Modifications of the SEPHIS Computer Code for Calculating the Purex Solvent Extraction System

S. B. Watson    R. H. Rainey
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MODIFICATIONS OF THE SEPHIS COMPUTER CODE FOR CALCULATING

THE PUREX SOLVENT EXTRACTION SYSTEM

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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.

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830

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UNION CARBIDE CORPORATION
for the
U. S. ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION

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TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>1</td>
</tr>
<tr>
<td>I. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>II. NOTATION AND TERMINOLOGY</td>
<td>3</td>
</tr>
<tr>
<td>III. PROGRAM MODIFICATIONS</td>
<td>5</td>
</tr>
<tr>
<td>IV. USER INFORMATION</td>
<td>13</td>
</tr>
<tr>
<td>V. APPLICATION OF THE SEPHIS PROGRAM TO PUREX SOLVENT EXTRACTION</td>
<td>23</td>
</tr>
<tr>
<td>EXTRAC TION PROCESSING PROBLEMS</td>
<td></td>
</tr>
<tr>
<td>BIBLIOGRAPHY</td>
<td>29</td>
</tr>
<tr>
<td>APPENDICES</td>
<td>31</td>
</tr>
<tr>
<td>A. Program Listing</td>
<td>31</td>
</tr>
<tr>
<td>B. Sample Input and Output</td>
<td>49</td>
</tr>
</tbody>
</table>
MODIFICATIONS OF THE SEPHIS COMPUTER CODE FOR CALCULATING
THE PUREX SOLVENT EXTRACTION SYSTEM

S. B. Watson and R. H. Rainey

ABSTRACT

The SEPHIS computer program was developed to simulate the countercurrent solvent extraction. This report gives modifications in the program which result in improved fit to experimental data, a decrease in computer storage requirements, and a decrease in execution time. Methods for applying the computer program to practical solvent extraction problems are explained.

I. INTRODUCTION

SEPHIS, a computer program for Solvent Extraction Processes Having Interacting Solutes, was developed by W. S. Groenier for the purpose of studying the application of a 15% TBP solvent extraction system for recovering irradiated LMFBR fuel. Due to the success of the program in helping to establish optimum flowsheet conditions by simulation of the extraction process, the program has been widely used. In particular, G. L. Richardson of HEDL adapted the SEPHIS program to the conventional Purex process and also has made valuable changes in program structure. The Richardson version of SEPHIS has undergone additional modifications at ORNL. The purposes of this report are to describe additional program modifications, to give instructions for use of the program, and to indicate some of its various applications.

A modification of the SEPHIS program is being made for the simulation of the Acid Thorex flowsheet.
The changes in the Purex solvent extraction version of SEPHIS would not have been possible without the generous assistance of G. L. Richardson, who provided a copy of his computer program, and of W. S. Groenier, who gave valuable guidance in the operation of the program. This work is funded by the HTGR program.
II. NOTATION AND TERMINOLOGY

The symbols used in Section III are defined as follows:

- $U$ - molar uranium concentration,
- $Pu$ - molar plutonium concentration,
- $H$ - molar acid concentration,
- $S$ - molar unextractable salt nitrate concentration,
- $u$ - molal uranium concentration,
- $pu$ - molal plutonium concentration,
- $h$ - molal acid concentration,
- $s$ - molal salt nitrate concentration,
- $M$ - total molarity of the solution,
- $m$ - total molality of the solution,
- $W$ - molar water concentration in the TBP phase - Eq. (3),
- $w$ - molal water concentration in the TBP phase - Eq. (4),
- $F$ - volume fraction of TBP in dry, solute-free solvent,
- $T$ - molarity of TBP in dry, solute-free solvent,
- $t$ - temperature, °C,
- $K$ - pseudo-mass equilibrium constant - Eqs. (8)-(11),
- $n$ - total nitrate salting strength in the aqueous phase (molal) - Eq. (15),
- $r$ - reductant concentration (molal),
- $D$ - distribution coefficient, (i.e., $D = \frac{U}{U_a}$),

Subscripts:

- $a$ - aqueous phase,
- $o$ - organic phase,
os - solute molarity in solute-saturated solvent,

u - uranium,

pu - plutonium,

h1 - acid associated with 1 molecule of TBP,

h2 - acid associated with 2 molecules of TBP.
III. PROGRAM MODIFICATIONS

The details of the original SEPHIS program are available in Ref. 1; therefore, they will not be repeated in this report. At the time of the preparation of this report, the modifications by Richardson\textsuperscript{2} have not been published. This program started with the Richardson version of the program; consequently, portions of his program are described in this report for completeness. The changes have been both in the program structure and in the mathematical modeling of the system. The complete modified program listing is given in Appendix A.

Programming changes

The following programming changes are present in the current version of SEPHIS:

1. Many of the variable names have been altered to enhance program readability. A listing of these changes is unnecessary since comment cards within the program specify the meanings of the majority of variables.

2. Common blocks have been reorganized for more efficient use of computer storage.

3. The multidimensional variables which contain the calculated concentrations for each stage have been reduced in size. Previously, these variables retained concentrations for each stage for 100 time intervals. Now only those concentrations for the previous and the current time intervals are stored. This modification resulted in a reduction of about 100 K of computer core storage.
4. The subroutines have been renamed, and computational capability of certain subroutines has been altered. SEPHIS presently consists of the following routines:

MAIN reads program description cards, initializes arrays, performs molarity and molality conversions, prints results, and analyzes the approach to steady-state operation.

PROFIL defines feed streams and initial profile, if not zero.

FLWS defines outgoing streams, calculates phase ratios, flow ratios, recycle flows, interstage flows, and stage volumes for each stage.

STAGES performs stage calculations for the current time interval.

UCOR calculates the distribution coefficients required by STAGES.

PLTR and PPL generate Calcomp plots (profile graphs and transient graphs). PLTR and PPL invoke the ORGRAPH\textsuperscript{5} plotting package which is available at ORNL, and the subroutines in the package are not printed in Appendix A.

**Modeling changes**

Modifications to the modeling of the extraction system for the uranium, plutonium, and nitric acid are summarized as follows:

1. As before, calculations are valid for three transferring components; however, the current version also includes the salting effect from nonextractable nitrate salts.
2. Provisions have been made for estimating the partitioning of plutonium from uranium by entering the reductant normality as a negative plutonium concentration. The code does not, however, include the effects of kinetics, which is an important consideration in actual processing facilities.

3. Stage calculations are performed on a solute-free basis. The relationship between solute-free concentrations (small letters) and molarities (capital letters) for aqueous and organic solutions is given below (taken from Ref. 2 with slight modifications):

\[
\frac{m_a}{M_a} = \frac{1.0}{1.0 - 0.0724U_a - 0.13Pu_a - 0.0309H_a - 0.031S_a} = 1.0 + 0.0724u_a + 0.13pu_a + 0.0309h_a + 0.031s_a
\]  

(1)

\[
\frac{m_o}{M_o} = \frac{1.0}{1.0 - 0.097U_o - 0.139Pu_o - 0.043H_o - 0.0174W_o} = 1.0 + 0.097u_o + 0.139pu_o + 0.043h_o + 0.0174w_o
\]  

(2)

where \( W_o \) and \( w_o \) are calculated water concentrations in the TBP phase defined by

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

(3)
\[ w_0 = (4.2 - 0.015t) \left( 1.0 - \frac{2u_0}{T} - \frac{2pu_0}{T} - \frac{0.6h_0}{T} \right)^{1.69} \]  

(4)

\[ U_{os}, Pu_{os}, \text{ and } H_{os} \text{ are molarities of uranium, plutonium, and acid, respectively, required to saturate the TBP. They are defined by:} \]

\[ U_{os} = \frac{0.5T}{1.0 + 0.046T} \]  

(5)

\[ Pu_{os} = \frac{0.5T}{1.0 + 0.09T} \]  

(6)

\[ H_{os} = \frac{T(1.0 - 0.00609(3.95 - 0.0144t)^{1.65})}{(1.0 + 0.043T)} \]  

(7)

4. Profile temperature may vary with the time interval.

5. The program accounts for the amount of water the TBP extracts.

6. The criterion for convergence of stage calculations has been somewhat modified. As in the original SEPHIS stage, calculations are performed using an iterative procedure in each stage for each time interval. If convergence ((observed-calculated)/calculated < .001) is achieved within 20 iterations, the computation is considered to be complete in the current version of SEPHIS. If the computation fails to converge, the last calculated values are accepted. This is based on the assumption that steady-state values may be obtained even though there was failure to converge in a transient period. (It should be emphasized that, when the 20th iteration is reported in the printout, it may have no physical significance.)
7. The definition of steady state as given by Groenier is also used in the current version of SEPHIS with additional complexities. Additional convergence criteria have been added to the program to obtain less precise answers where convenience required over 100 iterations.

8. Richardson developed a new method for calculating distribution coefficients in an attempt to extend the code to higher temperatures and TBP concentrations than the restrictions of 25°C and 15% TBP imposed by the earlier code. The following is taken in part from his work and includes some additional details.

The equilibrium correlation was based on deriving empirical equations for the following pseudo-mass-action equilibrium constants:

\[ K_u = \frac{(\text{UO}_2(\text{NO}_3)^2 \cdot 2\text{TBP})_o}{(\text{UO}_2^2\text{Pu}_a)(\text{TBP})_o} = K_u^2(\text{NO}_3)^2_a \]  

(8)

\[ K_{pu} = \frac{(\text{Pu}(\text{NO}_3)_4 \cdot 2\text{TBP})_o}{(\text{Pu}^4\text{Pu}_a)(\text{TBP})_o} = K_{pu}^4(\text{NO}_3)^4_a \]  

(9)

\[ K_{h1} = \frac{(\text{HNO}_3 \cdot \text{TBP})_o}{(\text{H}^+ \text{Pu}_a)(\text{TBP})_o} = K_{h1}^1(\text{NO}_3)^1_a \]  

(10)

\[ K_{h2} = \frac{(\text{HNO}_3 \cdot 2\text{TBP})_o}{(\text{H}^+ \text{Pu}_a)(\text{TBP})_o} = K_{h2}^2(\text{NO}_3)^2_a \]  

(11)
This program and Richardson's program are based on a fitting of the K values above. Groenier's program was based on a fitting of the K' values. The basic empirical equilibrium expressions were derived at 100% TBP equilibrated at 25°C, giving the following equations:

\[ K^* \text{ (12)} = 3.7n^{1.57}_{a} + 1.4n^{3.9}_{a} + 0.011n^{7.3}_{a} \]

\[ K^*_{h1} = 0.135n^{0.82}_{a} + 0.0052n^{3.44}_{a} \text{ (13)} \]

\[ K^*_{h2} = K^*_{h2} \text{ (14)} \]

where

\[ n_a = h_a + 2u_a + 4pu_a + s_a \text{ (15)} \]

The plutonium constant was determined as a function of the uranium constant at 25°C.

\[ K^*_{pu} = K^*_{u}(0.20 + 0.55F^{1.25} + 0.0074n^{2}_{a}) \text{ (16)} \]

