration procedure is repeated for the same time increment, but in the opposite direction. If either of the other two mixer integration techniques is specified, NDIREC% is returned to its previous value and the Subprogram ends.

D.3 Listing of the STAGES Subprogram

```
200 SUB STAGES (NDIREC%)  'Calculates concentrations in each stage for
    every time increment.
210 SHARED NTOST%, CTBP, NEWOUT%, SPH, IFAST%, IRXN%, DTHETA, IVOLM%,
    IVOLS%, IPRO%, TEMPI, ISOL5%, NSTR%, ISTR%, JSTR%, IPROCE%, LN%, V%,
    PQ$, QQ$, R$, RR$, T, CODUM(), CODUMM()
220 SHARED TPROF(), ATS(), OTS()
230 SHARED TEMPC, ARY(), DTRY()
240 SHARED X(), Y(), XS(), YS()
250 SHARED ANET(), ONET(), AT(), OT()
260 SHARED XFD(), YFD(), AFDRT(), OFDRT(), AFDTEM(), OFDTEM(), ALVRT(),
    OLVRT()
270 SHARED AVOL(), OVOL(), ASVOL(), OSVOL()
280 SHARED AQ(), ORG(), TEMP, CONVA, CONVO, TCONC%
290 SHARED RXNTRM(), AIN(), OIN()
300 DIM F(6), PHI(6), TX(6), DELTAX(6), DELTAY(3)
310 CCD = .001: TCONC% = 1
320 MSCAN% = 0
330 FOR NSCAN% = 1 TO NTOST%
340  J% = NSCAN%
350  IF NDIREC% < 0 THEN J% = NTOST% - NSCAN% + 1
360  LOCATE 6, 66: PRINT USING "###"; J%;
370  JJ% = J% - 1: JJJ% = J% + 1: CODUM(J%) = 0!
380  FOR I% = 1 TO 3
390   DELTAX(I%) = 0!: DELTAY(I%) = 0!: CODUMM(I%, J%) = 0!
400   AIN(I%) = AFDRT(J%) * XFD(I%, J%): OIN(I%) = OFDRT(J%) * YFD(I%, J%)
410   IF J% = 1 THEN 450
420   AIN(I%) = AIN(I%) + ANET(JJ%) * XS(JJ%, 3, I%, 1)
430   DELTAX(I%) = (XS(JJ%, 3, I%, 2) - XS(JJ%, 3, I%, 1)) * ANET(JJ%)
440   IF IFAST% <> 2 THEN AIN(I%) = AIN(I%) + (XS(JJ%, 3, I%, 2) - XS(JJ%,
      3, I%, 1)) * ANET(JJ%) / 2!
450   IF J% = NTOST% THEN 490
460   OIN(I%) = OIN(I%) + ONET(JJJ%) * YS(JJJ%, 3, I%, 1)
470   DELTAY(I%) = (YS(JJJ%, 3, I%, 2) - YS(JJJ%, 3, I%, 1)) * ONET(JJJ%)
480   IF IFAST% <> 2 THEN OIN(I%) = OIN(I%) + (YS(JJJ%, 3, I%, 2) -
      YS(JJJ%, 3, I%, 1)) * ONET(JJJ%) / 2!
490   IF NSTR% <> 1 THEN 560
500   IF J% <> JSTR% AND J% <> (ISTR% - 1) THEN 560
510   IF J% = (ISTR% - 1) THEN OIN(I%) = OFDRT(J%) * YFD(I%, J%)
520   IF J% = (ISTR% - 1) THEN DELTAY(I%) = 0!
```

```
530   IF J% = JSTR% THEN OIN(I%) = OIN(I%) + ONET(ISTR%) * YS(ISTR%, 3, I%,
      1)
540   IF J% = JSTR% THEN DELTAY(I%) = DELTAY(I%) + (YS(ISTR%, 3, I%, 2) -
      YS(ISTR%, 3, I%, 1)) * ONET(ISTR%)
550   IF J% = JSTR% AND IFAST% <> 2 THEN OIN(I%) = OIN(I%) + (YS(ISTR%, 3,
      I%, 2) - YS(ISTR%, 3, I%, 1)) * ONET(ISTR%) / 2!
560   IF ABS(AIN(I%)) < 1E-15 THEN AIN(I%) = 0!
570   IF ABS(OIN(I%)) < 1E-15 THEN OIN(I%) = 0!
580   TX(I%) = X(I%, J%, 2): ARY(I%) = X(I%, J%, 2): AQ(I%) = X(I%, J%, 2):
      ORG(I%) = Y(I%, J%, 2)
590  NEXT I%
600  FOR I% = 4 TO V%
610   DELTAX(I%) = 0!: CODUMM(I%, J%) = 0!
620   AIN(I%) = AFDRT(J%) * XFD(I%, J%)
630   IF J% = 1 THEN 670
640   AIN(I%) = AIN(I%) + ANET(JJ%) * XS(JJ%, 3, I%, 1)
650   DELTAX(I%) = (XS(JJ%, 3, I%, 2) - XS(JJ%, 3, I%, 1)) * ANET(JJ%)
660   IF IFAST% <> 2 THEN AIN(I%) = AIN(I%) + (XS(JJ%, 3, I%, 2) - XS(JJ%,
      3, I%, 1)) * ANET(JJ%) / 2!
670   IF ABS(AIN(I%)) < 1E-15 THEN AIN(I%) = 0!
680   TX(I%) = X(I%, J%, 2): ARY(I%) = X(I%, J%, 2): AQ(I%) = X(I%, J%, 2)
690  NEXT I%
700  TEMP = TPROF(J%, 2)
710  IF IPROCE% <> 0 THEN 740
720  CALL MOLALP  'The MOLALP Subprogram is called here.
730  GOTO 750
740  CALL MOLALT  'The MOLALT Subprogram is called here.
750  AQVOL = AVOL(J%) / CONVA: ORVOL = OVOL(J%) / CONVO
760  AQSVOL = ASVOL(J%) / CONVA: ORSVOL = OSVOL(J%) / CONVO
770  AHTIN = AFDRT(J%) * AFDTEM(J%): OHTIN = OFDRT(J%) * OFDTEM(J%)
780  IF J% <> 1 THEN AHTIN = AHTIN + ANET(JJ%) * ATS(JJ%, 3, 1)
790  IF J% <> 1 THEN AHTIN = AHTIN + (ATS(JJ%, 3, 2) - ATS(JJ%, 3, 1)) *
     ANET(JJ%) / 2!
800  IF J% <> NTOST% THEN OHTIN = OHTIN + ONET(JJJ%) * OTS(JJJ%, 3, 1)
810  IF J% <> NTOST% THEN OHTIN = OHTIN + (OTS(JJJ%, 3, 2) - OTS(JJJ%, 3,
     1)) * ONET(JJJ%) / 2!
820  IF NSTR% = 1 AND J% = (ISTR% - 1) THEN OHTIN = OFDRT(J%) * OFDTEM(J%)
830  IF NSTR% = 1 AND J% = JSTR% THEN OHTIN = OHTIN + ONET(ISTR%) *
     OTS(ISTR%, 3, 1)
840  IF NSTR% = 1 AND J% = JSTR% THEN OHTIN = OHTIN + (OTS(ISTR%, 3, 2) -
     OTS(ISTR%, 3, 1)) * ONET(ISTR%) / 2!
850  TPROF(J%, 2) = TPROF(J%, 1) + DTHETA * (AHTIN + SPH * OHTIN - (AT(J%)
     + SPH * OT(J%)) * TPROF(J%, 1)) / (AQVOL + SPH * ORVOL)
860  TEMPC = TPROF(J%, 2)
870  IMCHEM% = 0
880  IF IFAST% = 1 THEN 2300
890  IF IFAST% = 2 THEN 1980
900 REM The Runge-Kutta method begins here.
910  MCK% = 0
920  IF IPROCE% <> 0 THEN 950
930  CALL UCORPU  'The UCORPU Subprogram is called here.
940  GOTO 960
950  CALL UCORTH  'The UCORTH Subprogram is called here.
960  FOR I% = 1 TO 3
```

```
970   F(I%) = (AIN(I%) + OIN(I%) - (AT(J%) + OT(J%) * DTRY(I%)) * X(I%, J%,
      1)) / (AQVOL + ORVOL * DTRY(I%))
980   ARY(I%) = X(I%, J%, 1) + DTHETA * F(I%) / 2!
990  NEXT I%
1000  FOR I% = 4 TO V%
1010   F(I%) = (AIN(I%) - AT(J%) * X(I%, J%, 1)) / AQVOL
1020   ARY(I%) = X(I%, J%, 1) + DTHETA * F(I%) / 2!
1030  NEXT I%
1040  MCK% = MCK% + 1
1050  IF IPROCE% <> 0 THEN 1080
1060  CALL UCORPU  'The UCORPU Subprogram is called here.
1070  GOTO 1090
1080  CALL UCORTH  'The UCORTH Subprogram is called here.
1090  MDEX% = 0
1100  FOR I% = 1 TO V%
1110   IF ABS(ARY(I%)) < .000001 THEN 1140
1120   DIF = ABS((TX(I%) - ARY(I%)) / ARY(I%))
1130   IF DIF > CCD THEN MDEX% = 1
1140   TX(I%) = ARY(I%)
1150  NEXT I%
1160  IF MDEX% = 1 AND MCK% < 5 THEN 960
1170  FOR I% = 1 TO V%
1180   X(I%, J%, 2) = ARY(I%): PHI(I%) = F(I%)
1190  NEXT I%
1200  FOR I% = 1 TO 3
1210   F(I%) = (AIN(I%) + OIN(I%) - (AT(J%) + OT(J%) * DTRY(I%)) * X(I%,
       J%, 2)) / (AQVOL + ORVOL * DTRY(I%))
1220   ARY(I%) = X(I%, J%, 1) + DTHETA * F(I%) / 2!
1230  NEXT I%
1240  FOR I% = 4 TO V%
1250   F(I%) = (AIN(I%) - AT(J%) * X(I%, J%, 2)) / AQVOL
1260   ARY(I%) = X(I%, J%, 1) + DTHETA * F(I%) / 2!
1270  NEXT I%
1280  MCK% = MCK% + 1
1290  IF IPROCE% <> 0 THEN 1320
1300  CALL UCORPU  'The UCORPU Subprogram is called here.
1310  GOTO 1330
1320  CALL UCORTH  'The UCORTH Subprogram is called here.
1330  MDEX% = 0
1340  FOR I% = 1 TO V%
1350   IF ABS(ARY(I%)) < .000001 THEN 1380
1360   DIF = ABS((TX(I%) - ARY(I%)) / ARY(I%))
1370   IF DIF > CCD THEN MDEX% = 1
1380   TX(I%) = ARY(I%)
1390  NEXT I%
1400  IF MDEX% = 1 AND MCK% < 10 THEN 1200
1410  FOR I% = 1 TO V%
1420   X(I%, J%, 2) = ARY(I%): PHI(I%) = PHI(I%) + 2! * F(I%)
1430  NEXT I%
1440  FOR I% = 1 TO 3
1450   F(I%) = (AIN(I%) + OIN(I%) - (AT(J%) + OT(J%) * DTRY(I%)) * X(I%,
       J%, 2)) / (AQVOL + ORVOL * DTRY(I%))
1460   ARY(I%) = X(I%, J%, 1) + DTHETA * F(I%)
1470  NEXT I%
1480  FOR I% = 4 TO V%
```

```
1490   F(I%) = (AIN(I%) - AT(J%) * X(I%, J%, 2)) / AQVOL
1500   ARY(I%) = X(I%, J%, 1) + DTHETA * F(I%)
1510  NEXT I%
1520  MCK% = MCK% + 1
1530  IF IPROCE% <> 0 THEN 1560
1540  CALL UCORPU  'The UCORPU Subprogram is called here.
1550  GOTO 1570
1560  CALL UCORTH  'The UCORTH Subprogram is called here.
1570  MDEX% = 0
1580  FOR I% = 1 TO V%
1590   IF ABS(ARY(I%)) < .000001 THEN 1620
1600   DIF = ABS((TX(I%) - ARY(I%)) / ARY(I%))
1610   IF DIF > CCD THEN MDEX% = 1
1620   TX(I%) = ARY(I%)
1630  NEXT I%
1640  IF MDEX% = 1 AND MCK% < 15 THEN 1440
1650  FOR I% = 1 TO V%
1660   X(I%, J%, 2) = ARY(I%): PHI(I%) = PHI(I%) + 2! * F(I%)
1670  NEXT I%
1680  FOR I% = 1 TO 3
1690   F(I%) = (AIN(I%) + OIN(I%) - (AT(J%) + OT(J%) * DTRY(I%)) * X(I%,
       J%, 2)) / (AQVOL + ORVOL * DTRY(I%))
1700   ARY(I%) = X(I%, J%, 1) + (PHI(I%) + F(I%)) * DTHETA / 6!
1710  NEXT I%
1720  FOR I% = 4 TO V%
1730   F(I%) = (AIN(I%) - AT(J%) * X(I%, J%, 2)) / AQVOL
1740   ARY(I%) = X(I%, J%, 1) + (PHI(I%) + F(I%)) * DTHETA / 6!
1750  NEXT I%
1760  MCK% = MCK% + 1
1770  IF IPROCE% <> 0 THEN 1800
1780  CALL UCORPU  'The UCORPU Subprogram is called here.
1790  GOTO 1810
1800  CALL UCORTH  'The UCORTH Subprogram is called here.
1810  MDEX% = 0
1820  FOR I% = 1 TO V%
1830   IF ABS(ARY(I%)) < .000001 THEN 1860
1840   DIF = ABS((TX(I%) - ARY(I%)) / ARY(I%))
1850   IF DIF > CCD THEN MDEX% = 1
1860   TX(I%) = ARY(I%)
1870  NEXT I%
1880  IF MDEX% = 1 AND MCK% < 20 THEN 1680
1890  FOR I% = 1 TO 3
1900   IF ARY(I%) <= 1E-20 THEN ARY(I%) = 0!
1910   Y(I%, J%, 2) = DTRY(I%) * ARY(I%): X(I%, J%, 2) = ARY(I%)
1920  NEXT I%
1930  FOR I% = 4 TO V%
1940   IF ARY(I%) <= 1E-20 THEN ARY(I%) = 0!
1950   X(I%, J%, 2) = ARY(I%)
1960  NEXT I%
1970  GOTO 2580
1980 REM The fast method begins here.
1990  MCK% = 0
2000  MDEX% = 0
2010  IF IPROCE% <> 0 THEN 2040
2020  CALL UCORPU  'The UCORPU Subprogram is called here.
```

```
2030  GOTO 2050
2040  CALL UCORTH  'The UCORTH Subprogram is called here.
2050  FOR I% = 1 TO 3
2060   WGHT = DTHETA * (AT(J%) + DTRY(I%) * OT(J%)) / (AQVOL + DTRY(I%) *
       ORVOL)
2070   ARY(I%) = X(I%, J%, 1) * EXP(-WGHT) + (AIN(I%) + OIN(I%) +
       RXNTRM(I%, J%)) * (1! - EXP(-WGHT)) / (AT(J%) + DTRY(I%) * OT(J%)) +
       (DELTAX(I%) + DELTAY(I%)) * (EXP(-WGHT) + WGHT - 1!) / (WGHT *
       (AT(J%) + DTRY(I%) * OT(J%)))
2080   DIF = 0!
2090   IF ABS(ARY(I%)) >= .000001 THEN DIF = ABS((X(I%, J%, 2) - ARY(I%)) /
       ARY(I%))
2100   IF DIF > CCD THEN MDEX% = 1
2110   IF ARY(I%) < 1E-10 THEN ARY(I%) = 0!
2120   X(I%, J%, 2) = ARY(I%): Y(I%, J%, 2) = ARY(I%) * DTRY(I%)
2130  NEXT I%
2140  FOR I% = 4 TO V%
2150   WGHT = DTHETA * AT(J%) / AQVOL
2160   ARY(I%) = X(I%, J%, 1) * EXP(-WGHT) + (AIN(I%) + RXNTRM(I%, J%)) *
       (1! - EXP(-WGHT)) / AT(J%) + DELTAX(I%) * (EXP(-WGHT) + WGHT - 1!) /
       (WGHT * AT(J%))
2170   DIF = 0!
2180   IF ABS(ARY(I%)) >= .000001 THEN DIF = ABS((X(I%, J%, 2) - ARY(I%)) /
       ARY(I%))
2190   IF DIF > CCD THEN MDEX% = 1
2200   IF ARY(I%) < 1E-10 THEN ARY(I%) = 0!
2210   X(I%, J%, 2) = ARY(I%)
2220  NEXT I%
2230  MCK% = MCK% + 1
2240  IF MDEX% = 1 AND MCK% < 15 THEN 2000
2250  IF IMCHEM% = 1 OR IRXN% = 0 OR IPROCE% = 1 THEN 2630
2260  IMCHEM% = IMCHEM% + 1
2270  IF ISOL5% = 0 THEN 1980
2280  CALL MCHEMP(J%, AQVOL!, ORVOL!) 'The MCHEMP Subprogram is called
      here.
2290  GOTO 1980
2300 REM The trapezoidal method begins here.
2310  MCK% = 0
2320  MDEX% = 0
2330  IF IPROCE% <> 0 THEN 2360
2340  CALL UCORPU  'The UCORPU Subprogram is called here.
2350  GOTO 2370
2360  CALL UCORTH  'The UCORTH Subprogram is called here.
2370  FOR I% = 1 TO 3
2380   DVOLS = AQVOL + DTRY(I%) * ORVOL: DFLOS = AT(J%) + DTRY(I%) * OT(J%)
2390   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!)
2400   IF X(I%, J%, 2) <= 1E-20 THEN X(I%, J%, 2) = 0!
2410   Y(I%, J%, 2) = X(I%, J%, 2) * DTRY(I%)
2420   IF ABS(X(I%, J%, 2)) < 1E-09 THEN 2450
2430   DIF = ABS((X(I%, J%, 2) - ARY(I%)) / X(I%, J%, 2))
2440   IF DIF >= CCD THEN MDEX% = 1
2450   ARY(I%) = X(I%, J%, 2)
2460  NEXT I%
```

```
2470  FOR I% = 4 TO V%
2480   DVOLS = AQVOL: DFLOS = AT(J%)
2490   X(I%, J%, 2) = (AQVOL * X(I%, J%, 1) + DTHETA * (AIN(I%) - (AT(J%) *
       X(I%, J%, 1)) / 2!)) / (DVOLS + DTHETA * DFLOS / 2!)
2500   IF X(I%, J%, 2) <= 1E-20 THEN X(I%, J%, 2) = 0!
2510   IF ABS(X(I%, J%, 2)) < 1E-09 THEN 2540
2520   DIF = ABS((X(I%, J%, 2) - ARY(I%)) / X(I%, J%, 2))
2530   IF DIF >= CCD THEN MDEX% = 1
2540   ARY(I%) = X(I%, J%, 2)
2550  NEXT I%
2560  MCK% = MCK% + 1
2570  IF MDEX% = 1 AND MCK% <= 20 THEN 2320
2580  FACTA = 0!: FACTO = 0!
2590  IF IRXN% = 0 THEN 2630
2600  IF IPROCE% = 1 THEN 2630
2610  IF ISOL5% = 0 THEN 2630
2620  CALL MCHEMP(J%, AQVOL!, ORVOL!)  'The MCHEMP Subprogram is called
      here.
2630 REM The settlers are integrated here (trapezoidal method).
2640  FACTA = 150!: FACTO = 150!
2650  IF AQSVOL > 0! THEN FACTA = 3! * AT(J%) * DTHETA / AQSVOL
2660  IF ORSVOL > 0! THEN FACTO = 3! * OT(J%) * DTHETA / ORSVOL
2670  ATS(J%, 1, 2) = ATS(J%, 1, 1) * EXP(-FACTA) + TPROF(J%, 1) * (1! -
      EXP(-FACTA)) + (TPROF(J%, 2) - TPROF(J%, 1)) * (EXP(-FACTA) + FACTA -
      1!) / FACTA
2680  OTS(J%, 1, 2) = OTS(J%, 1, 1) * EXP(-FACTO) + TPROF(J%, 1) * (1! -
      EXP(-FACTO)) + (TPROF(J%, 2) - TPROF(J%, 1)) * (EXP(-FACTO) + FACTO -
      1!) / FACTO
2690  FOR I% = 1 TO 3
2700   CNGINV = 0!
2710   IF (X(I%, J%, 2) + Y(I%, J%, 2)) > .000001 THEN 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)))
2720   CNGINV = 100! * ABS(CNGINV)
2730   IF CODUM(J%) < CNGINV THEN CODUM(J%) = CNGINV
2735   IF CODUMM(I%, J%) < CNGINV THEN CODUMM(I%, J%) = CNGINV
2740   XS(J%, 1, I%, 2) = XS(J%, 1, I%, 1) * EXP(-FACTA) + X(I%, J%, 1) *
       (1! - EXP(-FACTA)) + (X(I%, J%, 2) - X(I%, J%, 1)) * (EXP(-FACTA) +
       FACTA - 1!) / FACTA
2750   IF XS(J%, 1, I%, 2) <= 1E-20 THEN XS(J%, 1, I%, 2) = 0!
2760   YS(J%, 1, I%, 2) = YS(J%, 1, I%, 1) * EXP(-FACTO) + Y(I%, J%, 1) *
       (1! - EXP(-FACTO)) + (Y(I%, J%, 2) - Y(I%, J%, 1)) * (EXP(-FACTO) +
       FACTO - 1!) / FACTO
2770   IF YS(J%, 1, I%, 2) <= 1E-20 THEN YS(J%, 1, I%, 2) = 0!
2780  NEXT I%
2790  FOR I% = 4 TO V%
2800   CNGINV = 0!
2810   IF X(I%, J%, 2) > .000001 THEN CNGINV = AVOL(J%) * (X(I%, J%, 2) -
       X(I%, J%, 1)) / (DTHETA * AVOL(J%) * X(I%, J%, 2))
2820   CNGINV = 100! * ABS(CNGINV)
2830   IF CODUM(J%) < CNGINV THEN CODUM(J%) = CNGINV
2835   IF CODUMM(I%, J%) < CNGINV THEN CODUMM(I%, J%) = CNGINV
```

```
2840   XS(J%, 1, I%, 2) = XS(J%, 1, I%, 1) * EXP(-FACTA) + X(I%, J%, 1) *
       (1! - EXP(-FACTA)) + (X(I%, J%, 2) - X(I%, J%, 1)) * (EXP(-FACTA) +
       FACTA - 1!) / FACTA
2850   IF XS(J%, 1, I%, 2) <= 1E-20 THEN XS(J%, 1, I%, 2) = 0!
2860  NEXT I%
2870  FOR KZ% = 2 TO 3
2880   KZB% = KZ% - 1
2890   ATS(J%, KZ%, 2) = ATS(J%, KZ%, 1) * EXP(-FACTA) + ATS(J%, KZB%, 1) *
       (1! - EXP(-FACTA)) + (ATS(J%, KZB%, 2) - ATS(J%, KZB%, 1)) * (EXP(-
       FACTA) + FACTA - 1!) / FACTA
2900   OTS(J%, KZ%, 2) = OTS(J%, KZ%, 1) * EXP(-FACTO) + OTS(J%, KZB%, 1) *
       (1! - EXP(-FACTO)) + (OTS(J%, KZB%, 2) - OTS(J%, KZB%, 1)) * (EXP(-
       FACTO) + FACTO - 1!) / FACTO
2910   FOR I% = 1 TO 3
2920    XS(J%, KZ%, I%, 2) = XS(J%, KZ%, I%, 1) * EXP(-FACTA) + XS(J%,
        KZB%, I%, 1) * (1! - EXP(-FACTA)) + (XS(J%, KZB%, I%, 2) - XS(J%,
        KZB%, I%, 1)) * (EXP(-FACTA) + FACTA - 1!) / FACTA
2930    IF XS(J%, KZ%, I%, 2) <= 1E-20 THEN XS(J%, KZ%, I%, 2) = 0!
2940    YS(J%, KZ%, I%, 2) = YS(J%, KZ%, I%, 1) * EXP(-FACTO) + YS(J%,
        KZB%, I%, 1) * (1! - EXP(-FACTO)) + (YS(J%, KZB%, I%, 2) - YS(J%,
        KZB%, I%, 1)) * (EXP(-FACTO) + FACTO - 1!) / FACTO
2950    IF YS(J%, KZ%, I%, 2) <= 1E-20 THEN YS(J%, KZ%, I%, 2) = 0!
2960   NEXT I%
2970   FOR I% = 4 TO V%
2980    XS(J%, KZ%, I%, 2) = XS(J%, KZ%, I%, 1) * EXP(-FACTA) + XS(J%,
        KZB%, I%, 1) * (1! - EXP(-FACTA)) + (XS(J%, KZB%, I%, 2) - XS(J%,
        KZB%, I%, 1)) * (EXP(-FACTA) + FACTA - 1!) / FACTA
2990    IF XS(J%, KZ%, I%, 2) <= 1E-20 THEN XS(J%, KZ%, I%, 2) = 0!
3000   NEXT I%
3010  NEXT KZ%
3020  IF IRXN% = 0 THEN 3060
3030  IF IPROCE% = 1 THEN 3060
3040  IF ISOL5% = 0 THEN 3060
3050  CALL SCHEMP(J%, AQSVOL!, ORSVOL!)  'The SCHEMP Subprogram is called
      here.
3060 NEXT NSCAN%
3070 NDIREC% = -NDIREC%
3080 MSCAN% = MSCAN% + 1
3090 IF IFAST% = 2 AND MSCAN% < 2 THEN 330
3100 IF IFAST% <> 2 THEN NDIREC% = -NDIREC%
3110 END SUB
```