The code provides correction factors for other TBP concentrations and temperatures:

\[ K^*_{u} = K^*_{u}(4F^{-0.17} - 3)e^{(2500\tau)} \text{ (17)} \]

\[ K^*_{pu} = K^*_{pu}(4F^{-0.17} - 3)e^{(-200\tau)} \text{ (18)} \]

\[ K^*_{h1} = K^*_{h2} = K^*_{h1}(1.0 - 0.54e^{-15F})e^{(340\tau)} \text{ (19)} \]
where \( \tau = \frac{1}{\tau_o} - \frac{1}{298} \) and \( \tau_o \) = equilibrium temperature, \(^\circ\)K. The change in the distribution with TBP concentration is estimated as follows:

\[
D_u = \frac{(UO_2(NO_3)_2 \cdot 2TBP)_o}{(UO_2^{2+})_a} = K_u(TBP)_o^2 \tag{20}
\]

\[
D_{pu} = \frac{(Pu(NO_3)_4 \cdot 2TBP)_o}{(Pu^{4+})_a} = K_{pu}(TBP)_o^2 \tag{21}
\]

\[
D_{h1} = \frac{(HNO_3 \cdot TBP)_o}{(H^+)_a} = K_{h1}(TBP)_o \tag{22}
\]

\[
D_{h2} = \frac{(HNO_3 \cdot 2TBP)_o}{(H^+)_a} = K_{h2}(TBP)_o^2 \tag{23}
\]

Free (uncomplexed) TBP concentration is calculated as follows:

\[
(TBP)_o = T - 2(UO_2(NO_3)_2 \cdot 2TBP)_o - 2(Pu(NO_3)_4 \cdot 2TBP)_o - (HNO_3 \cdot TBP)_o - 2(HNO_3 \cdot 2TBP)_o. \tag{24}
\]

Substitution of Eqs. (20) through (23) into (24) produces

\[
(TBP)_o = T - 2K_{ua}(TBP)_o^2 - 2K_{pu_a}(TBP)_o^2 - k_{h1}h_a(TBP)_o^2 - 2K_{h2}h_a(TBP)_o^2. \]

Solving the quadratic equation gives
(TBP)₀ = \frac{-(k₁h₁ + 1) + \sqrt{(k₁h₁ + 1)^2 + 8(Ku_a + Kp₂u_a + Kp₂h_a)(3.651F)}}{4(Ku_a + Kp₂u_a + Kp₂h_a)}

assuming T = 3.651F.

Thus, given uₐ, pₐ, hₐ, sₐ, and r, the distribution coefficients are calculated by forming nₐ which is used to evaluate (12) - (19), then solving (25) for (TBP)₀ and replacing it in (20) - (23).
IV. USER INFORMATION

The current version of SEPHIS is written in the IBM System/360 and System/370 FORTRAN IV language. The program is compiled using the H-level compiler and has been executed on both the IBM 360/91 and 360/75 at ORNL. The program requires about 140 K (K = 1024 bytes; bytes = 8 bits) of core storage for execution. Approximately 1/20 sec. of computing time on the IBM 360/91 is required for each time interval when calculating 10 stages.

The remainder of this section describes the content of the card input which must be prepared in order to execute the program and the output produced by the program. Sample input and the corresponding output are presented in Appendix B.

Input

The input data are to be prepared in the order shown in Table 1. Referring to Table 1, "Subroutine" indicates the subroutine in which the card is read. "Card Number" denotes the order within the group (Program Cards, Feed Stream Cards, etc.) or quantity of cards for each group to be input. "Columns" refers to the actual columns on the card in which the data must be punched. "Remarks, Variables, etc." gives an explanation as to the variable name, definition, and form of the data to be punched on the cards. The FORMAT descriptor indicates the content and length of the fields on the card. In the FORMAT descriptor the letter "A" denotes alphabetic data; "I" refers to integer data (no decimal point) which must always be right-justified in the field; "F"
Table 1. Input to SEPHIS Code

<table>
<thead>
<tr>
<th>Subroutine</th>
<th>Card Number</th>
<th>Columns</th>
<th>Remarks, Variables, etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAIN</td>
<td>1</td>
<td>FÔRMAT (10A4)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1-40</td>
<td>TITLE - problem title</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>FÔRMAT (F8.0,9I2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1-8</td>
<td>CTBP - volume fraction of dry TBP</td>
<td></td>
</tr>
<tr>
<td></td>
<td>9-10</td>
<td>NTØST - total number of stages - must not exceed 25</td>
<td></td>
</tr>
<tr>
<td></td>
<td>11-12</td>
<td>IPRØ - 0 for a zero initial concentration profile 1 for a non-zero initial profile</td>
<td></td>
</tr>
<tr>
<td></td>
<td>13-14</td>
<td>IRATIØ - 0 if phase ratio = flow ratio 1 if phase ratio values are to be input</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-16</td>
<td>ICALC - 0 for shutdown calculations (no U or Pu in feed streams) 1 for start-up or interruption</td>
<td></td>
</tr>
<tr>
<td></td>
<td>17-18</td>
<td>IØUT - 0 if there are no extra outgoing streams 1 if there are outgoing streams in addition to end streams</td>
<td></td>
</tr>
<tr>
<td></td>
<td>19-20</td>
<td>IVØL - 0 stage volumes are equal</td>
<td></td>
</tr>
</tbody>
</table>
Table 1. (continued)

<table>
<thead>
<tr>
<th>Subroutine</th>
<th>Card Number</th>
<th>Columns</th>
<th>Remarks, Variables, etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAIN (cont.)</td>
<td></td>
<td>IVØL - 1</td>
<td>1 stage volumes are unequal but according to total flow</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2 stage volumes are independently unequal</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3 stage volumes are equal and specified</td>
</tr>
<tr>
<td></td>
<td>21-22</td>
<td>IPR - 0</td>
<td>print out all time intervals</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1 print only last interval</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-1 print every 20th time interval</td>
</tr>
<tr>
<td></td>
<td>23-24</td>
<td>IPNCH - 0</td>
<td>no punched card output desired</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1 final profile output punched on cards</td>
</tr>
<tr>
<td></td>
<td>25-26</td>
<td>ICALPL - 0</td>
<td>no Calcomp plots</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1 profile graphs (log of concentration vs stage number at 1/8 steady state, 1/4 steady state, 1/2 steady state, and steady state)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2 transient graphs (concentration vs time interval at specified stages for each time block)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3 plot both 1 and 2</td>
</tr>
</tbody>
</table>

(Options 2 or 3 should be used for HAN* calculations to correct for stage residence time) (*Hydroxylamine Nitrate - Ref. 3)
Table 1. (continued)

<table>
<thead>
<tr>
<th>Subroutine</th>
<th>Card Number</th>
<th>Columns</th>
<th>Remarks, Variables, etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Feed Stream Cards</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PRØFIL</td>
<td>One card for each input stream</td>
<td></td>
<td>FORMAT (2I2,5F8.0,i2,F8.0)</td>
</tr>
<tr>
<td></td>
<td>1-2</td>
<td>I</td>
<td>stage number that feed enters</td>
</tr>
<tr>
<td></td>
<td>3-4</td>
<td>JHAS</td>
<td>1 for aqueous feed</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0 for organic feed</td>
</tr>
<tr>
<td></td>
<td>5-12</td>
<td>FDRT</td>
<td>feed flow rate (volume units)</td>
</tr>
<tr>
<td></td>
<td>13-20</td>
<td>CØN1</td>
<td>uranium content (g/l)</td>
</tr>
<tr>
<td></td>
<td>21-28</td>
<td>CØN2</td>
<td>plutonium content (g/l)</td>
</tr>
<tr>
<td></td>
<td>29-36</td>
<td>CØN3</td>
<td>acid molarity</td>
</tr>
<tr>
<td></td>
<td>37-44</td>
<td>TEMP</td>
<td>temperature in degrees C</td>
</tr>
<tr>
<td></td>
<td>45-46</td>
<td>INDEX</td>
<td>1 more cards to follow</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0 last card</td>
</tr>
<tr>
<td></td>
<td>47-54</td>
<td>CØN4</td>
<td>nitrate normality from inextractable salts, including the reductant</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(Enter Pu reductant normality as negative Pu concentration)</td>
</tr>
<tr>
<td><strong>Initial Profile Cards</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(required only for non-zero initial profile)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PRØFIL</td>
<td>One card for each stage</td>
<td></td>
<td>FORMAT (8F8.0)</td>
</tr>
<tr>
<td></td>
<td>1-8</td>
<td>X(1,J,1)</td>
<td>aqueous-phase uranium concentration in stage J (g/l)</td>
</tr>
</tbody>
</table>
### Table 1. (continued)

<table>
<thead>
<tr>
<th>Subroutine</th>
<th>Card Number</th>
<th>Columns</th>
<th>Remarks, Variables, etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRØFIL (cont.)</td>
<td></td>
<td>9-16</td>
<td>( X(2,J,1) ) - aqueous-phase plutonium concentration in stage ( J ) (g/l)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>17-24</td>
<td>( X(3,J,1) ) - aqueous-phase nitric acid concentration in stage ( J ) (M)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25-32</td>
<td>( Y(1,J,1) ) - organic-phase uranium concentration in stage ( J ) (g/l)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>33-40</td>
<td>( Y(2,J,1) ) - organic-phase plutonium concentration in stage ( J ) (g/l)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>41-48</td>
<td>( Y(3,J,1) ) - organic-phase nitric acid concentration in stage ( J ) (M)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>49-56</td>
<td>TPRØF((J,1)) - temperature in stage ( J )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>57-64</td>
<td>( X(4,J,1) ) - aqueous-phase nitrate concentration in stage ( J ) (M)</td>
</tr>
</tbody>
</table>

#### Outgoing Stream Data
(other than aqueous raffinate and organic product)

<table>
<thead>
<tr>
<th>FLOWS</th>
<th>One card for each outgoing stream</th>
<th>FORMAT (2I2,F8.0,I2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>.1-2</td>
<td>I - stage number that stream leaves</td>
<td></td>
</tr>
<tr>
<td>3-4</td>
<td>JHAS - 1 for aqueous stream 0 for organic stream</td>
<td></td>
</tr>
<tr>
<td>5-12</td>
<td>ØTRT - exit flow rate (volume units)</td>
<td></td>
</tr>
<tr>
<td>13-14</td>
<td>INDEX - 1 more cards follow 0 last card</td>
<td></td>
</tr>
</tbody>
</table>
Table 1. (continued)

<table>
<thead>
<tr>
<th>Subroutine</th>
<th>Card Number</th>
<th>Columns</th>
<th>Remarks, Variables, etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Phase Ratio Cards</strong>&lt;br&gt;(used only if phase ratio ≠ flow ratio)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>FLØWS</td>
<td></td>
<td>FØRMAT (I2,F8.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>One card for each region of constant phase ratio</td>
<td>1-2</td>
<td>I - number of stages having phase ratio shown</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3-12</td>
<td>RATIØ - aqueous/organic phase ratio</td>
</tr>
<tr>
<td><strong>Stage Volumes</strong>&lt;br&gt;(for IVØL=2 and IVØL=3)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>FLØWS</td>
<td></td>
<td></td>
<td>For IVØL=2 stage volumes are unequal and not flow related</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>1-8</td>
<td>STVØL(1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>:</td>
<td>:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>72-80</td>
<td>STVØL(10)</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1-8</td>
<td>STVØL(11)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>:</td>
<td>:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>72-80</td>
<td>STVØL(20)</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1-8</td>
<td>STVØL(21)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>:</td>
<td>:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>32-40</td>
<td>STVØL(25)</td>
</tr>
</tbody>
</table>

Only NTØST stage volumes need to be entered; that is, 1 to 3 cards are needed for input.
Table 1. (continued)

<table>
<thead>
<tr>
<th>Subroutine</th>
<th>Card Number</th>
<th>Columns</th>
<th>Remarks, Variables, etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>FLOWS</strong></td>
<td></td>
<td></td>
<td>For $IVOL=3$ stage volumes are equal and specified</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>1-8</td>
<td>$VOL$ - stage volume for all stages</td>
</tr>
<tr>
<td><strong>Graph Cards</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>(ICALPL=1,2,3)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>PLØTR</strong></td>
<td></td>
<td></td>
<td><strong>Profile graphs</strong> (ICALPL=1 or 3)</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>1-80</td>
<td>$TTL$ - title for all profile graphs</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>1-80</td>
<td>$XTAG$ - x-axis label for all profile graphs</td>
</tr>
<tr>
<td>One card for each profile graph</td>
<td>1-80</td>
<td>$YTAG$ - y-axis label for each profile graph</td>
<td></td>
</tr>
<tr>
<td><strong>Transient graphs</strong> (ICALPL=2 or 3)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>1-2</td>
<td>$NSTA(1)$ - stage no. for 1st set of transient graph</td>
</tr>
<tr>
<td>:</td>
<td></td>
<td>:</td>
<td>:</td>
</tr>
<tr>
<td>49-50</td>
<td></td>
<td></td>
<td>$NSTA(25)$ - stage no. for 25th set of transient graphs</td>
</tr>
<tr>
<td>Two graphs are plotted for each I such that $NSTA(I)\neq0$. For $NSTA(I)=0$ no graphs are plotted.</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 1. (continued)

<table>
<thead>
<tr>
<th>Subroutine</th>
<th>Card Number</th>
<th>Columns</th>
<th>Remarks, Variables, etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLØTR (cont.)</td>
<td>2</td>
<td>1-80</td>
<td>FØRMAT (10A8)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TTL - title for all transient graphs</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1-80</td>
<td>FØRMAT (10A8)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>XTAG - x-axis label for all transient graphs</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>One card for each transient graph</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1-80</td>
<td>FØRMAT (10A8)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>YTAG - y-axis label for each transient graph</td>
</tr>
</tbody>
</table>

Note: Character strings input as TTL, XTAG, and YTAG must end with $.

**Next Case**

<table>
<thead>
<tr>
<th>MAIN</th>
<th>1</th>
<th>FØRMAT (2I2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1-2</td>
<td>ICHNGE - 0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>next case is new</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1 new Feed Stream Cards and Outgoing Stream Data required for each feed and exit stream - no Program Cards, Initial Profile Cards, Phase Ratio Cards, or Stage Volume Cards are required</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2 stop</td>
</tr>
<tr>
<td></td>
<td>3-4</td>
<td>IDIF - 0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>no changes in Program Card parameters</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- 1 changes in at least one of these Program Card parameters - ICALC, IØUT, IPR, IPNCH, ICALPL (these parameters are explained in the section Program Cards)</td>
</tr>
</tbody>
</table>
Table 1. (continued)

<table>
<thead>
<tr>
<th>Subroutine</th>
<th>Card Number</th>
<th>Columns</th>
<th>Remarks, Variables, etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2</td>
<td>1-2</td>
<td>FORMAT (5I2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3-4</td>
<td>ICALC</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5-6</td>
<td>IØUT</td>
</tr>
<tr>
<td></td>
<td></td>
<td>7-8</td>
<td>IPNCH</td>
</tr>
<tr>
<td></td>
<td></td>
<td>9-10</td>
<td>ICALPL</td>
</tr>
</tbody>
</table>

If IDIF = 1, input a card of the following form; if IDIF = 0, omit this card.

See Program Cards for explanation of these parameters.
indicates a real number with or without a signed exponent (decimal point should be punched). The variable names are those used in the FORTRAN program. Two examples of sample input are included in Appendix B.

Output

Two examples of program printout are given in Appendix B. A general explanation of these examples and hence all output is herein described.

The first page of printed output provides a synopsis of input and various initial conditions. Included are the feed stream data, initial profile, phase ratios, and stage flows. The remainder of the printout consists of transient behavior results for each time interval. Printout for each time interval includes aqueous- and organic-phase concentrations, aqueous and organic flows, temperature, and number of iterations required for convergence in the stage calculations; all of which are printed for each stage.

After every time interval which is a multiple of 100 and upon convergence of the transient calculations, the percent steady state and the time intervals at which 90%, 95%, 99%, and 99.5% steady state have been reached are printed.

If desired, output may also be obtained in the form of Calcomp plots. Profile graphs (concentration vs stage number) and/or transient graphs (concentration vs time interval) may be produced by (1) requesting plots on the "Program Cards" and (2) entering the correct input as prescribed in "Graph Cards" (see Input).
V. APPLICATION OF THE SEPHIS PROGRAM TO PUREX
SOLVENT EXTRACTION PROCESSING PROBLEMS

The procedure used in the SEPHIS calculations makes this program very useful for several types of design, optimization, and evaluation problems in a solvent extraction system. Starting with any combination of concentrations of uranium, plutonium, and nitric acid in each stage of a countercurrent contactor and any combination of feed stream compositions and flow rates, the program calculates the step-by-step change in the concentration of the uranium, plutonium, and nitric acid of each stage. This type calculation provides a means of evaluating both transient and steady-state effects of start-up or shutdown procedures, of modifications of flowsheet conditions, of operational changes due to equipment malfunction, of errors in operational procedure, etc. A comparison of the steady-state concentrations of uranium, plutonium, and nitric acid calculated by the original and the revised computer codes with the values determined by a laboratory countercurrent batch extraction is given in Table 2. Examples of calculations at transient conditions are given in Appendix B. The concentrations of uranium, plutonium, and nitric acid resulting from these calculations may be used in evaluating product losses, in determining the critical (nuclear) safety of the equipment, in estimating the loading of the solvent so that decontamination from fission products may be estimated from other data, etc. Due to the reflux of extracting components in a multistaged countercurrent contactor system, the concentration of any extractable material may reach a higher value in the column than in the feed or exit streams.
Table 2. Comparison of Steady-State Purex Conditions Calculated by the Original and Revised SEPHIS Programs with Data from a Laboratory Experiment

Flowsheet Conditions: Scrub: 2 M HNO₃, 0.3 volume, stage 1; Feed: 27.7 g U/l, 4.43 g Pu/l, 3.2 M HNO₃, 1.0 volume, stage 4; Organic: 15.3 v/o TBP--84.7 v/o n-dodecane, 1.8 volume, stage 11.

<table>
<thead>
<tr>
<th>Stage</th>
<th>Uranium (g/l)</th>
<th>Plutonium (g/l)</th>
<th>Acid (M)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Original¹</td>
<td>Experimental²</td>
<td>Revised³</td>
</tr>
<tr>
<td>Aqueous Phase</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>21.0</td>
<td>18.5</td>
<td>18.8</td>
</tr>
<tr>
<td>2</td>
<td>28.2</td>
<td>23.0</td>
<td>24.6</td>
</tr>
<tr>
<td>3</td>
<td>30.6</td>
<td>18.5</td>
<td>24.5</td>
</tr>
<tr>
<td>4</td>
<td>24.5</td>
<td>18.2</td>
<td>19.1</td>
</tr>
<tr>
<td>5</td>
<td>2.57</td>
<td>2.72</td>
<td>1.43</td>
</tr>
<tr>
<td>6</td>
<td>0.12x10⁻³</td>
<td>0.11</td>
<td>6.67x10⁻²</td>
</tr>
<tr>
<td>7</td>
<td>5.69x10⁻⁴</td>
<td>0.01</td>
<td>2.97x10⁻⁴</td>
</tr>
<tr>
<td>8</td>
<td>2.53x10⁻⁷</td>
<td>1.31x10⁻⁷</td>
<td>2.63x10⁻⁷</td>
</tr>
<tr>
<td>9</td>
<td>1.13x10⁻⁷</td>
<td>5.86x10⁻⁷</td>
<td>2.81x10⁻⁷</td>
</tr>
<tr>
<td>10</td>
<td>5.10x10⁻⁸</td>
<td>2.63x10⁻⁸</td>
<td>3.03x10⁻⁸</td>
</tr>
<tr>
<td>11</td>
<td>2.80x10⁻⁸</td>
<td>1.29x10⁻⁸</td>
<td>3.95x10⁻⁸</td>
</tr>
</tbody>
</table>

| Organic Phase | | | | | | | | | |
| 1     | 37.6          | 38.8           | 36.9     | 2.46    | 2.53         | 2.41     | 0.12     | 0.21         | 0.09    |
| 2     | 41.1          | 42.1           | 39.9     | 3.33    | 2.91         | 3.11     | 0.10     | 0.21         | 0.08    |
| 3     | 42.3          | 43.6           | 40.9     | 3.98    | 3.05         | 3.48     | 0.09     | 0.24         | 0.09    |
| 4     | 42.7          | 43.7           | 40.9     | 4.33    | 3.21         | 3.54     | 0.12     | 0.26         | 0.13    |
| 5     | 17.7          | 13.9           | 13.6     | 5.22    | 2.65         | 3.27     | 0.27     | 0.29         | 0.30    |
| 6     | 1.85          | 1.28           | 1.02     | 1.38    | 0.50         | 0.68     | 0.41     | 0.34         | 0.39    |
| 7     | 9.17x10⁻²     | 0.07           | 4.72x10⁻²| 0.16    | 0.074        | 8.88x10⁻²| 0.44     | 0.34         | 0.40    |
| 8     | 4.11x10⁻⁴     | 0.02           | 2.10x10⁻⁵| 1.77x10⁻²| 0.009      | 1.11x10⁻²| 0.44     | 0.34         | 0.40    |
| 9     | 1.83x10⁻⁷     | 9.33x10⁻⁷      | 1.89x10⁻⁷| 0.002   | 1.37x10⁻⁷   | 0.44     | 0.35     | 0.40         | 0.40    |
| 10    | 8.12x10⁻⁹     | 4.14x10⁻⁷      | 2.00x10⁻⁴| 0.001   | 1.68x10⁻⁴   | 0.44     | 0.34     | 0.39         | 0.39    |
| 11    | 3.48x10⁻⁸     | 1.78x10⁻⁷      | 1.90x10⁻⁵| 0.004   | 1.86x10⁻⁵   | 0.40     | 0.30     | 0.34         | 0.34    |

¹The original SEPHIS code as reported in ORNL-4746.
²Laboratory data reported, p. 11, ORNL-4746.
³SEPHIS code in its present form.
Changes in operating conditions can then result in transient high concentrations in the exit streams. During such transient conditions nuclear criticality in tankage may be approached, a situation that would not occur during steady-state conditions. The SEPHIS program may be used to detect such occurrences. The program perhaps has its greatest utility as an aid to the planning of laboratory tests designed to determine optimum values for flowsheet parameters and as a diagnostic tool when operating solvent extraction systems.