D.7 Print Subprograms (PRTPU and PRTTH)

Statements	Description
PRTPU:	
4980-5860	Subprogram PRTPU provides a hard-copy printout of results for a given modeling problem. The index TCONC% is set at 1 indicating that solute-free units will be converted to molar units. Solute concentrations and phase flow rates in the mixers for the current time increment being printed are converted to molar

Statements	Description
	units through the MOLALP Subprogram. Phase densities are estimated using correlations discussed in Sect. 2.5. Extraction factors for each transferring solute are also calculated. The molar concentrations in each stage are then converted to units appropriate for the printout (g/L for heavy metals) and printed. Phase densities, phase flow rates, temperatures, extraction factors, degree of solvent saturation, and maximum solute inventory changes per minute are also printed for each stage. A counter (LN%) keeps track of each line printed and printer paper is advanced as appropriate. The Subprogram then ends.
PRTTH: 5910-6770	Subprogram PRTTH provides a hard-copy printout of results for a given modeling problem. The index TCONC% is set at 1 indicating that solute-free units will be converted to molar units. Solute concentrations and phase flow rates in the mixers for the current time increment being printed are converted to molar units through the MOLALT Subprogram. Phase densities are not calculated. Extraction factors for each transferring solute are calculated and molar concentrations in each stage are converted to units appropriate for the printout (g/L for heavy metals) and printed. Phase flow rates, temperatures, extraction factors, degree of solvent saturation, and maximum solute inventory changes per minute are printed for each stage. A counter (LN%) keeps track of each line printed and printer paper is advanced as appropriate. The Subprogram then ends.

D.8 Listing of the Print Subprograms (PRTPU and PRTTH)

```
4980 SUB PRTPU  'Prints the results for Purex.
4990 SHARED NTOST%, CTBP, NEWOUT%, SPH, IFAST%, IRXN%, DTHETA, IVOLM%,
     IVOLS%, IPRO%, TEMPI, ISOL5%, NSTR%, ISTR%, JSTR%, IPROCE%, LN%, V%,
     PQ$, QQ$, R$, RR$, T, CODUM(), CODUMM()
5000 SHARED TPROF(), ATS(), OTS()
5010 SHARED X(), Y(), XS(), YS()
5020 SHARED ANET(), ONET(), AT(), OT()
5030 SHARED XFD(), YFD(), AFDRT(), OFDRT(), AFDTEM(), OFDTEM(), ALVRT(),
     OLVRT()
5040 SHARED AQ(), ORG(), TEMP, CONVA, CONVO, TCONC%
5050 SHARED ADEN(), ODEN(), AOUT(), OOUT(), EXT1(), EXT2(), EXT3(), TSAT()
5060 GOSUB 5720  'To set up Purex aqueous results chart
5070 TCONC% = 1
5075 SOLDEN = 1000! * (CTBP * 266.32 / 273.6 + (1! - CTBP) * 170.34 /
     227.5)
5080 FOR I% = 1 TO NTOST%
5090  IF LN% < 55 THEN 5110
5100  LPRINT CHR$(12); : LN% = 0: GOSUB 5720
5110  FOR J% = 1 TO V%
```

```
5120  AQ(J%) = X(J%, I%, 2)
5130 NEXT J%
5140 FOR J% = 1 TO 3
5150  ORG(J%) = Y(J%, I%, 2)
5160 NEXT J%
5170 TEMP = TPROF(I%, 2)
5180 CALL MOLALP  'The MOLALP Subprogram is called here.
5190 ADEN(I%) = (997.07 + 394.04 * AQ(2) + 492.02 * (AQ(3) + AQ(4)) +
     63.01 * AQ(1) + 213.1 * AQ(6)) / (1000! + 72.4 * AQ(2) + 130! *
     (AQ(3) + AQ(4)) + 30.9 * AQ(1) + 31! * AQ(6))
5200 AOUT(I%) = AT(I%) * CONVA: OOUT(I%) = OT(I%) * CONVO
5210 FOR J% = 1 TO V%
5220  X(J%, I%, 2) = AQ(J%) / CONVA
5230 NEXT J%
5240 FOR J% = 1 TO 3
5250  Y(J%, I%, 2) = ORG(J%) / CONVO
5260 NEXT J%
5270 X(2, I%, 2) = X(2, I%, 2) * 238!: X(3, I%, 2) = X(3, I%, 2) * 239!
5280 X(4, I%, 2) = X(4, I%, 2) * 239!
5290 LPRINT USING " ### "; I%;
5300 FOR J% = 1 TO V%
5310  LPRINT USING QQ$; X(J%, I%, 2);
5320 NEXT J%
5330 LPRINT USING QQ$; ADEN(I%); AOUT(I%); : LPRINT USING RR$; TPROF(I%,
     2)
5340 IF ABS(ALVRT(I%)) < .000001 THEN 5390
5350 PROFLO = CONVA * ALVRT(I%)
5360 LPRINT USING " ### "; I%;
5370 LPRINT "   PRODUCT STREAM"; SPACE$(74);
5380 LPRINT USING QQ$; PROFLO: LN% = LN% + 1
5390 LN% = LN% + 1
5400 NEXT I%
5410 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 5430
5420 LPRINT CHR$(12); : LN% = 0
5430 GOSUB 5790  'To set up Purex organic results chart
5440 FOR I% = 1 TO NTOST%
5450  IF LN% < 55 THEN 5470
5460  LPRINT CHR$(12); : LN% = 0: GOSUB 5790
5470  EXT1(I%) = 0!: EXT2(I%) = 0!: EXT3(I%) = 0!
5480  TSAT(I%) = (2! * Y(2, I%, 2) + 2! * Y(3, I%, 2) + Y(1, I%, 2)) * 100!
      / T
5490  Y(2, I%, 2) = Y(2, I%, 2) * 238!: Y(3, I%, 2) = Y(3, I%, 2) * 239!
5500  IF AOUT(I%) <= .000001 THEN 5560
5510  EXT1(I%) = OOUT(I%) / AOUT(I%)
5520  IF X(2, I%, 2) > 1E-10 THEN EXT2(I%) = EXT1(I%) * Y(2, I%, 2) / X(2,
      I%, 2)
5530  IF (X(3, I%, 2) + X(4, I%, 2)) > 1E-10 THEN EXT3(I%) = EXT1(I%) *
      Y(3, I%, 2) / (X(3, I%, 2) + X(4, I%, 2))
5540  IF X(1, I%, 2) > 1E-10 THEN EXT1(I%) = EXT1(I%) * Y(1, I%, 2) / X(1,
      I%, 2)
5550  IF X(1, I%, 2) <= 1E-10 THEN EXT1(I%) = 0!
5560  WO = (4.2 - .015 * TEMP) * (CTBP ^ 1.69) * (T - 2! * Y(2, I%, 1) - 2!
      * Y(3, I%, 1) - .6 * Y(1, I%, 1)) / T
```

```
5565  ODEN(I%) = (SOLDEN + 18.02 * WO + 394.04 * Y(2, I%, 1) + 492.02 *
      Y(3, I%, 1) + 63.01 * Y(1, I%, 1)) / (1000! + 17.4 * WO + 97! * Y(2,
      I%, 1) + 139! * Y(3, I%, 1) + 43! * Y(1, I%, 1))
5570  IF ABS(OLVRT(I%)) < .000001 THEN 5620
5580  PROFLO = OLVRT(I%) * OOUT(I%) / OT(I%)
5590  LPRINT USING " ### "; I%;
5600  LPRINT "   PRODUCT STREAM"; SPACE$(73);
5610  LPRINT USING QQ$; PROFLO: LN% = LN% + 1
5620  LPRINT USING " ### "; I%;
5630  FOR J% = 1 TO 3
5640   LPRINT USING QQ$; Y(J%, I%, 2);
5650  NEXT J%
5660  LPRINT USING QQ$; EXT2(I%); EXT3(I%); EXT1(I%); ODEN(I%); OOUT(I%); :
      LPRINT USING RR$; TSAT(I%); : LPRINT USING QQ$; CODUM(I%)
5670  LN% = LN% + 1
5680 NEXT I%
5690 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 5710
5700 LPRINT CHR$(12); : LN% = 0
5710 GOTO 5860
5720 REM Subroutine to set up Purex aqueous results chart.
5730  LPRINT " AQUEOUS PHASE:"
5740  LPRINT " STAGE  NITRIC ACID    URANIUM      PU (IV)      PU (III)
      REDUCTANT   NITRATE ION    DENSITY     FLOW RATE    TEMP"
5750  LPRINT "  NO.        (M)          (g/L)         (g/L)         (g/L)
      (M)           (M)         (g/mL)        (L/min)       (C)"
5760  LPRINT " -----  -----------  -----------  -----------  -----------  -
      ----------  -----------  -----------  -----------  ------"
5770  LN% = LN% + 4
5780 RETURN
5790 REM Subroutine to set up Purex organic results chart.
5800  LPRINT " ORGANIC PHASE:"
5810  LPRINT " STAGE  NITRIC ACID    URANIUM      PU (IV)      U EXTRACT
      PU EXTRACT   H+ EXTRACT     DENSITY     FLOW RATE   TBPSAT
      INVENTORY"
5820  LPRINT "  NO.        (M)          (g/L)         (g/L)         FACTOR
      FACTOR        FACTOR        (g/mL)        (L/min)       (%)     CHANGE
      (%)"
5830  LPRINT " -----  -----------  -----------  -----------  -----------  -
      ----------  -----------  -----------  -----------  ------  ----------
      -"
5840  LN% = LN% + 4
5850 RETURN
5860 END SUB
```

```
5910 SUB PRTTH  'Prints the results for Thorex.
5920 SHARED NTOST%, CTBP, NEWOUT%, SPH, IFAST%, IRXN%, DTHETA, IVOLM%,
     IVOLS%, IPRO%, TEMPI, ISOL5%, NSTR%, ISTR%, JSTR%, IPROCE%, LN%, V%,
     PQ$, QQ$, R$, RR$, T, CODUM(), CODUMM()
5930 SHARED TPROF(), ATS(), OTS()
5940 SHARED X(), Y(), XS(), YS()
5950 SHARED ANET(), ONET(), AT(), OT()
5960 SHARED XFD(), YFD(), AFDRT(), OFDRT(), AFDTEM(), OFDTEM(), ALVRT(),
     OLVRT()
5970 SHARED AQ(), ORG(), TEMP, CONVA, CONVO, TCONC%
5980 SHARED ADEN(), ODEN(), AOUT(), OOUT(), EXT1(), EXT2(), EXT3(), TSAT()
```

```
5990 TCONC% = 1
6000 GOSUB 6630  'To set up Thorex aqueous results chart
6010 FOR I% = 1 TO NTOST%
6020  IF LN% < 55 THEN 6040
6030  LPRINT CHR$(12); : LN% = 0: GOSUB 6630
6040  FOR J% = 1 TO V%
6050   AQ(J%) = X(J%, I%, 2)
6060  NEXT J%
6070  FOR J% = 1 TO 3
6080   ORG(J%) = Y(J%, I%, 2)
6090  NEXT J%
6100  TEMP = TPROF(I%, 2)
6110  CALL MOLALT  'The MOLALT Subprogram is called here.
6120  AOUT(I%) = AT(I%) * CONVA: OOUT(I%) = OT(I%) * CONVO
6130  FOR J% = 1 TO V%
6140   X(J%, I%, 2) = AQ(J%) / CONVA
6150  NEXT J%
6160  FOR J% = 1 TO 3
6170   Y(J%, I%, 2) = ORG(J%) / CONVO
6180  NEXT J%
6190  X(2, I%, 2) = X(2, I%, 2) * 238!: X(3, I%, 2) = X(3, I%, 2) * 232!
6200  LPRINT USING " ### "; I%;
6210  FOR J% = 1 TO V%
6220   LPRINT USING QQ$; X(J%, I%, 2);
6230  NEXT J%
6240  LPRINT SPACE$(38); : LPRINT USING QQ$; AOUT(I%); : LPRINT USING RR$;
      TPROF(I%, 2)
6250  IF ABS(ALVRT(I%)) < .000001 THEN 6290
6260  PROFLO = CONVA * ALVRT(I%)
6270  LPRINT USING " ### "; I%; : LPRINT "   PRODUCT STREAM";
6280  LPRINT SPACE$(74); : LPRINT USING QQ$; PROFLO: LN% = LN% + 1
6290  LN% = LN% + 1
6300 NEXT I%
6310 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 6330
6320 LPRINT CHR$(12); : LN% = 0
6330 GOSUB 6700  'To set up Thorex organic results chart
6340 FOR I% = 1 TO NTOST%
6350  IF LN% < 55 THEN 6370
6360  LPRINT CHR$(12); : LN% = 0: GOSUB 6700
6370  EXT1(I%) = 0!: EXT2(I%) = 0!: EXT3(I%) = 0!
6380  TSAT(I%) = (2! * Y(2, I%, 2) + 3! * Y(3, I%, 2) + Y(1, I%, 2)) * 100!
      / T
6390  Y(2, I%, 2) = Y(2, I%, 2) * 238!: Y(3, I%, 2) = Y(3, I%, 2) * 232!
6400  IF AOUT(I%) <= .000001 THEN 6460
6410  EXT1(I%) = OOUT(I%) / AOUT(I%)
6420  IF X(2, I%, 2) > 1E-10 THEN EXT2(I%) = EXT1(I%) * Y(2, I%, 2) / X(2,
      I%, 2)
6430  IF X(3, I%, 2) > 1E-10 THEN EXT3(I%) = EXT1(I%) * Y(3, I%, 2) / X(3,
      I%, 2)
6440  IF X(1, I%, 2) > 1E-10 THEN EXT1(I%) = EXT1(I%) * Y(1, I%, 2) / X(1,
      I%, 2)
6450  IF X(1, I%, 2) <= 1E-10 THEN EXT1(I%) = 0!
6460  IF ABS(OLVRT(I%)) < .000001 THEN 6510
6470  PROFLO = OLVRT(I%) * OOUT(I%) / OT(I%)
6480  LPRINT USING " ### "; I%;
```

```
6490  LPRINT "   PRODUCT STREAM"; SPACE$(73);
6500  LPRINT USING QQ$; PROFLO: LN% = LN% + 1
6510  LPRINT USING " ### "; I%;
6520  FOR J% = 1 TO 3
6530   LPRINT USING QQ$; Y(J%, I%, 2);
6540  NEXT J%
6550  LPRINT USING QQ$; EXT2(I%); EXT3(I%); EXT1(I%); : LPRINT SPACE$(12);
      : LPRINT USING QQ$; OOUT(I%); : LPRINT USING RR$; TSAT(I%); : LPRINT
      USING QQ$; CODUM(I%)
6560  IF Y(3, I%, 2) > SQR(4.311727E-02 - 3.317647E-05 * (TPROF(I%, 2) -
      55.03183) ^ 2! + .36719 * (Y(1, I%, 2) - .3455787) ^ 2!) * 232! THEN
      6570 ELSE 6580
6570  LPRINT " *****  3 Phases Possible in the above stage": LN% = LN% + 1
6580  LN% = LN% + 1
6590 NEXT I%
6600 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 6620
6610 LPRINT CHR$(12); : LN% = 0
6620 GOTO 6770
6630 REM Subroutine to set up Thorex aqueous results chart.
6640  LPRINT " AQUEOUS PHASE:"
6650  LPRINT " STAGE  NITRIC ACID    URANIUM      THORIUM    NITRATE ION
      FLOW RATE    TEMP"
6660  LPRINT "  NO.       (M)          (g/L)        (g/L)          (M)
      (L/min)      (C)"
6670  LPRINT " -----  -----------  -----------  -----------  -----------
      -----------  -------"
6680  LN% = LN% + 4
6690 RETURN
6700 REM Subroutine to set up Thorex organic results chart.
6710  LPRINT " ORGANIC PHASE (The indication of 3 phases is within a 10%
      tolerance):"
6720  LPRINT " STAGE  NITRIC ACID    URANIUM      THORIUM     U EXTRACT
      TH EXTRACT   H+ EXTRACT                  FLOW RATE   TBPSAT
      INVENTORY"
6730  LPRINT "  NO.       (M)          (g/L)        (g/L)        FACTOR
      FACTOR       FACTOR                    (L/min)      (%)    CHANGE
      (%)"
6740  LPRINT " -----  -----------  -----------  -----------  -----------  -
      ----------  -----------                -----------  ------  ----------
      -"
6750  LN% = LN% + 4
6760 RETURN
6770 END SUB
```

D.9 Conversion Factor Subprograms (MOLALP and MOLALT)

Statements	Description
MOLALP:	
80- 110	This Subprogram provides factors for conversions between molar and solute-free concentrations (CONV). If the value of TCONC% passed to the Subprogram is -1, the conversion factors

Statements	Description

generated will be used to convert from molar to solute-free values; if +1 the opposite conversion is to be made. The basis for the conversion factors is discussed in Sect. 2.4.

120- 150 For the case where TCONC% = -1, the terms UOS, PUOS, and HOS are developed for use in calculating the term WO, which has to do with the solubility of water in the organic phase.

$$UOS = T / (2 + 0.092\ T) \tag{D.36}$$

$$PUOS = T / (2 + 0.18\ T) \tag{D.37}$$

$$HOS = \frac{T\ [1 - 0.00609\ (3.95 - 0.0144\ TEMP)\ (CTBP)^{1.65}]}{1 + 0.043\ T} \tag{D.38}$$

$$WO = (3.95 - 0.0144\ T)\ (CTBP)^{1.65} \left[1 - \frac{ORG(2)}{UOS} - \frac{ORG(3)}{PUOS} - 0.65\ \frac{ORG(1)}{HOS}\right] \tag{D.39}$$

where T = molar concentration of TBP in the solvent,
TEMP = solution temperature, °C,
CTBP = volume fraction TBP in the solvent,
ORG(1) = Organic nitric acid concentration, M,
ORG(2) = Organic uranium concentration, M, and
ORG(3) = Organic plutonium concentration, M.

Program control then transfers to statement 170.

160 For the case where TCONC% = +1, the term WO is calculated directly.

$$WO = (4.2 - 0.015\ TEMP)\ (CTBP)^{1.69}\ [T - 2\ ORG(2) - 2\ ORG(3) - 0.6\ ORG(1)]\ /\ T \tag{D.40}$$

170- 190 The conversion factors CONVO and CONVA are for the organic and aqueous phases respectively. They are used as shown below.

If TCONC% = -1:

For flow rates: $\text{solute-free units} = \dfrac{\text{molar units}}{\text{CONV}}$

For concentrations:

solute-free units = (molar units) (CONV)

Statements	Description
	If TCONC% = +1:
	For flow rates: molar units = (solute-free units) (CONV)
	For concentrations: $\text{molar units} = \dfrac{\text{solute-free units}}{\text{CONV}}$
	$\text{CONVO} = \left[1 + \text{TCONC\%}\ [0.097\ \text{ORG}(2) + 0.139\ \text{ORG}(3) + 0.043\ \text{ORG}(1) + 0.0174\ \text{WO}]\right]^{\text{TCONC\%}}$ (D.41)
	$\text{CONVA} = \left[1 + \text{TCONC\%}\ [0.0724\ \text{AQ}(2) + 0.13\ \text{AQ}(3) + 0.0309\ \text{AQ}(1) + 0.031\ \text{AQ}(6)]\right]^{\text{TCONC\%}}$ (D.42)
	where AQ(1) = aqueous nitric acid concentration, M, AQ(2) = aqueous uranium concentration, M, and AQ(3) = aqueous plutonium concentration, M.
MOLALT: 5870-5900	No conversion factors have yet been developed for Thorex solutions. Consequently,
	CONVA = 1 (D.43)
	CONVO = 1 (D.44)

D.10 Listing of the Conversion Factor Subprograms (MOLALP and MOLALT)

```
80 SUB MOLALP  'Provides molar/molal conversion factors.
90 SHARED NTOST%, CTBP, NEWOUT%, SPH, IFAST%, IRXN%, DTHETA, IVOLM%,
   IVOLS%, IPRO%, TEMPI, ISOL5%, NSTR%, ISTR%, JSTR%, IPROCE%, LN%, V%,
   PQ$, QQ$, R$, RR$, T, CODUM(), CODUMM()
100 SHARED AQ(), ORG(), TEMP, CONVA, CONVO, TCONC%
110 IF TCONC% = 1 THEN 160
120 UOS = T / (2! + .092 * T): PUOS = T / (2! + .18 * T)
130 HOS = T * (1! - .00609 * (3.95 - .0144 * TEMP) * (CTBP ^ 1.65)) / (1! +
    0.043 * T)
140 WO = (3.95 - .0144 * TEMP) * (CTBP ^ 1.65) * (1! - ORG(2) / UOS -
    ORG(3) / PUOS - .65 * ORG(1) / HOS)
150 GOTO 170
160 WO = (4.2 - .015 * TEMP) * (CTBP ^ 1.69) * (T - 2! * ORG(2) - 2! *
    ORG(3) - .6 * ORG(1)) / T
170 CONVO = (1! + TCONC% * (.097 * ORG(2) + .139 * ORG(3) + .043 * ORG(1) +
    0.0174 * WO)) ^ TCONC%
180 CONVA = (1! + TCONC% * (7.240001E-02 * AQ(2) + .13 * AQ(3) + .0309 *
    AQ(1) + .031 * AQ(6))) ^ TCONC%
```

```
190 END SUB
```

```
5870 SUB MOLALT  'Provides molar/molal conversion factors.
5880 SHARED AQ(), ORG(), TEMP, CONVA, CONVO, TCONC%
5890 CONVA = 1!: CONVO = 1!
5900 END SUB
```

D.11 Chemical Reaction Subprograms (MCHEMP and SCHEMP)

Statements	Description
MCHEMP:	
3410-3500	Chemical reactions occuring in the mixer are considered to take place only at the aqueous-phase composition, but the solute in the organic phase acts to buffer the aqueous-phase concentration. This results from the additional mass transfer that occurs to satisfy equilibrium conditions. Three reaction mechanisms are available for selection through the Problem Definition file, all involve the reduction of Pu(IV) to Pu(III). These mechanisms are discussed in Sect. 2.6. In these initial statements, stoichiometric constants are defined for the reactions.
3510-3610	The total amount of solute in the mixer (SOLAMT) is calculated from mixer phase volumes and concentrations; a pseudo-volume (SOLVOL) is also calculated. The variable RX is set equal to the mixer aqueous solute concentration. Program flow is then routed to statement 4000 if instantaneous reduction of Pu is specified, statement 3860 if Pu reduction by U(IV) is specified, or continues to statement 3620 if Pu reduction by hydroxylamine nitrate is specified.
3620-3850	Reduction by hydroxylamine nitrate. The assumed reaction is: $2\ NH_3OH^+ + 2\ Pu^{4+} = 2\ Pu^{3+} + N_2 + 2\ H_2O + 4\ H^+$ (D.45)
3620-3650	A test is made to see if essential solute concentrations are significant. If not, control transfers to statement 4000 for an instantaneous reduction. Otherwise, the ratio of Pu(IV) to reductant and the total nitrate content are calculated.
3660	The reaction rate constant is calculated using the relationship discussed in Sect. 2.6.3.
3670-3830	The rate equation is integrated by assuming constant acidity and nitrate concentration. The proper root of the equation is localized by a binary search.
3840-3850	The amount of reacted solute is calculated and control is transferred to statement 4060.