The number of theoretical stages required to give a specified loss or separation of uranium and plutonium with a given flowsheet may be determined by varying the number of stages used in the calculation until the desired results are obtained. Similarly, the height equivalent to a theoretical stage in a solvent extraction column or the stage efficiency of a mixer-settler can be determined by adjusting the numbers of stages in the calculations until the calculated effluent concentrations match experimental data. In these calculations it is well to remember the interdependence of the two parts of a compound extraction cascade when analyzing the variation in the reflux of the extractable species with operating conditions. It is therefore necessary to simultaneously determine the number of stages in each end of a compound cascade when performing calculations.

The time unit given by the program is that for one volumetric displacement of an ideal mixer-settler contactor. The real-time equivalent, therefore, is equal to the volume of one theoretical stage divided by the sum of the flow rates to the stage. An example of such a calculation...
is given in Table 3, where the calculational time unit is equivalent to 0.85 min of real time. In this example, the column contained 11-1/4 theoretical stages and the time for the volumetric displacement of the column is about 10 min.
Table 3. Calculation of the Time for the Volumetric Displacement of a Theoretical Stage in a Pulsed Column

<table>
<thead>
<tr>
<th>Column Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 in. pipe, schedule 40, ID 6.065 in.</td>
</tr>
<tr>
<td>Pulse plates, 1/8 in. thick, 23% free space, 6 in. diam., 2 in. spacing</td>
</tr>
<tr>
<td>Support rods, 3 ea., 1/4 in. diameter</td>
</tr>
<tr>
<td>Total length, 36 ft.</td>
</tr>
<tr>
<td>HETS, 3.2 ft.</td>
</tr>
</tbody>
</table>

Flow rate at 80% flooding, 1 in. pulse, 60 pulse/min. = 1600 gal/hr/ft²

Volume of a Theoretical Stage

\[
\left[\left(\frac{6.065}{2}\right)^2 \times \pi \times 3.2 \times 12\right] - \left[\left(\frac{6}{2}\right)^2 \times \pi \times 0.125 \times \frac{3.2 \times 12}{2} \times 0.77\right] + 3\left[\left(\frac{25}{2}\right)^2 \times \pi \times 3.2 \times 12\right] = 1047 \text{ in.}^3 \text{ or } 0.6059 \text{ ft.}^3
\]

Flow rate through column

\[
1600 \frac{\text{gal}}{\text{ft}^2 \cdot \text{hr}} \times \frac{\text{ft}^3}{7.48 \text{ gal}} \times \frac{\text{hr}}{60 \text{ min}} \times \left[\left(\frac{6.056}{2} \times 12\right) \times \pi\right] \text{ ft}^2 = 0.7153 \frac{\text{ft}^3}{\text{min}}
\]

Displacement Time

\[
0.6059 \text{ ft}^3 \times \frac{\text{min}}{0.7154 \text{ ft}^3} = 0.85 \text{ min}
\]
BIBLIOGRAPHY


APPENDIX A

Program Listing
PROGRAM SEPHIS

* ORAL MODIFICATION OF THE RICHARDSON-WANCE REVISED VERSION

* TRANSIENT STAGE CALCULATIONS FOR PURE SOLVENT EXTRACTION PROCESS.

* CALCULATIONS VALID FOR 3 TRANSFERRING COMPONENTS. INCLUDE SALTING

* OUT FROM NON-TRANSFERRING STAGE.

* CALCULATIONS CAN BE MADE BY ENTERING THE REDUCTANT FORMALITY AS A

* NEGATIVE PLUTONIUM CONCENTRATION ON THE APPROPRIATE FEED CASE.

* COMPONENT 1 = URBAN. COMPONENT 2 = PLUTONIUM. COMPONENT 4 = SALT BITRATE

* STAGE VOLUMES EQUAL UNLESS NOTED OTHERWISE.

DIMENSION TITLE(10)
DIMENSION AA(25),TT(25),0.0(25),RATIO(25)
DIMENSION CPA(4),CP0(4)
COMMON/PL/PLTXC,IT,OUT,IVOL,RECT(25),ICMNGC,ALVTP(25),OLVT(25)
COMMON/STG/STGLO,CMDCS(25),AB(25),GT(25),OT(25)
COMMON/IND/IND(25),ND(25),RD(25),0.0(25),IPRO(25)
COMMON/FL/FL,FLOR(25),F(25,2),FPD(25,2),FPD(25,4),FPD(25,4)
COMMON/CTP/CTB,ART(4),STRY(25),RO(25),RFP(25)

ISTAGE = 0

WRITE(100,1),TITLE,CTB,WTOST,IPRO,IND,ICMNC,OUT,IVOL,IFP,IPWCH,
1 ICALPL

10 CONTINUE

READ 100,TITLE,CTB,WTOST,IPRO,IND,ICALC,OUT,IVOL,IFP,IPWCH,
1 ICALPL

C TITLE IS THE PROBLEM TITLE. 40 SPACES ARE ALLOWED.
C WTOST = TOTAL NUMBER OF STAGES, MUST NOT EXCEED 25
C NSOL = NUMBER OF SOLUTES, MUST BE 4
C CTB = VOLUME FRACTION OF OUT TRP
C IPRO = 0 FOR A ZERO INITIAL CONCENTRATION PROFILE
C 1 FOR A NON-ZERO INITIAL PROFILE
C IBC = 0 IF PHASE RATIO CARDS FOLLOW
C 1 IF PHASE RATIO CARDS FOLLOW
C ICALC = 0 FOR SHUT-DOWN CONDITIONS (NO OUT OR IN FEED STREAMS)
C 1 FOR START-UP OR INTERRUPTION
C 0.0 IF THERE ARE NO EXTRA OUTGOING STREAMS
C 0 IF STAGE VOLUMES ARE UNEQUAL BUT ACCORDING TO TOTAL FLOW
C 1 IF STAGE VOLUMES ARE INDEPENDENTLY UNEQUAL
C 3 IF STAGE VOLUMES ARE EQUAL AND SPECIFIED. OPTIONS 2 OR 3
C SHOULDBE USED FOR NEW CALCULATIONS TO CONVERG FOR STAGE
C RESIDENCE TIME.
C IPF = 0 TO PRINT ALL TIME INTERVALS
C -1 TO PRINT ONLY LAST INTERVAL
C -1 TO PRINT EVERY 20TH TIME INTERVAL
C ICMNC = 0 IF NEXT CASE IS NEW
C 1 IF NEXT CASE INVOLVES ONLY A CHANGE IN FEED FLOWS, COMP, AND TEMP
C 2 STOP
C IPWCH = 0 IF NO PUNCHED CARD OUTPUT DESIRED
C 1 FOR FINAL PROFILE OUTPUT OR PUNCHED CARDS
C ICALPL = 0 NO CALCORP PLOTS
C = 1 PROFILE GRAPHS OF LOGARITHMS OF CONCENTRATION
C VS STAGE NUMBER AT STAGE STATE, 1/2, 1/4, AND 1/8 OF STAGE STATE TIME
C = 2 TRANSIENT GRAPHS OF CONCENTRATION VS TIME AT
C SPECIFIED STAGES FOR EACH TIME BLOCK
C = 3 PLOT BOTH 1 AND 2
C 0 CLEAR
C 1 CLEAR
C ZEROS OF ABSTAS
DO 15 J=1,WTOST
CDOBN(J)=0.0
STVOL(J)= 0.0
DO 15 K=1,2
NH(J,K)= 0.0
YPB(J,K)= 25.0
DO 15 J=1,NSOL
DF(J)= 0.0
Y(J,J,K)=0.0
15 CONTINUE
ICMRG = 0

11 CONTINUE

DO 30 J=1,WTOST
A(J)= 0.0
O(J)= 0.0
APRD(J)= 0.0
OFTRD(J)= 0.0
ALIVT(J)= 0.0
OLVT(J)= 0.0
30 CONTINUE

DO 40 J=1,WTOST
A(J)= 0.0
O(J)= 0.0
APRD(J)= 0.0
OFTRD(J)= 0.0
ALIVT(J)= 0.0
OLVT(J)= 0.0
40 CONTINUE
RHFD(J) = 0.0
APDTEM(J) = 25.0
OPDTEM(J) = 25.0
CONTUE
DO 30 I=1,NSOLU
CPA(I)=C.
CPO(I)=0.
DO 30 J=1,NTOST
XPD(1.1) = 0.0
YPD(1,1) = 0.0
CONTUE
30

C PROFIL SETS INITIAL CONCENTRATIONS FOR TIME ZERO, ALSO DEFINES FEED STREAMS
C
C CALL PROFIL

C WRITE FEED STREAM DATA

PRINT 1002, TITLE
WRITE(6,1003) I,APDRT(1) ,APDRT(2),APDRT(3),APDRT(4),APDRT(5),APDRT(6),APDRT(7),APDRT(8),APDRT(9),APDRT(10),APDRT(11)
1 APDTEM(1)

C CONVERT TO MOLARITY

XPD(1,1) = XPD(1,1)/236.
XPD(2,1) = XPD(2,1)/239.

C AQUEOUS STAGE FLOW RATES (APDRT) AND AQUEOUS CONTENT OF STAGE (XPD) CONVERTED FROM VOLUME UNITS TO SOLUTE-FREE VOLUME UNITS

DENOM = 1.0-0.072*XPD(1,1)-0.13*XPD(2,1)-0.0309*XPD(3,1)
1-0.03*XPD(4,1)
IF(XPD(1,1).LT.0.0) DENOM = DENOM + 1.0
ADPT(1) = APDRT(1)/DENOM
DO 35 J = 1,6
XPD(J,1) = XPD(J,1)/DENOM
35
CONTUE

C SET ACID IN ALL STAGES TO SCRUB ACID CONCENTRATION

IP(IPRT(1).EQ.0) X(3,1,1) = XPD(3,1)
IP(OPDRT(1).LE.0.) GO TO 50
PRINT 1005,CTBP,I,YFD(1,1),YPD(2,1),YPD(3,1),YPO(4,1),OFDRT(I),1,OPDTEM(1)

C CONVERT TO MOLARITY

YPD(1,1) = YPD(1,1)/238.
YPD(2,1) = YPD(2,1)/239.