Statements	Description
3860-3990	Reduction by U(IV). The assumed reaction is: $2\ Pu^{4+} + U^{4+} + 2\ H_2O = 2\ Pu^{3+} + UO_2^{2+} + 4\ H^+$ (D.46)
3860-3870	A test is made to see if essential solute concentrations are significant. If not, control transfers to statement 4000 for an instantaneous reduction.
3880-3970	The rate equation is integrated assuming a constant nitric acid concentration. The rate constant is described in Sect. 2.6.2.
3980-3990	The amount of reacted solute is calculated and control is transferred to statement 4060.
4000-4050	Instantaneous reduction. The assumed reaction is: $Pu^{4+} + \text{reductant} = Pu^{3+}$ (D.47)
4000-4020	The amount of reacted solute is directly calculated assuming instantaneous conversion.
4030-4050	If the Fast integration technique for mixers is specified, the amount of reacted solute is calculated from solute quantities entering the mixer rather than solute quantities in inventory. Program flow then proceeds to statement 4060.
4060-4100	The amount and concentration of solute in the mixer is adjusted to account for that reacted (but not < 0), and the products from reactions (RXNTRM) are calculated for use in the Fast integration method for mixers.
4110	If the Fast integration method is specified, the Subprogram ends. Otherwise, program flow proceeds to statement 4120.
4120-4300	The UCOR Subprogram is called to obtain new distribution coefficients resulting from post-reaction solute concentrations. Up to 5 trials are allowed for obtaining equilibrium conditions. The Subprogram then ends.
SCHEMP:	
4310-4450	Chemical reactions occuring in the settler are less complicated as no interphase approximations are necessary. Zone concentrations determine the extent of reaction. The same three reaction mechanisms available in Subprogram MCHEMP are available here. In these initial statements, stoichiometric constants are defined for the reactions and the array variables RX and RY are set equal to the settler aqueous and organic solute concentrations in each zone.

Statements	Description
4460	Program flow is routed to statement 4850 if instantaneous reduction of Pu is specified, statement 4710 if Pu reduction by U(IV) is specified, or continues to statement 4470 if Pu reduction by hydroxylamine nitrate is specified.
4470-4500	Reduction by hydroxylamine nitrate. This is handled in the same manner as for reaction in the mixer. A test is made to see if essential solute concentrations are significant. If not, control transfers to statement 4850 for an instantaneous reduction. Otherwise, the ratio of Pu(IV) to reductant and the total nitrate content are calculated.
4510	The reaction rate constant is calculated using the relationship discussed in Sect. 2.6.3.
4520-4680	The rate equation is integrated by assuming constant acidity and nitrate concentration. The proper root of the equation is localized by a binary search.
4690-4700	The amount of reacted solute is calculated and control is transferred to statement 4890.
4710-4720	Reduction by U(IV). This is handled in the same manner as for reaction in the mixer. A test is made to see if essential solute concentrations are significant. If not, control transfers to statement 4850 for an instantaneous reduction.
4730-4820	The rate equation is integrated assuming a constant nitric acid concentration. The rate constant is described in Sect. 2.6.2.
4830-4840	The amount of reacted solute is calculated and control is transferred to statement 4890.
4850-4880	Instantaneous reduction. The amount of reacted solute is directly calculated assuming instantaneous conversion. Program flow then proceeds to statement 4890.
4890-4970	The concentrations of solute in the settler zones are adjusted to account for that reacted (but not < 0), and the Subprogram ends.

D.12 Listing of Chemical Reaction Subprograms (MCHEMP and SCHEMP)

```
3410 SUB MCHEMP (J%, AQVOL!, ORVOL!) 'Handles chemical reactions in the
     mixers.
```

```
3420 SHARED NTOST%, CTBP, NEWOUT%, SPH, IFAST%, IRXN%, DTHETA, IVOLM%,
     IVOLS%, IPRO%, TEMPI, ISOL5%, NSTR%, ISTR%, JSTR%, IPROCE%, LN%, V%,
     PQ$, QQ$, R$, RR$, T, CODUM(), CODUMM()
3430 SHARED TPROF(), ATS(), OTS()
3440 SHARED TEMPC, ARY(), DTRY()
3450 SHARED X(), Y(), XS(), YS()
3460 SHARED RXNTRM(), AIN(), OIN()
3470 DIM RX(6), SOLAMT(6), SOLVOL(6), STOIC(6, 3)
3480 STOIC(1, 2) = 2!: STOIC(1, 3) = 2!: STOIC(2, 2) = .5: STOIC(3, 1) = -
     1!
3490 STOIC(3, 2) = -1!: STOIC(3, 3) = -1!: STOIC(4, 1) = 1!: STOIC(4, 2) =
     1!
3500 STOIC(4, 3) = 1!: STOIC(5, 1) = -1!: STOIC(5, 2) = -.5: STOIC(5, 3) =
     -1!
3510 FOR I% = 1 TO 3
3520  SOLAMT(I%) = AQVOL * X(I%, J%, 2) + ORVOL * Y(I%, J%, 2)
3530  SOLVOL(I%) = AQVOL + DTRY(I%) * ORVOL
3540  RX(I%) = X(I%, J%, 2)
3550 NEXT I%
3560 FOR I% = 4 TO 6
3570  SOLAMT(I%) = AQVOL * X(I%, J%, 2)
3580  SOLVOL(I%) = AQVOL
3590  RX(I%) = X(I%, J%, 2)
3600 NEXT I%
3610 ON IRXN% GOTO 4000, 3860, 3620
3620 REM Reduction by hydroxylamine nitrate.
3630 IF RX(1) < 1E-10 OR RX(3) < 1E-10 OR RX(5) < 1E-10 THEN 4000
3640 FOR1# = SOLAMT(3) / SOLAMT(5)
3650 TOTNIT = RX(1) + 2! * RX(2) + 4! * RX(3) + 3! * RX(4) + RX(6) + .33
3660 RK# = (1.74 * EXP(31000! / 1.987 * (1! / 303.16 - 1! / (273.16 +
     TPROF(J%, 2))))) * RX(3) * DTHETA * (RX(5) / (RX(1) * RX(1) * TOTNIT))
     ^ 2!
3670 IF (1! / FOR1#) < 1! THEN EXTMAX = 1! / FOR1# ELSE EXTMAX = 1!
3680 EXTINC# = .25 * EXTMAX: EXTENT# = .5 * EXTMAX: B# = SOLAMT(3) /
     SOLVOL(4)
3690 A# = RX(4) + B#: AA# = A# * A#: BB# = A# * B#: CC# = B# * B#
3700 FOR I% = 1 TO 25
3710  A# = 1! / (1! - EXTENT#)
3720  IF FOR1# > .01# THEN 3750
3730  AMTINT# = AA# * A# * EXTENT# - 2! * BB# * LOG(A#) + CC# * EXTENT#
3740  GOTO 3800
3750  IF ABS(1# - FOR1#) < .01# THEN 3790
3760  B# = 1# - FOR1# * EXTENT#: C# = 1# / (1# - FOR1#)
3770  AMTINT# = -(FOR1# - A# * EXTENT# - FOR1# / B# + 2! * C# * FOR1# *
      LOG(A# * B#)) * AA# * C# * C# + 2! * BB# * C# * (FOR1# * EXTENT# / B#
      - C# * LOG(A# * B#)) + CC# * EXTENT# / B#
3780  GOTO 3800
3790  AMTINT# = AA# * (A# ^ 3! - 1!) / 3! - BB# * (A# ^ 2! - 1!) + CC# *
      (A# - 1!)
3800  IF AMTINT# > RK# THEN EXTENT1# = EXTENT# - EXTINC#
3810  IF AMTINT# < RK# THEN EXTENT1# = EXTENT# + EXTINC#
3820  EXTINC# = EXTINC# / 2#: EXDIF# = (EXTENT1# - EXTENT#) / EXTENT#:
      EXTENT# = EXTENT1#
3825  IF ABS(EXDIF#) < .00001# THEN 3840
3830 NEXT I%
```

```
3840 RXNAMT = EXTENT# * SOLAMT(3)
3850 GOTO 4060
3860 REM Reduction by U(IV).
3870 IF RX(3) < 1E-10 OR RX(5) < 1E-10 THEN 4000
3880 W = 1! - .5 ^ (6! * DTHETA): WW = 2! * SOLAMT(5) / SOLAMT(3)
3890 IF W > WW THEN 3910
3900 IF W <= 1! THEN EXTMAX = W: GOTO 3920 ELSE EXTMAX = 1!: GOTO 3920
3910 IF WW <= 1! THEN EXTMAX = WW ELSE EXTMAX = 1!
3920 RK = 170! * DTHETA * RX(5): RCU = SOLAMT(3) / (2! * SOLAMT(5))
3930 RHO = RX(1) * RX(1): REXP = 1E+30
3940 IF (RK * (1! - RCU)) < (70! * RHO) THEN REXP = EXP(RK * (1! - RCU) /
     RHO)
3950 EXTENT = RK / (RK + RHO)
3960 IF ABS(1! - RCU) > .05 THEN EXTENT = (1! - REXP) / (RCU - REXP)
3970 IF EXTENT > EXTMAX THEN EXTENT = EXTMAX
3980 RXNAMT = SOLAMT(3) * EXTENT
3990 GOTO 4060
4000 REM Instantaneous reduction.
4010 W = -SOLAMT(3) / STOIC(3, IRXN%): WW = -SOLAMT(5) / STOIC(5, IRXN%)
4020 IF W < WW THEN RXNAMT = W ELSE RXNAMT = WW
4030 IF IFAST% <> 2 THEN 4060
4040 W = -(AIN(3) + OIN(3)) / STOIC(3, IRXN%): WW = -AIN(5) / STOIC(5,
     IRXN%)
4050 IF W < WW THEN RXNAMT = DTHETA * W ELSE RXNAMT = DTHETA * WW
4060 FOR I% = 1 TO 6
4070  SOLAMT(I%) = SOLAMT(I%) + RXNAMT * STOIC(I%, IRXN%)
4080  IF SOLAMT(I%) < 0! THEN SOLAMT(I%) = 0!
4090  ARY(I%) = SOLAMT(I%) / SOLVOL(I%): RXNTRM(I%, J%) = RXNAMT *
      STOIC(I%, IRXN%) / DTHETA
4100 NEXT I%
4110 IF IFAST% = 2 THEN 4300
4120 FOR ITRY% = 1 TO 5
4130  ICK% = 0
4140  CALL UCORPU  'The UCORPU Subprogram is called here.
4150  FOR I% = 1 TO 3
4160   X(I%, J%, 2) = SOLAMT(I%) / (AQVOL + DTRY(I%) * ORVOL)
4170   IF ABS(X(I%, J%, 2) - ARY(I%)) > (.0001 * X(I%, J%, 2)) THEN ICK% =
       1
4180   ARY(I%) = X(I%, J%, 2)
4190   IF X(I%, J%, 2) <= 1E-20 THEN X(I%, J%, 2) = 0!
4200   Y(I%, J%, 2) = X(I%, J%, 2) * DTRY(I%)
4210  NEXT I%
4220  FOR I% = 4 TO V%
4230   X(I%, J%, 2) = SOLAMT(I%) / AQVOL
4240   IF ABS(X(I%, J%, 2) - ARY(I%)) > (.0001 * X(I%, J%, 2)) THEN ICK% =
       1
4250   ARY(I%) = X(I%, J%, 2)
4260   IF X(I%, J%, 2) <= 1E-20 THEN X(I%, J%, 2) = 0!
4270  NEXT I%
4280  IF ICK% = 0 THEN 4300
4290 NEXT ITRY%
4300 END SUB
```

```
4310 SUB SCHEMP (J%, AQSVOL!, ORSVOL!)  'Handles chemical reactions in the
     settlers.
```

```
4320 SHARED NTOST%, CTBP, NEWOUT%, SPH, IFAST%, IRXN%, DTHETA, IVOLM%,
     IVOLS%, IPRO%, TEMPI, ISOL5%, NSTR%, ISTR%, JSTR%, IPROCE%, LN%, V%,
     PQ$, QQ$, R$, RR$, T, CODUM(), CODUMM()
4330 SHARED TPROF(), ATS(), OTS()
4340 SHARED X(), Y(), XS(), YS()
4350 DIM RX(6), RY(3), STOICX(6, 3)
4360 FOR KZ% = 1 TO 3
4370  FOR I% = 1 TO 6
4380   RX(I%) = XS(J%, KZ%, I%, 2)
4390  NEXT I%
4400  FOR I% = 1 TO 3
4410   RY(I%) = YS(J%, KZ%, I%, 2)
4420  NEXT I%
4430  STOICX(1, 2) = 2!: STOICX(1, 3) = 2!: STOICX(2, 2) = .5: STOICX(3, 1)
      = -1!
4440  STOICX(3, 2) = -1!: STOICX(3, 3) = -1!: STOICX(4, 1) = 1!: STOICX(4,
      2) = 1!
4450  STOICX(4, 3) = 1!: STOICX(5, 1) = -1!: STOICX(5, 2) = -.5: STOICX(5,
      3) = -1!
4460  ON IRXN% GOTO 4850, 4710, 4470
4470 REM Reduction by hydroxylamine nitrate.
4480  IF RX(1) < 1E-10 OR RX(3) < 1E-10 OR RX(5) < 1E-10 THEN 4850
4490  FOR1# = RX(3) / RX(5)
4500  TOTNIT = RX(1) + 2! * RX(2) + 4! * RX(3) + 3! * RX(4) + RX(6) + .33#
4510  RK# = (1.74 * EXP(31000! / 1.987 * (1! / 303.16 - 1! / (273.16 +
      TPROF(J%, 2))))) * RX(3) * DTHETA * (RX(5) / (RX(1) * RX(1) *
      TOTNIT)) ^ 2!
4520  IF (1! / FOR1#) < 1! THEN EXTMAX = 1! / FOR1# ELSE EXTMAX = 1!
4530  EXTINC# = .25 * EXTMAX: EXTENT# = .5 * EXTMAX: B# = RX(3): A# = RX(4)
      + B#
4540  AA# = A# * A#: BB# = A# * B#: CC# = B# * B#
4550  FOR I% = 1 TO 25
4560   A# = 1! / (1! - EXTENT#)
4570   IF FOR1# > .01# THEN 4600
4580   AMTINT# = AA# * A# * EXTENT# - 2! * BB# * LOG(A#) + CC# * EXTENT#
4590   GOTO 4650
4600   IF ABS(1# - FOR1#) < .01# THEN 4640
4610   B# = 1# - FOR1# * EXTENT#: C# = 1# / (1# - FOR1#)
4620   AMTINT# = -(FOR1# - A# * EXTENT# - FOR1# / B# + 2! * C# * FOR1# *
       LOG(A# * B#)) * AA# * C# * C# + 2! * BB# * C# * (FOR1# * EXTENT# /
       B# - C# * LOG(A# * B#)) + CC# * EXTENT# / B#
4630   GOTO 4650
4640   AMTINT# = AA# * (A# ^ 3! - 1!) / 3! - BB# * (A# ^ 2! - 1!) + CC# *
       (A# - 1!)
4650   IF AMTINT# > RK# THEN EXTENT1# = EXTENT# - EXTINC#
4660   IF AMTINT# < RK# THEN EXTENT1# = EXTENT# + EXTINC#
4670   EXTINC# = EXTINC# / 2#: EXDIF# = (EXTENT1# - EXTENT#) / EXTENT#:
       EXTENT# = EXTENT1#
4675   IF ABS(EXDIF#) < .00001# THEN 4690
4680  NEXT I%
4690  DELX = RX(3) * EXTENT#: DELY = 0!
4700  GOTO 4890
4710 REM Reduction by U(IV).
4720  IF RX(3) < 1E-10 OR RX(5) < 1E-10 THEN 4850
4730  W = 1! - .5 ^ (6! * DTHETA): WW = 2! * RX(5) / RX(3)
```

```
4740  IF W > WW THEN 4760
4750  IF W <= 1! THEN EXTMAX = W: GOTO 4770 ELSE EXTMAX = 1!: GOTO 4770
4760  IF WW <= 1! THEN EXTMAX = WW ELSE EXTMAX = 1!
4770  RK = 170! * DTHETA * RX(5): RCU = RX(3) / (2! * RX(5))
4780  RHO = RX(1) * RX(1): REXP = 1E+30
4790  IF (RK * (1! - RCU)) < (70! * RHO) THEN REXP = EXP(RK * (1! - RCU) /
      RHO)
4800  EXTENT = RK / (RK + RHO)
4810  IF ABS(1! - RCU) > .05 THEN EXTENT = (1! - REXP) / (RCU - REXP)
4820  IF EXTENT > EXTMAX THEN EXTENT = EXTMAX
4830  DELX = RX(3) * EXTENT: DELY = 0!
4840  GOTO 4890
4850 REM Instantaneous reduction.
4860  W = -RX(3) / STOICX(3, IRXN%): WW = -RX(5) / STOICX(5, IRXN%)
4870  IF W < WW THEN DELX = W ELSE DELX = WW
4880  DELY = 0!
4890  FOR I% = 1 TO 6
4900   XS(J%, KZ%, I%, 2) = XS(J%, KZ%, I%, 2) + STOICX(I%, IRXN%) * DELX
4910   IF XS(J%, KZ%, I%, 2) <= 1E-20 THEN XS(J%, KZ%, I%, 2) = 0!
4920  NEXT I%
4930  FOR I% = 1 TO 3
4940   IF YS(J%, KZ%, I%, 2) <= 1E-20 THEN YS(J%, KZ%, I%, 2) = 0!
4950  NEXT I%
4960 NEXT KZ%
4970 END SUB
```

APPENDIX E
SECOM.BI—THE "INCLUDE" FILE

The Main Module (SECALC.BAS) and the Secondary Module (SECAL1.BAS) Basic programs are compiled and linked using Microsoft QuickBASIC, Version 4.0, to produce a directly executable file (SECALC.EXE). The following "Include" file is required for the linking step.

E.1 Listing of File SECOM.BI (The "Include" File for SECALC)

```
DECLARE SUB MOLALP ()
DECLARE SUB MOLALT ()
DECLARE SUB UCORPU ()
DECLARE SUB UCORTH ()
DECLARE SUB STAGES (NDIREC%)
DECLARE SUB MCHEMP (J%, AQVOL!, ORVOL!)
DECLARE SUB SCHEMP (J%, AQSVOL!, ORSVOL!)
DECLARE SUB PRTPU ()
DECLARE SUB PRTTH ()
COMMON /CONTR1/ NTOST%, CTBP, NEWOUT%, SPH, IFAST%, IRXN%, DTHETA, IVOLM%,
       IVOLS%, IPRO%, TEMPI, ISOL5%, NSTR%, ISTR%, JSTR%, IPROCE%, LN%, V%,
       PQ$, QQ$, R$, RR$, T, CODUM(), CODUMM()
COMMON /TEMPS/ TPROF(), ATS(), OTS()
COMMON /DISTRB/ TEMPC, ARY(), DTRY()
COMMON /CONCS/ X(), Y(), XS(), YS()
COMMON /FLOWS/ ANET(), ONET(), AT(), OT()
COMMON /STREAM/ XFD(), YFD(), AFDRT(), OFDRT(), AFDTEM(), OFDTEM(),
       ALVRT(), OLVRT()
COMMON /VOLS/ AVOL(), OVOL(), ASVOL(), OSVOL()
COMMON /MOLALC/ AQ(), ORG(), TEMP, CONVA, CONVO, TCONC%
COMMON /RXNS/ RXNTRM(), AIN(), OIN()
COMMON /CONTR2/ ADEN(), ODEN(), AOUT(), OOUT(), EXT1(), EXT2(), EXT3(),
       TSAT()
```