C ORGANIC STAGE FLOW RATES (OPDRT) AND ORGANIC CONTENT OF STAGE (YPD) CONVERTED FROM VOLUME UNITS TO SOLUTE-FREE VOLUME UNITS

WO = (3.95-0.014*OPDTEM(I))*CTBP**1.65
WS = WO*(1.0-0.0639*W0)/(1.0-0.043*W0)
WC = WO*(1.0-0.057*XPD(1,1)-0.135*XPD(2,1)-0.043*XPD(3,1)-0.0174*WC)
OPDRT(I) = OPDRT(I)*DENOM
DO 50 J = 1,6
YPD(J,1) = YPD(J,1)/DENOM
50 CONTUE

C ORGANIC STAGE FLOW (OPDRT) AND ORGANIC CONTENT

C OF STAGE (YPD) CONVERTED FROM VOLUME UNITS TO SOLUTE-FREE VOLUME UNITS

C SET ACID IN ALL STAGES TO SCRUB ACID CONCENTRATION

IP(IPRT(1).EQ.0) X(3,1,1) = XPD(3,1)
IP(OPDRT(1).LE.0.) GO TO 50
PRINT 1005,CTBP,I,YFD(1,1),YPD(2,1),YPD(3,1),YPD(4,1),OPDRT(I),1,OPDTEM(I)

C CONVERT TO MOLARITY

C PRINT OUTGOING STREAMS (ALVBT AND OLVT) IN SOLUTE-FREE VOLUME UNITS

C PRINT OUTGOING STREAMS (ALVBT AND OLVT) IN SOLUTE-FREE VOLUME UNITS
IF NO EXTRA OUTGOING STREAMS, AVOID PRINT OF ALVFR AND OLVFT

DO 45 I=1,NST
IF(ALVFR(I).LE.0.) GO TO 45
PRINT 1670,ALVFR(I)
CONTINUE
DO 45 I=1,NST
IF(ALVFT(I).LE.0.) GO TO 45
PRINT 1670,ALVFT(I)
CONTINUE

50 CONTINUE

PRINT INITIAL PROFILE BEFORE UNIT CONVERSION

CONTINUE

PRINT 1009
PRINT 1010,J,X(I,J,1) ,X(2,J,1) ,X(3,J,1) ,Y(1,J,1) ,Y(2,J,1) ,Y(3,J,1) ,T(I,1)
CONTINUE

IF(IPRO .EQ.0. AND. ICHNGE. EQ. 0) GO TO 85

DO 80 J=1,NST
X(1,J,1)=X(1,J,1)/238.
Y(1,J,1)=Y(1,J,1)/238.
X(2,J,1)=X(2,J,1)/239.
Y(2,J,1)=Y(2,J,1)/239.
CONTINUE

X(2,J,1) = X(2,J,1) + RN(J,1)

PRINT 1011
GO TO 95
90 CONTINUE
PRINT 1012
95 CONTINUE

C A IS AQUEOUS INTERSTAGE FLOW
C O IS ORGANIC INTERSTAGE FLOW
C AA IS TOTAL AQUEOUS FLOW LEAVING STAGE
C AO IS TOTAL ORGANIC FLOW LEAVING STAGE
C RCYA IS AQUEOUS RECYCLE TO SATISFY PHASE RATIO
C RCYO IS ORGANIC RECYCLE TO SATISFY PHASE RATIO
C AT IS TOTAL AQUEOUS FLOW WITHIN A STAGE
C OT IS TOTAL ORGANIC FLOW WITHIN A STAGE
C TP IS TOTAL FLOW ON TO A STAGE
C
C CALCULATION

IF NUMBER SHOTDOYN (ICALC=O), CHECK

140 CONTINUE

150 CONTINUE

C PRINT STAGE FLOWS

C DO 120 J=1,NSTOST

C PRINT 1015, J, RATIO(J), AA(J), AR(J), BCTR(J), AT(J)

C 120 CONTINUE

C PRINT 1016

C DO 125 J=1,NSTOST

C PRINT 1017, J, TT(J), STYOL(J), AO(J), OR(J), BCTR(J), CT(J)

C 125 CONTINUE

WRITE(6, 1018)

C M - IS 100 OR LAST TIME INTERVAL

C ICEN - COUNTS BY 100'S NUMBER OF ITERATIONS

C BDF - ADF FOR PREVIOUS TIME INTERVAL

C CDF - SET EQUAL TO ADF IF ADF-BDF (CONVERGENCE HAS OCCURRED)

C DDF - DETERMINES DDF,PPDF,PPPPDF,PPPPPDF (PERCENT STEADY STATE)

C K = 100

C ICEN = 0

C BDF = 0.

C CDF = 0.

C DDF = 0.10

C INITIALIZATION OF TOTAL MOLES IN (SOLIN) AND TOTAL MOLES OUT (SOLOUT)

C DO 130 I = 1,3

C SOLIN(I) = 0.0

C SOLOUT(I) = 0.0

C 130 CONTINUE

C DO 135 I = 1,3

C SOLIN(I) = SOLIN(I) + APROP(I) * TPDP(I) + OFDR(T) + TPDP(I) * TPDP(I)

C IF (TPDP(I) .LT. 0) SOLIN(I) = SOLIN(I) - APROP(I) * TPDP(I)

C 135 CONTINUE

C SPH = 0.399 * CTBP + 0.321 *(1.0 - CTBP)

C K = TIME INTERVAL COUNTER (MOD 100)

C CONTINUE

C K = 1

C PERFORMS STAGE CALCULATIONS FOR EACH TIME INTERVAL

C CALL STAGES(SPH)

C DO 150 J=1,NSTOST

C TPROF(J,1) = TPROF(J,2)

C DO 150 I=1,4

C IF (I .LT. 1.0) 999999

C Y(J,1) = X(J,1) * 1.0

C 999999

C BNP(J,1) = BNP(J,2)

C 150 CONTINUE

C IF NUMBER OF TIME INTERVALS IS LESS THAN THE NUMBER OF STAGES,

C ONLY CALCULATION OF SOLIN,SOLOUT, AND PERCENT STEADY STATE

C IF (ICEN.NQ.0. AND .K.LT.NSTOST) GO TO 210

C IF SHUTDOWN (ICALC=0), CHECK FOR NEAR ZERO CONCENTRATION

C IF (ICALC.EQ.1) GO TO 160

C FOR SHUTDOWN, ICALC=0, TEST FOR COMPONENTS 1 AND 2 = 0, NOT COMPONENT 3

C DO 155 J=1,NSTOST

C IF (Y(J,1).GT.0.0000001) GO TO 210

C IF (Y(J,1).LT.0.0000001) GO TO 210

C 155 CONTINUE

C GO TO 205

C CALCULATION OF PERCENT STEADY STATE

C CALCULATE TOTAL MOLES IN (SOLIN) AND TOTAL MOLES OUT (SOLOUT)

C CONTINUE

C DO 165 J=1,3

C SOLOUT(I) = A(NSTOST) * T(I,NSTOST,1) * (O(I) * Y(I,1,1)

C DO 165 J=1,NSTOST

C 165 CONTINUE

C
SOLOUT(1) = SOLOUT(1) + ALVRT(J) * X(I, J, 1) + OLVRT(J) * I(I, J, 1)

CONTINUE

DO 170 J = 1, NOST

SOLOUT(2) = SOLOUT(2) + ALVRT(J) * RN(J, 1)

CONTINUE

SOLOUT(2) = SOLOUT(2) - A(NTOST) * RN(UMST, 1)

DO 180 I = 1, 3

IF (SOLIN(I) .GT. O.) GO TO 175

DP(I) = O.

GO TO 180

CONTINUE

DP(I) = ABS((SOLIN(I) - SOLOUT(I)) / SOLIN(I))

CONTINUE

ADF = AMAX1(DP(1), DP(2), DP(3))

IF ADF = BD(1) (PERCENT STEADY STATE FOR CURRENT TIME INTERVAL) AS PREVIOUS TIME INTERVAL), TERMINATE CALCULATIONS

IF (ADP.NE.BDP) GO TO 185

CDP = ADF

GO TO 205

C 185 CONTINUE

IF (1.0 .GE. 3. AND. DDP.LT.0.004) DDP = 2.*DDP

IF (ADP.GT.DDP) GO TO 210

C 190 CONTINUE

IF (DDP.LT.0.100) GO TO 195

JX=K+100*I

PPFD = 100. * (1.0 - DDP)

DDP = 0.10

GO TO 210

C 195 CONTINUE

IF (ICEN.GT.0) GO TO 205

IF (IPR.EQ.0) GO TO 215

IF (IPR.EQ.-1.AND. (K.EQ.20.0.R.K.EQ.60.0.R.K.EQ.80.0.R.K.EQ.100.0)) GO TO 215

GO TO 255

C 215 CONTINUE

C DETERMINE IF TIME INTERVAL IS TO BE PRINTED

IF (IPR.EQ.0) GO TO 215

IF (IPR.EQ.-1.AND. (K.EQ.20.0.R.K.EQ.40.0.R.K.EQ.60.0.R.K.EQ.80.0.R.K.EQ.100.0)) GO TO 215

IF (IPR.EQ.1.AND. K.EQ.8) GO TO 215

GO TO 255

C 215 CONTINUE

C CONVERSION BACK TO VOLUME UNITS

DO 230 J = 1, NOST

X(I, J, 2) = X(I, J, 2) - RR(J, 2) * B(H(I, J, 2))

DEHH = 1.0E-05 * (X(I, J, 2) + 0.13*X(I, J, 2) + 0.0309*X(I, J, 2) + 0.031*I(I, J, 2))
CONVERT TOTAL HOLES IN AND OUT TO G/L AND PRINT

IF INCREHENT TIPIE INTERVAL COUNTER

CONVERT TO G/L

CONTINUE

DO 225 J = 1,3

IF (ALVRT(J) .GT.0.) PRINT 1021, AOUT(J)

T(J,2) = T(J,2) / DENO

OOUT(J) = -ALVRT(J) / DENO

CONVERT TO G/L

DO 235 JJ = 1,4

Y(I,J,2) = Y(I,J,2) / DENO

CPO(J,J) = MAX(Y(J,J,2), CPO(J,J))

CONTINUE

PRINT FOR A GIVEN TIME INTERVAL

PRINT 1019

GO TO 240

CONTINUE

PRINT 1022, J, (T(J,2) , I=1,3), AOUT(J)

IF (ALVRT(J) .GT.0.) PRINT 1021, AOUT(J)

CONTINUE

PRINT 1023

GO TO 250

CONTINUE

PRINT 1024, J, (T(J,2), I=1,3), OOUT(J), CODIN(J), TPROF(J,2)

CONTINUE

IF LESS THAN OR EQUAL TO M, PERFORM STAGE CALCULATIONS FOR ANOTHER

TIME INTERVAL

IF (K.EQ.M) GO TO 145

IF SHUTDOWN (ICALC=0), BYPASS PRINTOUT OF PERCENT STEADY STATE

IF (ICALC.EQ.0) GO TO 260

PRINT PERCENT STEADY STATE AFTER EVERY 100 TIME INTERVALS

AND OTHER CASES WHEN K=M

APDF = 100. * (1.0 - ADP)

PRINT 1025, APDF

IF (DPP.LT.0.0) PRINT 1026, PPDF, JK

IF (DPP.LT.0.005) PRINT 1026, PPDF, JJJJK

IF (DPP.LT.0.0005) PRINT 1026, PPPPDF, JJJJK

IF (DPP.LT.0.00005) PRINT 1026, PPPPPDF, JJJJK

IF (DPP.LT.0.000005) PRINT 1026, PPPPPPDF, JJJJK

IF (DPP.LT.0.0000005) PRINT 1026, PPPPPPPDF, JJJJK

IF (DPP.LT.0.00000005) PRINT 1026, PPPPPPPPDF, JJJJK

IF (DPP.LT.0.000000005) PRINT 1026, PPPPPPPPPDF, JJJJK

PRINT 1026

CONTINUE

PRINT 1028

CONTINUE

PRINT TOTAL HOLES IN AND OUT TO G/L AND PRINT
CHANGE SPEED AND EXIT STREAM, EVEN IF NO CHARGE IS MADE. NO PROFILE CARDS ARE REQUIRED. IF CHANGE = 1, NEW FEED STREAM AND OUT CARDS ARE REQUIRED FOR EACH CASE. FEED AND EXIT STREAM, EVEN IF NO CHANGE IS MADE. NO PROFILE CARDS ARE REQUIRED.