APPENDIX F
SEPRNT.BAS—THE PROBLEM PRINTING PROGRAM

```
10 REM PROGRAM SEPRNT -- Solvent Extraction Process Having Interacting
   Solutes -- Printing of Problem Final Result
20 REM $DYNAMIC
30 WIDTH "scrn:", 80
40 SCREEN 0, 1, 0, 0
50 KEY OFF: CLS
60 R1% = 1: C1% = 1: R2% = 23: C2% = 79: GOSUB 2970  'To draw double box
70 R1% = 10: C1% = 25: R2% = 14: C2% = 55: GOSUB 3110  'To draw single box
80 FOR I% = 1 TO 24
90  LOCATE 10, I%: PRINT CHR$(196);
100 NEXT I%
110 FOR I% = 56 TO 78
120  LOCATE 10, I%: PRINT CHR$(196);
130 NEXT I%
140 LOCATE 10, 1: PRINT CHR$(199);
150 LOCATE 10, 25: PRINT CHR$(194);
160 LOCATE 10, 55: PRINT CHR$(194);
170 LOCATE 10, 79: PRINT CHR$(182); : COLOR 0, 7
180 LOCATE 3, 29: PRINT "PC - S E P H I S - MOD4"; : COLOR 7, 0
190 LOCATE 4, 31: PRINT "Version 2.11 (1990)";
200 LOCATE 6, 13: PRINT "A Solvent Extraction Process Having Interacting
    Solutes";
210 LOCATE 8, 17: PRINT "For Uranium, Plutonium, Thorium, and Nitric Acid";
220 LOCATE 9, 16: PRINT "Mass Transfer in Purex- or Thorex-type
    Flowsheets";
230 LOCATE 11, 34: PRINT "W.S. Groenier";
240 LOCATE 12, 30: PRINT "Fuel Recycle Division";
250 LOCATE 13, 26: PRINT "Oak Ridge National Laboratory"; : COLOR 0, 7
260 LOCATE 17, 26: PRINT "*** PROBLEM PRINTING ONLY ***"; : COLOR 7, 0
265 LOCATE 19, 17: PRINT "Problem Definition and Results files are needed";
266 LOCATE 20, 20: PRINT "Choose the location for these files below";
270 LOCATE 24, 1: INPUT ; "Do you want to continue (Y/N)? ", REPLY$
280 IF REPLY$ <> "Y" THEN CLS : GOTO 2670
290 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
295 INPUT ; "Will the files be on a diskette (Y/N)? ", REPLY$
296 IF REPLY$ <> "Y" THEN 320
297 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 24, 1
300 PRINT "Insert diskette -- Press any key to continue.";
310 K$ = INKEY$: IF K$ = "" THEN 310
320 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 25, 1: PRINT SPACE$(79); :
    LOCATE 24, 1
330 PRINT "Enter Drive (Path) and FILENAME of Problem Definition data
    file.";
335 LOCATE 25, 1: INPUT ; "Make your entry here. ", DATFIL1$
```

```
340 LOCATE 24, 1: PRINT SPACE$(79); : LOCATE 25, 1: PRINT SPACE$(79); :
    LOCATE 24, 1
350 PRINT "Enter Drive (Path) and FILENAME of Problem Results data file.";
354 LOCATE 25, 1: INPUT ; "Make your entry here. ", DATFIL2$
355 DATFIL1$ = DATFIL1$ + ".DAT"
356 DATFIL2$ = DATFIL2$ + ".DAT"
360 CLS : P$ = "###.#": Q$ = "####.##": PP$ = "###.##": PQ$ = "
    ##.##^^^^": R$ = "     ###.#": RR$ = "    ###.#": QQ$ = "    ##.##^^^^":
    PPP$ = "###.####"
380 ON ERROR GOTO 3670
390 OPEN DATFIL1$ FOR INPUT AS #1
400 OPEN DATFIL2$ FOR INPUT AS #2
410 LOCATE 15, 1: PRINT "Have printer ON and READY -- Then press any key.";
420 K$ = INKEY$: IF K$ = "" THEN 420
430 CLS
440 ON ERROR GOTO 3760: LPRINT CHR$(15);
450 WIDTH "lpt1:", 135
460 INPUT #1, DAT1$, TIM1$
470 INPUT #1, TITLE$, NTOST%, CTBP, TEMPI, NSTR%, ISTR%, JSTR%, IRXN%,
    IPROCE%, DTHETA, DPRINT%, TSTOP%, TOL, NEWOUT%, IVOLM%, IVOLS%, IPRO%,
    IFAST%
480 DIM CON(6), X(6, NTOST%), Y(3, NTOST%), ADEN(NTOST%), AOUT(NTOST%),
    TPROF(NTOST%), EXT1(NTOST%), EXT2(NTOST%), EXT3(NTOST%), ODEN(NTOST%),
    OOUT(NTOST%), TSAT(NTOST%), CODUM(NTOST%)
490 LPRINT "PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11:";
    SPACE$(63); DAT1$; " "; TIM1$
500 LPRINT : LPRINT "     Problem:  "; TITLE$
510 LPRINT
520 IF IPROCE% = 0 THEN LPRINT SPACE$(10); "PUREX PROCESS."
530 IF IPROCE% = 1 THEN LPRINT SPACE$(10); "THOREX PROCESS."
540 LPRINT SPACE$(10); "Total stages:  "; NTOST%
550 LPRINT SPACE$(10); "Volume % TBP in solvent:  "; : LPRINT USING P$;
    CTBP * 100!
560 LPRINT SPACE$(10); "Initial or default temperature ("; CHR$(248); "C):
    ";
570 LPRINT USING P$; TEMPI
580 IF NSTR% = 0 THEN LPRINT SPACE$(10); "No unusual stage connections"
590 IF NSTR% = 1 THEN LPRINT SPACE$(10); "Organic taken from stage ";
    ISTR%; " feeds stage "; JSTR%; "."
600 IF IPROCE% = 1 THEN 660
610 ON (IRXN% + 1) GOTO 620, 630, 640, 650
620 LPRINT SPACE$(10); "No Plutonium reaction.": GOTO 660
630 LPRINT SPACE$(10); "Instantaneous reduction of Pu(IV).": GOTO 660
640 LPRINT SPACE$(10); "Reduction of Pu(IV) by U(IV).": GOTO 660
650 LPRINT SPACE$(10); "Reduction of Pu(IV) by hydroxylamine nitrate."
660 LPRINT SPACE$(10); "Minutes per time increment:  "; : LPRINT USING Q$;
    DTHETA
670 LPRINT SPACE$(10); "Minutes between printing of the concentration
    profile:  "; : LPRINT USING "####"; DPRINT%
680 LPRINT SPACE$(10); "Calculations will stop after ";
690 LPRINT USING "####"; TSTOP%;
700 LPRINT " minutes or when a tolerance of ";
710 LPRINT USING PPP$; TOL;
720 LPRINT " % per minute is reached."
730 ON IVOLM% GOTO 740, 750, 760
```

```
740 LPRINT SPACE$(10); "Mixer volumes are defined for each phase.": GOTO
    770
750 LPRINT SPACE$(10); "Total mixer volumes are defined (phase ratios =
    flow ratios).": GOTO 770
760 LPRINT SPACE$(10); "Mixer volumes = (phase flow)(unit time)."
770 ON IVOLS% GOTO 780, 790, 800
780 LPRINT SPACE$(10); "Settler volumes are defined for each phase.": GOTO
    810
790 LPRINT SPACE$(10); "Total settler volumes are defined (phase ratios =
    flow ratios).": GOTO 810
800 LPRINT SPACE$(10); "Settler volumes = (phase flow)(unit time)."
810 ON (IPRO% + 1) GOTO 820, 830, 840
820 LPRINT SPACE$(10); "Initial concentration profile is zero.": GOTO 850
830 LPRINT SPACE$(10); "Initial concentration profile is defined.": GOTO
    850
840 LPRINT SPACE$(10); "Initial concentration profile is from a previous
    problem."
850 ON (IFAST% + 1) GOTO 860, 870, 880
860 LPRINT SPACE$(10); "Runge-Kutta integration will be used.": GOTO 890
870 LPRINT SPACE$(10); "Trapezoidal integration will be used.": GOTO 890
880 LPRINT SPACE$(10); "Fast integration will be used."
890 IF NEWOUT% = 0 THEN LPRINT SPACE$(10); "No extra product streams."
900 IF NEWOUT% = 1 THEN LPRINT SPACE$(10); "Extra product stream(s)."
910 LPRINT : LPRINT SPACE$(10); "The FILESPEC for this Problem Definition
    data file is:  "; DATFIL1$
920 LPRINT SPACE$(10); "The FILESPEC for this Problem Results data file is:
    "; DATFIL2$: LPRINT
930 LPRINT "FEED AND PRODUCT STREAM DATA:"
940 LN% = 23
950 IF IPROCE% = 0 THEN GOSUB 3250  'To set up Purex feed & product chart
960 IF IPROCE% = 1 THEN GOSUB 3310  'To set up Thorex feed & product chart
970 INPUT #1, NST%, JHAS%, FDRT
980 IF JHAS% = 0 THEN V% = 3 ELSE IF IPROCE% = 0 THEN V% = 6 ELSE V% = 4
990 FOR I% = 1 TO V%
1000  INPUT #1, CON(I%)
1010 NEXT I%
1020 INPUT #1, TEMP, INDEX%
1030 IF JHAS% = 1 THEN LPRINT SPACE$(8); "AQUEOUS ";
1040 IF JHAS% = 0 THEN LPRINT SPACE$(4); : LPRINT USING P$; CTBP * 100!; :
     LPRINT " % TBP ";
1050 LPRINT USING "###"; NST%;
1060 FOR I% = 1 TO V%
1070  LPRINT USING PQ$; CON(I%);
1080 NEXT I%
1090 IF V% = 3 THEN LPRINT SPACE$(42);
1100 IF V% = 4 THEN LPRINT SPACE$(28);
1110 LPRINT USING PQ$; FDRT;
1120 LPRINT USING R$; TEMP
1130 LN% = LN% + 1
1140 IF INDEX% <> 1 THEN 1170
1150 IF LN% < 55 THEN 970
1160 LPRINT CHR$(12); : LN% = 0: GOTO 950
1170 IF NEWOUT% <> 1 THEN 1310
1180 IF LN% < 55 THEN 1220
1190 LPRINT CHR$(12); : LN% = 0
```

```
1200 IF IPROCE% = 0 THEN GOSUB 3250  'To set up Purex feed & product chart
1210 IF IPROCE% = 1 THEN GOSUB 3310  'To set up Thorex feed & product chart
1220 INPUT #1, NST%, JHAS%, OTRT, INDEX%
1230 IF JHAS% = 1 THEN LPRINT SPACE$(8); "AQUEOUS ";
1240 IF JHAS% = 0 THEN LPRINT SPACE$(8); "ORGANIC ";
1250 LPRINT USING "###"; NST%;
1260 LPRINT "      Product stream removed (actual flow rate to be
     computed)";
1270 LPRINT SPACE$(22); : LPRINT USING PQ$; OTRT
1280 LN% = LN% + 1
1290 IF INDEX% <> 1 THEN 1310
1300 IF LN% >= 55 THEN 1190 ELSE 1220
1310 IF IPRO% = 0 THEN 1720
1320 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 1340
1330 LPRINT CHR$(12); : LN% = 0
1340 LPRINT "INITIAL AQUEOUS PROFILE DATA:": LN% = LN% + 1
1350 IF IPROCE% = 0 THEN GOSUB 3370: V% = 6  'To set up Purex aqueous
     profile chart
1360 IF IPROCE% = 1 THEN GOSUB 3430: V% = 4  'To set up Thorex aqueous
     profile chart
1370 FOR I% = 1 TO NTOST%
1380  IF LN% < 55 THEN 1420
1390  LPRINT CHR$(12); : LN% = 0
1400  IF IPROCE% = 0 THEN GOSUB 3370  'To set up Purex aqueous profile
      chart
1410  IF IPROCE% = 1 THEN GOSUB 3430  'To set up Thorex aqueous profile
      chart
1420  FOR J% = 1 TO V%
1430   INPUT #1, CON(J%)
1440  NEXT J%
1450  INPUT #1, TEMP
1460  LPRINT SPACE$(16); : LPRINT USING "###"; I%;
1470  FOR J% = 1 TO V%
1480   LPRINT USING PQ$; CON(J%);
1490  NEXT J%
1500  IF V% = 6 THEN LPRINT SPACE$(14);
1510  IF V% = 4 THEN LPRINT SPACE$(42);
1520  LPRINT USING R$; TEMP
1530  LN% = LN% + 1
1540 NEXT I%
1550 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 1570
1560 LPRINT CHR$(12); : LN% = 0
1570 LPRINT "INITIAL ORGANIC PROFILE DATA:": LN% = LN% + 1
1580 IF IPROCE% = 0 THEN GOSUB 3550  'To set up Purex organic profile chart
1590 IF IPROCE% = 1 THEN GOSUB 3610  'To set up Thorex organic profile
     chart
1600 FOR I% = 1 TO NTOST%
1610  IF LN% < 55 THEN 1650
1620  LPRINT CHR$(12); : LN% = 0
1630  IF IPROCE% = 0 THEN GOSUB 3550  'To set up Purex organic profile
      chart
1640  IF IPROCE% = 1 THEN GOSUB 3610  'To set up Thorex organic profile
      chart
1650  FOR J% = 1 TO 3
1660   INPUT #1, CON(J%)
```

```
1670  NEXT J%
1680  LPRINT SPACE$(16); : LPRINT USING "###"; I%;
1690  LPRINT USING PQ$; CON(1); CON(2); CON(3)
1700  LN% = LN% + 1
1710 NEXT I%
1720 IF IVOLM% = 3 THEN 1930
1730 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 1750
1740 LPRINT CHR$(12); : LN% = 0
1750 LPRINT "MIXER VOLUME DATA (L):": LN% = LN% + 1
1760 GOSUB 3490  'To set up volume chart
1770 PX% = 0
1780 INPUT #1, NST%, VOLA, VOLO, INDEX%
1790 NS% = NST%: VLA = VOLA: VLO = VOLO: IDEX% = INDEX%
1800 IF IVOLM% <> 1 THEN 1830
1810 LPRINT SPACE$(16); : LPRINT USING "###"; NS%;
1820 LPRINT USING PQ$; VLA; VLO: GOTO 1850
1830 LPRINT SPACE$(16); : LPRINT USING "###"; NS%;
1840 LPRINT SPACE$(28); : LPRINT USING PQ$; VLA
1850 LN% = LN% + 1
1860 IF LN% < 55 THEN 1880
1870 IF NS% = NTOST% THEN 1930 ELSE LPRINT CHR$(12); : LN% = 0: GOSUB 3490
1880 IF PX% = 1 THEN 1910
1890 IF IDEX% <> 1 THEN 1920
1900 INPUT #1, NST%, VOLA, VOLO, INDEX%
1910 IF NST% = NS% + 1 THEN PX% = 0: GOTO 1790 ELSE NS% = NS% + 1: PX% = 1:
     GOTO 1800
1920 IF NS% <> NTOST% THEN NS% = NS% + 1: GOTO 1800
1930 IF IVOLS% = 3 THEN 2140
1940 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 1960
1950 LPRINT CHR$(12); : LN% = 0
1960 LPRINT "SETTLER VOLUME DATA (L):": LN% = LN% + 1
1970 GOSUB 3490  'To set up volume chart
1980 PX% = 0
1990 INPUT #1, NST%, VOLA, VOLO, INDEX%
2000 NS% = NST%: VLA = VOLA: VLO = VOLO: IDEX% = INDEX%
2010 IF IVOLS% <> 1 THEN 2040
2020 LPRINT SPACE$(16); : LPRINT USING "###"; NS%;
2030 LPRINT USING PQ$; VLA; VLO: GOTO 2060
2040 LPRINT SPACE$(16); : LPRINT USING "###"; NS%;
2050 LPRINT SPACE$(28); : LPRINT USING PQ$; VLA
2060 LN% = LN% + 1
2070 IF LN% < 55 THEN 2090
2080 IF NS% = NTOST% THEN 2140 ELSE LPRINT CHR$(12); : LN% = 0: GOSUB 3490
2090 IF PX% = 1 THEN 2120
2100 IF IDEX% <> 1 THEN 2130
2110 INPUT #1, NST%, VOLA, VOLO, INDEX%
2120 IF NST% = NS% + 1 THEN PX% = 0: GOTO 2000 ELSE NS% = NS% + 1: PX% = 1:
     GOTO 2010
2130 IF NS% <> NTOST% THEN NS% = NS% + 1: GOTO 2010
2140 LPRINT CHR$(12);
2150 INPUT #2, TITLE$
2160 INPUT #2, DAT2$, TIM2$, TOTIME
2170 LPRINT "PROBLEM RESULTS FOR SEPHIS MOD4, Ver. 2.11:"; SPACE$(71);
     DAT2$; " "; TIM2$
```

```
2180 LPRINT : LPRINT "     Problem:  "; TITLE$: LPRINT : LPRINT "
     (mixer concentrations shown)"
2190 LPRINT : LPRINT "TIME = "; : LPRINT USING Q$; TOTIME; : LPRINT "
     MINUTES"
2200 LN% = 5
2210 IF IPROCE% = 0 THEN GOSUB 2690: V% = 6  'To set up Purex aqueous
     results chart
2220 IF IPROCE% = 1 THEN GOSUB 2760: V% = 4  'To set up Thorex aqueous
     results chart
2230 FOR I% = 1 TO NTOST%
2240  INPUT #2, J%, X(1, J%), X(2, J%), X(3, J%), Y(1, J%), Y(2, J%), Y(3,
      J%), X(4, J%), X(5, J%), X(6, J%), ADEN(J%), AOUT(J%), TPROF(J%),
      EXT2(J%), EXT3(J%), EXT1(J%), ODEN(J%), OOUT(J%), TSAT(J%), CODUM(J%)
2250 NEXT I%
2260 FOR I% = 1 TO NTOST%
2270  IF LN% < 55 THEN 2310
2280  LPRINT CHR$(12); : LN% = 0
2290  IF IPROCE% = 0 THEN GOSUB 2690  'To set up Purex aqueous results
      chart
2300  IF IPROCE% = 1 THEN GOSUB 2760  'To set up Thorex aqueous results
      chart
2310  LPRINT USING " ### "; I%;
2320  FOR J% = 1 TO V%
2330   LPRINT USING QQ$; X(J%, I%);
2340  NEXT J%
2350  IF IPROCE% = 0 THEN LPRINT USING QQ$; ADEN(I%); AOUT(I%); : LPRINT
      USING RR$; TPROF(I%)
2360  IF IPROCE% = 1 THEN LPRINT SPACE$(38); : LPRINT USING QQ$; AOUT(I%);
      : LPRINT USING RR$; TPROF(I%)
2370  LN% = LN% + 1
2380 NEXT I%
2390 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 2410
2400 LPRINT CHR$(12); : LN% = 0
2410 IF IPROCE% = 0 THEN GOSUB 2830  'To set up Purex organic results chart
2420 IF IPROCE% = 1 THEN GOSUB 2900  'To set up Thorex organic results
     chart
2430 FOR I% = 1 TO NTOST%
2440  IF LN% < 55 THEN 2480
2450  LPRINT CHR$(12); : LN% = 0
2460  IF IPROCE% = 0 THEN GOSUB 2830  'To set up Purex organic results
      chart
2470  IF IPROCE% = 1 THEN GOSUB 2900  'To set up Thorex organic results
      chart
2480  LPRINT USING " ### "; I%;
2490  FOR J% = 1 TO 3
2500   LPRINT USING QQ$; Y(J%, I%);
2510  NEXT J%
2520  IF IPROCE% = 0 THEN LPRINT USING QQ$; EXT2(I%); EXT3(I%); EXT1(I%);
      ODEN(I%); OOUT(I%); : LPRINT USING RR$; TSAT(I%); : LPRINT USING QQ$;
      CODUM(I%)
2530  IF IPROCE% = 1 THEN LPRINT USING QQ$; EXT2(I%); EXT3(I%); EXT1(I%); :
      LPRINT SPACE$(12); : LPRINT USING QQ$; OOUT(I%); : LPRINT USING RR$;
      TSAT(I%); : LPRINT USING QQ$; CODUM(I%)
2540  LN% = LN% + 1
2550 NEXT I%
```

```
2560 IF LN% < 50 THEN LPRINT : LN% = LN% + 1: GOTO 2580
2570 LPRINT CHR$(12);
2580 IF IPROCE% <> 0 THEN 2610
2590 LPRINT "Valid ranges:": LPRINT "     0.0 to 5.0 M H+": LPRINT "
     0.0 to 200 gU/L": LPRINT "     0.0 to 100 gPu/L": LPRINT "     10 to
     30% TBP": LPRINT "     10 to 40"; CHR$(248); "C"
2600 GOTO 2620
2610 LPRINT "Valid ranges:": LPRINT "     0.0 to 3.0 M H+": LPRINT "
     0.0 TO 20.0 gU/L": LPRINT "     0.0 to 150 gTh/L": LPRINT "     ~30%
     TBP": LPRINT "     15 to 70"; CHR$(248); "C"
2620 INPUT #2, TIM2$, TIM3$
2630 LPRINT : LPRINT "Run Time is from "; TIM2$; " to "; TIM3$
2640 LPRINT CHR$(12);
2650 LPRINT CHR$(18);
2660 CLS : CLOSE #1: CLOSE #2
2670 RUN "sephis"
2680 END
2690 REM Subroutine to set up Purex aqueous results chart.
2700  LPRINT " AQUEOUS PHASE:"
2710  LPRINT " STAGE  NITRIC ACID    URANIUM      PU (IV)     PU (III)
      REDUCTANT   NITRATE ION    DENSITY     FLOW RATE    TEMP"
2720  LPRINT "  NO.       (M)          (g/L)         (g/L)         (g/L)
      (M)          (M)         (g/mL)        (L/min)       (C)"
2730  LPRINT " -----  -----------  -----------  -----------  -----------  -
      ----------  -----------  -----------  -----------  ------"
2740  LN% = LN% + 4
2750 RETURN
2760 REM Subroutine to set up Thorex aqueous results chart.
2770  LPRINT " AQUEOUS PHASE:"
2780  LPRINT " STAGE  NITRIC ACID    URANIUM      THORIUM    NITRATE ION
      FLOW RATE    TEMP"
2790  LPRINT "  NO.       (M)          (g/L)         (g/L)          (M)
      (L/min)      (C)"
2800  LPRINT " -----  -----------  -----------  -----------  -----------
      -----------  ------"
2810  LN% = LN% + 4
2820 RETURN
2830 REM Subroutine to set up Purex organic results chart.
2840  LPRINT " ORGANIC PHASE:"
2850  LPRINT " STAGE  NITRIC ACID    URANIUM      PU (IV)     U EXTRACT
      PU EXTRACT   H+ EXTRACT     DENSITY     FLOW RATE   TBPSAT
      INVENTORY"
2860  LPRINT "  NO.       (M)          (g/L)         (g/L)        FACTOR
      FACTOR       FACTOR       (g/mL)        (L/min)       (%)    CHANGE
      (%)"
2870  LPRINT " -----  -----------  -----------  -----------  -----------  -
      ----------  -----------  -----------  -----------  ------  ----------
      -"
2880  LN% = LN% + 4
2890 RETURN
2900 REM Subroutine to set up Thorex organic results chart.
2910  LPRINT " ORGANIC PHASE:"
2920  LPRINT " STAGE  NITRIC ACID    URANIUM      THORIUM     U EXTRACT
      TH EXTRACT   H+ EXTRACT                  FLOW RATE   TBPSAT
      INVENTORY"
```

```
2930  LPRINT "  NO.        (M)          (g/L)         (g/L)         FACTOR
      FACTOR        FACTOR                      (L/min)       (%)    CHANGE
      (%)"
2940  LPRINT " -----  -----------  -----------  -----------  -----------  -
      ----------  -----------                 -----------  ------  ----------
      -"
2950  LN% = LN% + 4
2960 RETURN
2970 REM Subroutine to draw a double box.
2980  FOR I% = R1% + 1 TO R2% - 1
2990   LOCATE I%, C1%: PRINT CHR$(186);
3000   LOCATE I%, C2%: PRINT CHR$(186);
3010  NEXT I%
3020  FOR J% = C1% + 1 TO C2% - 1
3030   LOCATE R1%, J%: PRINT CHR$(205);
3040   LOCATE R2%, J%: PRINT CHR$(205);
3050  NEXT J%
3060  LOCATE R1%, C1%: PRINT CHR$(201);
3070  LOCATE R1%, C2%: PRINT CHR$(187);
3080  LOCATE R2%, C1%: PRINT CHR$(200);
3090  LOCATE R2%, C2%: PRINT CHR$(188);
3100 RETURN
3110 REM Subroutine to draw a single box.
3120  FOR I% = R1% + 1 TO R2% - 1
3130   LOCATE I%, C1%: PRINT CHR$(179);
3140   LOCATE I%, C2%: PRINT CHR$(179);
3150  NEXT I%
3160  FOR J% = C1% + 1 TO C2% - 1
3170   LOCATE R1%, J%: PRINT CHR$(196);
3180   LOCATE R2%, J%: PRINT CHR$(196);
3190  NEXT J%
3200  LOCATE R1%, C1%: PRINT CHR$(218);
3210  LOCATE R1%, C2%: PRINT CHR$(191);
3220  LOCATE R2%, C1%: PRINT CHR$(192);
3230  LOCATE R2%, C2%: PRINT CHR$(217);
3240 RETURN
3250 REM Subroutine to set up chart for Purex feed & product stream data.
3260  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        PU (IV)
      PU (III)       REDUCTANT    NITRATE ION    FLOW RATE      TEMP"
3270  LPRINT SPACE$(17); "NO.        (M)          (g/L)          (g/L)
      (g/L)           (M)           (M)         (L/min)        (C)"
3280  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------   -----------   -----------   -----------    ------"
3290  LN% = LN% + 3
3300 RETURN
3310 REM Subroutine to set up chart for Thorex feed & product stream data.
3320  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        THORIUM
      NITRATE ION                                FLOW RATE       TEMP"
3330  LPRINT SPACE$(17); "NO.        (M)          (g/L)          (g/L)
      (M)                                       (L/min)        (C)"
3340  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------                               -----------    ------"
3350  LN% = LN% + 3
3360 RETURN
3370 REM Subroutine to set up Purex aqueous profile chart.
```

```
3380  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        PU (IV)
      PU (III)       REDUCTANT    NITRATE ION                   TEMP"
3390  LPRINT SPACE$(17); "NO.        (M)           (g/L)         (g/L)
      (g/L)            (M)          (M)                        (C)"
3400  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------   -----------   -----------                   ------"
3410  LN% = LN% + 3
3420 RETURN
3430 REM Subroutine to set up Thorex aqueous profile chart.
3440  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        THORIUM
      NITRATE ION                                               TEMP"
3450  LPRINT SPACE$(17); "NO.        (M)           (g/L)         (g/L)
      (M)                                                      (C)"
3460  LPRINT SPACE$(16); "-----  -----------   -----------   -----------
      -----------                                               ------"
3470  LN% = LN% + 3
3480 RETURN
3490 REM Subroutine to set up volume chart.
3500  LPRINT SPACE$(16); "STAGE    AQUEOUS       ORGANIC        TOTAL"
3510  LPRINT SPACE$(17); "NO.     VOLUME        VOLUME        VOLUME"
3520  LPRINT SPACE$(16); "-----  -----------   -----------   -----------"
3530  LN% = LN% + 3
3540 RETURN
3550 REM Subroutine to set up Purex organic profile chart.
3560  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        PU (IV)"
3570  LPRINT SPACE$(17); "NO.        (M)           (g/L)         (g/L)"
3580  LPRINT SPACE$(16); "-----  -----------   -----------   -----------"
3590  LN% = LN% + 3
3600 RETURN
3610 REM Subroutine to set up Thorex organic profile chart.
3620  LPRINT SPACE$(16); "STAGE  NITRIC ACID     URANIUM        THORIUM"
3630  LPRINT SPACE$(17); "NO.        (M)           (g/L)         (g/L)"
3640  LPRINT SPACE$(16); "-----  -----------   -----------   -----------"
3650  LN% = LN% + 3
3660 RETURN
3670 REM Error trapping routine.
3690  IF ERR = 64 THEN LOCATE 24, 1: PRINT "Bad file name"; : GOTO 3730
3700  IF ERR = 71 THEN LOCATE 24, 1: PRINT "Disk not ready"; : GOTO 3730
3710  IF ERR = 53 THEN LOCATE 24, 1: PRINT "File not found"; : GOTO 3730
3720  ON ERROR GOTO 0
3730  PRINT " - Press any key to continue";
3740  K$ = INKEY$: IF K$ = "" THEN 3740
3750  RESUME 290
3760 REM Error trapping routine.
3780  IF ERR = 24 THEN LOCATE 25, 1: PRINT "Your printer is not ready"; :
      GOTO 3800
3790  ON ERROR GOTO 0
3800  PRINT " - Check it and press any key";
3810  K$ = INKEY$: IF K$ = "" THEN 3810
3820  LOCATE 25, 1: PRINT SPACE$(79);
3840  RESUME
```

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