INITIAL PROFILE IS SET AS THAT AT END OF LAST CALCULATION.

1  PROG 0
DO 285 J=1,A
DO 285 J=1,NOST
IP(IPNC.LE.0)
GO TO 280
READ 1034, IDCHG, IPDF
IF(IDPF.EQ.4) READ 1034, ICALC, IOUT, IPR, IFRCH, ICALPL
IF(ICEN.EQ.0) GO TO 10
CALL PLOTR (M+100+ICEN,ICALPL,NWJST,CFA,CPO)
IF(IPNCH.LE.0) PRINT 1032, TIMINT
TIMINT=STVOL (1)
IF(IPG.EQ.1) READ 103U,ICALC,1OUT,IPR,IPRC,ICALPL
DO 285 1=1,4
X (I,1),X (I,2),X (I,3),X (I,4),X (I,5),X (I,6),X (I,7),X (I,8) =X (I, J, 2)
DO 285 J=1,NTOST
1 PORMAT(UOX,IO,
1018 PORMAT('0PRASE RATIOS EQUAL PLOW RATIOS',31, 'STAGE NO.',ZX,'A/C EAASE RATIO',/)
1018 PORMAT('0PRASE RATIOS EQUAL PLOW RATIOS',31, 'STAGE NO.',ZX,'A/C EAASE RATIO',/)
1015 PORMAT(2X,12,0X,1PE9.3,17X,U (211E9.3))
1016 PORMAT(2X,12,0X,1PE9.3,17X,U (211E9.3))
1017 PORMAT(2X,12,0X,1PE9.3,17X,U (211E9.3))
1018 PORMAT(2X,12,0X,1PE9.3,17X,U (211E9.3))
1019 PORMAT(2X,12,0X,1PE9.3,17X,U (211E9.3))
1020 PORMAT(2X,12,0X,1PE9.3,17X,U (211E9.3))
1021 PORMAT(2X,12,0X,1PE9.3,17X,U (211E9.3))
SUBROUTINE PROF1
COMMON/PROF/ IPRO, X(4,25,2), Y(4,25,2), XFD(4,25), YFD(4,25), [...
1 CONTINUE RETURN
C
10 CONTINUE RETURN
C
30 CONTINUE IF (INDEX.EQ.1) GO TO 10
C
C FOR IPRO = 0, THE ZERO PROFILE IS ALREADY IN X AND Y ARRAYS
C
END

DATA /10 CONTINUE PROF 140/
10 CONTINUE
1027 FORMAT ('(G/L)',7X,'(H)',5X,'OP STAGE')
1029 FORMAT ('TOTAL U CONCENTRATION IN (G/L) INDEX ',3 X, 'STAGE')
1030 FORMAT ('TOTAL U PLUTONIUM IN ',2X, 'TOTAL G/L URANIUM IN:',2X,IPE11.4,
1031 FORMAT ('TOTAL MOLES HNO3 IN ':,5X, 'PE11.4', 1, ' ', OUT(,411.4)
1032 FORMAT ('MINUTES/TIME INTERVAL:',F7.3)
1033 FORMAT ('(F8.6,F8.7,F8.6,F8.4)
1034 FORMAT (512)
C
C
SUBROUTINE PROF1
COMMON/PROF/ IPRO, X(4,25,2), Y(4,25,2), [...
1 CONTINUE RETURN
C
10 CONTINUE RETURN
C
30 CONTINUE IF (INDEX.EQ.1) GO TO 10
C
C FOR IPRO = 0, THE ZERO PROFILE IS ALREADY IN X AND Y ARRAYS
C
END

DATA /10 CONTINUE PROF 140/
10 CONTINUE
1027 FORMAT ('(G/L)',7X,'(H)',5X,'OP STAGE')
1029 FORMAT ('TOTAL U CONCENTRATION IN (G/L) INDEX ',3 X, 'STAGE')
1030 FORMAT ('TOTAL U PLUTONIUM IN ',2X, 'TOTAL G/L URANIUM IN:',2X, IPE11.4,
1031 FORMAT ('TOTAL MOLES HNO3 IN ':,5X, 'PE11.4', 1, ' ', OUT(,411.4)
1032 FORMAT ('MINUTES/TIME INTERVAL:',F7.3)
1033 FORMAT ('(F8.6,F8.7,F8.6,F8.4)
1034 FORMAT (512)
C
C
SUBROUTINE PROF1
COMMON/PROF/ IPRO, X(4,25,2), Y(4,25,2), XFD(4,25), YFD(4,25), PROF 40
1 PROF 40
C
C DEFINE FEED STREAMS
C
I = STAGE NUMBER THAT FEED ENTERS JHAS = 1 FOR AQUEOUS FEED
C FPRO = FEED FLOW RATE (VOLUME UNITS) 0 FOR ORGANIC FEED
C COM1 = URANIUM CONTENT IN G/L INDEX = 1 IF MORE FEED CARDS FOLLOW
C COM2 = PLUTONIUM CONTENT IN G/L 0 FOR LAST CARD
C CCOME = ACID Molarity FROM INEXTRACTABLE SALTS, INCLUDING THE REDUCTANT
C CEMER PU REDUCTANT NORMALITY AS NEGATIVE PU CONCENTRATION.
C
1 CONTINUE RETURN
C
1 PROFI 10
C
10 CONTINUE RETURN
C
30 CONTINUE IF (INDEX.EQ.1) GO TO 10
C
C ORGANIC FEED
C
C
10 CONTINUE RETURN
C
C AQUEOUS FEED
C
20 CONTINUE CONTINUE
APROF(I) = PROF
1 CONTINUE IF (INDEX.EQ.1) GO TO 10
C
C FOR IPRO = 0, THE ZERO PROFILE IS ALREADY IN X AND Y ARRAYS
C
END
SUBROUTINE PLOYS (STVOL)
COMMON/PLYS/IRATIO, IOUT, IVOL, RECY(25), ICNCHG, ALVRT(ZS), GLVRT(25)
COMMON/PEED/NTOST, AFDRT(25), OPDRT(25)
COMMON/REC/A(25), 0(25), RRI0(25), RCYCA(25), RCPC0(25)
DIMENSION STVOL(25)

C DEFINE OUTGOING STREAMS OTHER THAN AQUEOUS RAPPINATE AND ORGANIC PRODUCT
C I = STAGE NUMBER THAT STREAM LEAVES JHAS = 1 FOR AQUEOUS STREAM
C INDEX = 1 IF MORE CARDS FOLLOW 0 FOR LAST CARD OTRT = EXIT FLOW RATE (VOLUME UNITS)
C (FLOWS GIVEN IN SOLUTE-FREE VOLUME UNITS)

10 CONTINUE
READ 1001, I, JHAS, OTRT, INDEX
IF(JHAS.EQ.1) GO TO 15
C ORGANIC STREAM
OLVRT(1) = OTRT
GO TO 20
C AQUEOUS STREAM
15 CONTINUE
ALVRT(1) = OTRT
C MORE CARDS?
20 CONTINUE
IF(INDEX.EQ.1) GO TO 10
C WE DO NOT PROVIDE FOR RETURNING STREAMS
C SET AQUEOUS AND ORGANIC INTERSTAGE FLOW (1 AND 0)
25 CONTINUE
DO 35 J=1, NTOST
IF(J.GT.1) GO TO 30
A(J) = A(J-1) + ALVRT(1) - ATRT(1)
A(J) = A(J-1) + ATRT(1) - ALVRT(1)
A(J) = A(J-1) + ATRT(1) - ALVRT(1)
A(J) = A(J-1) + ATRT(1) - ALVRT(1)
GO TO 35
30 CONTINUE
35 CONTINUE
C THE INTERSTAGE FLOWS ARE NOW SET
C DEFINE PHASE RATIOS
30 DO 40 J=1, NTOST
RCYCR(J) = 0.0
RCYCO(J) = 0.0
40 CONTINUE
CALCULATE PHASE RATIO WHEN IRATIO=0, PHASE RATIO=FLOW RATIO
DO 45 I=1,NTOST
RAIO(I) = (ALVET(I)*A(I))/((OLVET(I)*O(I))
45 CONTINUE
GO TO 60
C
DO NOT REDEFINE PHASE RATIO IF ICHNGE=1
C
CONTINUE
IF(ICHNGE.EQ.1) GO TO 70
C
DEFINE PHASE RATIOS WHEN IRATIO=1, PHASE RATIOS DO NOT EQUAL
FLOW RATIOS
C
NUMBER OF STAGES HAVING PHASE RATIO SHOWN
READ 1002,I,RATIO
DO 55 J=K,I
RAIO(I) = RATIO
I=K+1
GO TO 50
C
CALCULATE NECESSARY RECYCLE FLOWS
C
TYPE 1 IS RECYCLE OF ONE PHASE ONLY, TO SATISFY PHASE RATIO
C
USED WHEN IRATIO = 1
C
TYPE 2 IS RECYCLE OF BOTH PHASES WITH PHASE RATIO RAIO(I)
C
TO ALLOW TOTAL STAGE FLOW TO EQUAL FLOMAX
C
USED WHEN IVOL = 0.2
C
RECYCLE VOLUMES AND RATIOS ARE SOLUTE-FREE VALUES
C
C
CONTINUE
IF(IVOL.EQ.1) GO TO 100
C
FLOTOT = TOTAL FLOW LEAVING A STAGE
C
FLOMAX = GREATEST TOTAL FLOW FROM A STAGE
C
60 CONTINUE
IF(IVOL.EQ.1) GO TO 100
DO 65 I=1,NTOST
FLOTOT = ALVET(I) + A(I) + OLVET(I) + O(I)
RECT(I) = FLOTOT
FLOMAX = MAX(1,FLOTOT,FLOMAX)
65 CONTINUE
IF(IVOL.EQ.0) GO TO 90
IF(IVOL.EQ.1) GO TO 100
IF(IVOL.EQ.2.OR.IVOL.EQ.3) GO TO 110
C
CALCULATE FLOMAX,BCTC1,BCTCO,RECT,FLOMAX FOR IRATIO=1
C
AND IVOL=0,1,2,3
C
FLO = TOTAL AQUEOUS FLOW LEAVING A STAGE
C
OLF = TOTAL ORGANIC FLOW LEAVING A STAGE
C
BFL = RATIO OF AQUEOUS TO ORGANIC FLOW LEAVING A STAGE (FLO/OLF)
C
BCTCA = AQUEOUS RECYCLE TO SATISFY PHASE RATIO
C
BCTCO = ORGANIC RECYCLE TO SATISFY PHASE RATIO
C
70 CONTINUE
DO 85 I=1,NTOST
AFL = ALVET(I) + A(I)
OLF = OLVET(I) + O(I)
BFL = AFL/OLF
85 CONTINUE
C
COMPARISON CP FLOW RATIO (BFL) TO PHASE RATIO (RAIO)
C
IF(BFL.GT.RAIO(J)) GO TO 75
IBL = BFL-RAIO(J) GO TO 80
FLOTOT=FLOTOT*(RAIO(J)+1.0)/(BFL+1.0)
BCTCA(J) = FLOTOT - APL - AFL
GO TO 80
75 CONTINUE
BCTC(J)=FLOTOT*BFL*(RAIO(J)+1.0)/(BFL*(1.0+RAIO(J))
BCTCO(J) = FLOTOT - APL - ABL
80 CONTINUE
RECT(J)=FLOTOT
FLOMAX = MAX(1,FLOTOT,FLOMAX)
85 CONTINUE
C
FLOMAX CONTAINS THE LARGEST TOTAL FLOW FROM A STAGE - STAGES HAVING APL < AFL
C
TOTAL FLOW LESS THAN FLOMAX MUST ENTER RECYCLE
C
OF TYPE 2
C
IF(IVOL.EQ.0) GO TO 90
IF(IVOL.EQ.1) GO TO 100
IF(IVOL.EQ.2.OR.IVOL.EQ.3) GO TO 110
C
90 CONTINUE
C
IVOL=0; IRATIO=0,1
DO 95 I=1,NTOST
   RECY(I) = FLOMAX - RECY(I)
95 CONTINUE
RETURN
C
C IVOL=1, IRATIO=0, 1
C
100 CONTINUE
   DO 105 I=1,NTOST
      RECY(I) = 0.0
   RETURN
105 CONTINUE
C
C DETERMINE STAGE VOLUME
STAGE VOLUMES ARE ZERO
C
C
C IF ICHANGE=0, READ STAGE VOLUMES
C IF ICHANGE=1, BYPASS READING OF STAGE VOLUMES
C
110 CONTINUE
   IF(ICHANGE.EQ.1) GO TO 125
   IF(VOL.EQ.2) GO TO 120
C
C IVOL=3; STAGE VOLUMES ARE EQUIVALENT AND SPECIFIED
IRATIO=O, 1
C
READ 1003, VOL
   DO 115 J=1,NTOST
      STVOL(J) = VOL
   115 CONTINUE
   GO TO 125
C
C IVOL=2; STAGE VOLUMES ARE INDEPENDENTLY UNEQUAL
C
120 CONTINUE
   READ 1004, (STVOL(J),J=1,NTOST)
C
C STAGE VOLUMES ARE SOLUTE-FREE VOLUMES
C
C CALCULATE LENGTH OF TIME INTERVAL (TIME) AND RECY FOR IVOL=2, 3
C
125 CONTINUE
   TIME=0.0
   DO 135 I=1,NTOST
      RECY(I) = RECY(I)/STVOL(I)
      TIME = MAX(TIME,RECY(I),TIME)
   135 CONTINUE
   FLOMAX = TIME
   DO 145 I=1,NTOST
      RECY(I) = (FLOMAX - RECY(I))*STVOL(I)
   145 CONTINUE
C
C 100 FORMAT(12F8.0)
1001 FORMAT(12F8.0,12)
1002 FORMAT(12F8.0)
1003 FORMAT(10F8.0)
1004 FORMAT(10F8.0)
C
RETURN
END

SUBROUTINE STAGES(SPA)
C DETERMINE AINV(4),CN(4)
C COMMON/STGS/, NSOLU,COOH(25),X(4,25),Y(9,25,2),1FD(4,25),YPO(4,25),
   .Y(9,25,2),IPRO,X(4,25,2),Y(9,25,2),1FD(4,25)
   .YPO(4,25),
C COMMON/REC/, A(25),0(25),RA(25),RCYCA(25),RCYCO(25)
C COMMON/DIST/,CTBP,ARY(4),MRT(0),TO,R1(25,2),RNFO(25)
   .TPROF(25,2),APOTEB(25) .OPOTEB(25)
C
C PERFORM STAGE CALCULATIONS FOR CURRENT TIME INTERVAL - CONSIDER
C INPUTS FROM ADJACENT STAGES, FEED STREAMS, AND MOST IMPORTANTLY
C STAGE VOLUMES - RECYCLE A RESULT OF STAGE FLOW RATES
C LESS THAN FLOMAX (TYPE 2) AND PHASE RATIO NOT EQUAL TO FLOW
C RATIO (TYPE 1)
C
C 100 FORMAT(12F8.0)
1001 FORMAT(12F8.0,12)
1002 FORMAT(12F8.0)
1003 FORMAT(10F8.0)

C AB - AQUEOUS RECYCLE TO FILL STAGE
C OR - ORGANIC RECYCLE TO FILL STAGE
C RBCA - AQUEOUS RECYCLE TO SATISFY PHASE RATIO
C RBCO - ORGANIC RECYCLE TO SATISFY PHASE RATIO
C AT - TOTAL AQUEOUS FLOW WITHIN A STAGE =
C ALLOW ONLY 20 ITERATIONS STA 1080
C STA 1090
C STA 1070
C STA 1030
C
C STAG 890
C COMPOSITION (ARY) AT THE STAGE EQUILIBRIUM TEMPERATURE (TEODC) STAG 880
C
C INDEX IS THE FIT COUNTER
C UCOR CALCULATES DISTRIBUTION RATIOS (DTRY) FOR EACH TRIAL AQUEOUS PHASE
C COMPOSITION (ARY) AT THE STAGE EQUILIBRIUM TEMPERATURE (TEODC) STAG 880
C
C CALL UCOR(TMPF(JJ),J)
C GO 70 J = 1,MTST

IF(J(GT.1)) GO TO 10

AR(J,J) = (APDRT(J) *ENP(J) * (AR(J) + BCTCA(J)) * RN(J,1)) / AT(J)
GO TO 15

10 CONTINUE

J(J,J) = (APDRT(J) *ENP(J) * (AR(J) + BCTCA(J)) * RN(J,1)) * RN(J,1)

1 A(JJ) = (RN(J,J) * RN(J,J)) / AT(J)

15 CONTINUE

DO 20 J = 1,NSOLU

A(J) = RN(J,J) * RN(J,J) / AT(J)

GO TO 20

20 CONTINUE

IF(J(J,J) = 1)

DO 30 J = 1,MTST

G(J) = EXPRT(J) * ENP(J) * (AR(J) + BCTCA(J)) * RN(J,1) * RN(J,1)
GO TO 35

30 CONTINUE

GIN(J) = EXPRT(J) * ENP(J) * (AR(J) + BCTCA(J)) * RN(J,1) * RN(J,1)

35 CONTINUE

AIR(J) = RN(J,J) * RN(J,J) / AT(J)

GIN(J) = AIR(J) *RN(J,J)

ABT(J) = X(J,J,1)

IF(ABT(J) LT.0.1)

40 CONTINUE

ABT(J) = X(J,J,1)

45 CONTINUE

ABT(J) = X(J,J,1)

50 CONTINUE

GO 50

50 CONTINUE

GO 50

55 CONTINUE

60 CONTINUE

TMPF(J,J) = AIRT(J) / (AIR(J) + BCYCA(J)) * RN(J,1)

C C = 0.001

CCD = 0.001

C MCK IS THE ITERATION COUNTER
C MDX IS THE FIT COUNTER
C MCK = 0

65 CONTINUE

MDX = 0

60 CONTINUE

GO TO 50

CALL UCOR(TMPF(JJ),J)
GO 70 J = 1,MTST

TSIN = AIR(J) + RATO(J) + GIN(J)

IF(TSIN LT.0.1)

DTF(J) = 0.

DTRY(J) = 0.

X(J,J,2) = YPD(J) / (RATO(J) + DTRY(J))

IF(X(J,J,2) LT.0.1)

GO TO 70

DI = (X(J,J,2) - ARY(J)) / X(J,J,2)

DIF = ABS(DI)

ARY(J) = X(J,J,2)

IF(DIF LE.0.01)

GO TO 70

CONTINUE

MDX = MDX + 1

70 CONTINUE

MCK = MCK + 1

C ALLOW ONLY 20 ITERATIONS
C STA 1020
C STA 1030
C STA 1040
C STA 1050
C STA 1060
C STA 1070
C STA 1080
C STA 1090
SUBROUTINE UCOR (TERPC, J)
COMMON/tISI/ CTBP, ARY(U), DTRY (4), TO, RN(25,2), RRFD(25)

UCOR 10
UCOR 20

ncnu
In

UCOR 20

/REDUCE 9 FOR EACH

UCOR 50

PUTOT=ARY(2)-RN(J,2)

IF(UAR.LT.0) UAM 0.

IF(HAR.LT.0) HAM = 0.

IF(SNITR.LT.0) SNITR = 0.

PUIII=PUTOT-eryuhn

IF(PUIII.LT.0) PUIII = 0.

TNM = HAM + 2.*0.11M + 2.*PUAM + SNITR + 4.*POIII

IF (TNM.EQ.0.0) TNM = 1.0

TERPRK = 1000./(TEMPC + 213.16)

DRT = TERPRK - 3.3539

UK = 3.7*TEM**1.0 + 1.4*TEM**3.9 + 0.01**TEM**7.3

DF = DF*TEM**(-0.17) - 3.

PK = PK*(2.0 + .55*TEM**1.25 + .0074*TEM**2)

IF (TEMPC .LT. 25.) PX = PX*EXP(2.5*TEM)

IF (TEMPC .GT. 25.) PK = PX*EXP(-2.2*TEM)

IF (TEMPC .LT. 25.) HK1 = HK1*EXP(0.34*TEM)

HK2 = HK1

A = 2.*(OK*URfl + PUK*POIR + HK2*EAII)

B = HK1*HAM + 1.

C = -1.

TF= -C/B

GO TO 15

CONTINUE

TF = (-A + SQRT(B**2 -4.*A*C))/(2.*A)

CONTINUE

DH1 = HK1*TF

DH2 = HK2*TF**2

DO = UK*TF**2

DPU = DPU*TF**2

DTRY (1) = DO

DTRY (2) = DPU

DTRY (3) = DH

RETURN

END
C I AND A-REDUCED AQUEOUS CONCENTRATIONS
C Y AND O-REDUCED ORGANIC CONCENTRATIONS
C TITLE-GRAPH TITLE
C YTAG-X AXIS LABEL
C XTAG-Y AXIS LABEL
C
C DIMENSION CFA(25),CFO(4),X(4),Y(4),A(25,4,4),O(25,4,4),MSTA(25)
C REAL*T TILG(10),TILX(10),TILA(10)
C REAL*8 TLEG(4)/'FRACTION', 'OF STATE', 'OF STATE', 'TIME' /,
C 1 DESCRI(13)/'STATE TIME','STAGE TIME','STATE SUBSTATE',
C 2 'STATE TIME','STAGE TIME','STATE', 'OPERATION',
C 3 'STATE TIME','STAGE TIME','STATE', 'OPERATION',
C 4 'STATE TIME', 'STAGE TIME', 'STATE', 'OPERATION',
C INTEGER*4 ISYIB(U)/1,2,3,4/,
C INTEGER*4 ISYIBP(4)/1,2,3,4/
C REAL*8 TLEG2(2)/'COMPONENT', 'TS$
C 1 DESCR2(U)/'URANIUM', 'PLUTONIUM', 'NITRIC ACIDS' /
C C ZERO REDUCED CONCENTRATION ARRAYS
C DO 10 I=1,25
C DO 10 J=1,4
C DO 10 K=1,U
C A(I,J,R) =O.
C A(I,J,R)=O.
C 10 CONTINUE
C C CALCULATE REDUCED CONCENTRATIONS
C UNIT 10 READS PRINTOUT FOR EACH TIME INTERVAL
C REIND 11 URITE(6,1001) CFA,CPO
C DO 25 I=1,ROUNT
C DO 25 J=1,NTOST
C READ(11) L,X,Y
C DO 20 R=1,U
C IF(CFI(K).EQ.O.) GO TO 15
C X(K)=X(K)/CFA(K)*100.
C IF(CFO(K).EQ.O.) GO TO 20
C Y(R)=Y(R)/CPO(K)*100.
C URITE(10) L.1.Y
C REIND 10
C REIND 11
C IP(ICALPL.EQ.2) GO TO 95
C 15 CONTINUE
C 20 CONTINUE
C 25 CONTINUE
C C WILL PLOT CURVES FOR EACH TIME INTERVAL
C C ASSIGN ARRAY INDEX FOR PLOT GRAPH
C DO 40 I=1,U
C II=U-I+1
C INDEX=2*KOUNT/2*II
C 30 CONTINUE
C DO 35 K=1,NTOST
C READ(10) L,(A(K,J),J=1,4), (O(K,J),J=1,4)
C 35 CONTINUE
C IF(L.NE.INDEX) GO TO 30
C REIND 10
C REIND 11
C IP(ICALPL.EQ.2) GO TO 95
C 40 CONTINUE
C C PLOT PROFILE GRAPHS
C READ(5,1003) TIL
C READ(5,1003) TILA
C xmin=1.
C xmax=NTOST
C C DETERMINE MIN AND MAX FOR Y AXIS
C YMAX=0.
C YMIN=1.1
C DO 45 I=1,NTOST
C DO 45 J=1,4
C DO 45 K=1,3
C YMAX=MAX(YMAX,A(I,J,K),O(I,J,K),YMIN)
C IF(A(I,J,K).EQ.O. AND. O(I,J,K).EQ.O.) GO TO 45
C O(I,J,K),YMIN)
C IF(O(I,J,K).EQ.O.) YMIN=MIN(YMIN,O(I,J,K),YMIN)
C IF(C(I,J,K).EQ.O.) YMIN=MIN(YMIN,C(I,J,K),YMIN)
C 45 CONTINUE
C DO 50 I=1,3
C C AQUEOUS
C DO 50 J=1,NTOST
C IF(A(I,J,3).GT.0.) GO TO 55
C 50 CONTINUE
C GO TO 90
CONTINUE
C
CALL PIXPLT(KMIN,KMAX,KMIN,KMAX,'VLOG','RECH',0.,0.,
1 BUFFER,4000,'S.R.WATSONS')
C
READ(5,1003) YTAG
CALL TITLE(O.4,TTL,YTAG,YTAG)
C
NKOST=NKOST-1
DO 51 J=1,NKOST
IF(A(J,J,J,L) .EQ.0.) CALL PPL(A(J,J,L),0-J1,INTOST,E51)
51 CONTINUE
C
DO 70 J=1,U
DO 70 JJ=1,INTOST
IF(A(J,JJ,J,L) .GT.0.) GO TO 75
70 CONTINUE
C
CALL PIXPLT(O.4,TTL,XTAG,YTAG)
DO 85 I=1,U
DO 85 JJ=1,INTOST
IF(A(I,J,J,L) .EQ.0.) CALL PPL(A(I,J,J,L),0-J1,INTOST,E85)
85 CONTINUE
C
CALL LEGEND(TLEG1,ISTMB4,DESCR1,2.1,1.5)
C
DO 90 I=1,U
DO 90 J=1,INTOST
IF(A(I,J,J,L) .EQ.0.) GO TO 90
90 CONTINUE
C
CALL PIXPLT(O.4,TTL,XTAG,YTAG)
DO 105 I=1,U
DO 105 J=1,INTOST
IF(A(I,J,J,L) .EQ.0.) CALL PPL(A(I,J,J,L),0-J1,INTOST,E105)
105 CONTINUE
C
C ORGANIC

C READ STAGES TO BE PLOTTED

C READ(5,1004) (NSTA(I),I=1,NKOST)

C WILL GENERATE 2 PLOTS FOR EACH NONZERO VALUE OF NSTA

C DO 130 I=1,NKOST

C IF(NSTA(I).EQ.0.) GO TO 130

C AQUEOUS

C CALL PIXPLT(KMIN,KMAX,KMIN,KMAX,'LINE','RECH',0.,0.,

1 BUFFER,4000,'S.R.WATSONS')

C READ(5,1003) YTAG

C CALL TITLE(O.4,TTL,YTAG,YTAG)

C DO 110 J=1,KOST

C IF(KMAX .GT. KOST) CALL QCSIZE(KMAX/10.,10.)

C KMIN=0.

C XMAX=KOST

C IF(KMAX .GT. KOST) CALL QCSIZE(KMAX/10.,10.)

C XMIN=0.

C XMAX=100.

C READ STAGES TO BE PLOTTED

C READ(5,1004) (NSTA(I),I=1,NKOST)

C CALL PIXPLT(KMIN,KMAX,KMIN,KMAX,'LINE','RECH',0.,0.,

1 BUFFER,4000,'S.R.WATSONS')

C READ(5,1003) YTAG

C CALL TITLE(O.4,TTL,YTAG,YTAG)

C DO 110 J=1,KOST

C IF(KMAX .GT. KOST) CALL QCSIZE(KMAX/10.,10.)

C XMIN=0.

C XMAX=100.

C AQUEOUS

C CALL PIXPLT(KMIN,KMAX,KMIN,KMAX,'LINE','RECH',0.,0.,

1 BUFFER,4000,'S.R.WATSONS')

C READ(5,1003) YTAG

C CALL TITLE(O.4,TTL,YTAG,YTAG)

C DO 110 J=1,KOST

C IF(KMAX .GT. KOST) CALL QCSIZE(KMAX/10.,10.)

C XMIN=0.

C XMAX=100.

C AQUEOUS

C CALL PIXPLT(KMIN,KMAX,KMIN,KMAX,'LINE','RECH',0.,0.,

1 BUFFER,4000,'S.R.WATSONS')

C READ(5,1003) YTAG
CALL TITLE(0,A,XTAG,YTAM)
DO 125 J=1,KOUNT
   DO 120 K=1,NTOST
      READ(10) L,X,Y
      IF(K.NE.NSTA(1)) GO TO 120
      XPOINT=L
      DO 115 II=1,3
         CALL PNTPLT(XPOINT,Y(II),II,-1)
      CONTINUE
   CONTINUE
   120 CONTINUE
   125 CONTINUE
   REWIND 10
   CALL LEGEND(TLEG2,ISTMB,3,DESCR2,2,-3.,1.)
   CONTINUE
   CALL ADVANS
   1001 FORMAT(' ',IP4X11.3,4X,4E11.3)
   1002 FORMAT(' ',4X,1P4E11.3,4X,4E11.3)
   1003 FORMAT(10X)
   1004 FORMAT(25X)
   CONTINUE
   RETURN
END

SUBROUTINE PPL(A,J,NTOST,*)
C
C PLOT NONZERO POINT ON THE CURVE
C
DIMENSION A(25)
DO 10 I=1,NTOST
   IDASH=0
   XPOINT=I
   IF(I.EQ.1) IDASH=-1
   IF(I.GT.1.AND.A(I-1).EQ.0.) IDASH=-1
   IF(A(I).GT.0.) CALL PNTPLT(XPOINT,A(I),J,IDASH)
   10 CONTINUE
RETURN 1
END
APPENDIX B

Sample Input and Output
Two Examples of Input to SEPHEX

<table>
<thead>
<tr>
<th>Case 1</th>
<th>CO EXTRACTION RUN</th>
<th>11 - 20</th>
<th>21 - 30</th>
<th>31 - 40</th>
<th>41 - 50</th>
<th>51 - 60</th>
<th>61 - 70</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 . 5 3 1 1</td>
<td>0 0 1 0 1</td>
<td>0 0 0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 1 0 5 . 1 E</td>
<td>1 0</td>
<td>0</td>
<td>2</td>
<td>2 5 . 1</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 1</td>
<td>1 6 7 7 E 1</td>
<td>4 4 3</td>
<td>3 2</td>
<td>2 5 . 1</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 1 0</td>
<td>1 8 . 0</td>
<td>0</td>
<td>0</td>
<td>2 5 . 0</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
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</table>

Case 2

<table>
<thead>
<tr>
<th>PU EXTRACTION</th>
<th>1 . 5 1 0</th>
<th>0 0 1 0 1</th>
<th>0 0 0</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1 1 1 1 E - 1</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>2 5 . 1</td>
</tr>
<tr>
<td>4 1</td>
<td>1</td>
<td>0</td>
<td>4 9 2 E 1</td>
<td>4 1</td>
</tr>
<tr>
<td>1 0 0</td>
<td>9 . E - 1</td>
<td>0</td>
<td>0</td>
<td>2 5</td>
</tr>
</tbody>
</table>

2
# OUTPUT - CASE 1

## CALCULATIONS FOR A SOLVENT EXTRACTION PROCESS HAVING 2 INTERACTING SOLUTES

### FEED STREAM DATA

<table>
<thead>
<tr>
<th>Stage No.</th>
<th>Uranium (G/L)</th>
<th>Fluoride (G/L)</th>
<th>NO3 (G/L)</th>
<th>SALT NO3 (G/L)</th>
<th>Flow Rate (VCl.OBu2)</th>
<th>Temp (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>2.0000E00</td>
<td>0</td>
<td>0.0000-01</td>
<td>25.0</td>
</tr>
<tr>
<td>15.3 - TBP</td>
<td>11</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.8000-00</td>
<td>25.0</td>
</tr>
</tbody>
</table>

### INITIAL PROFILE

<table>
<thead>
<tr>
<th>Stage No.</th>
<th>Uranium (G/L)</th>
<th>Fluoride (G/L)</th>
<th>NO3 (G/L)</th>
<th>SALT NO3 (G/L)</th>
<th>Flow Rate (VCl.OBu2)</th>
<th>Temp (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>2.1317E-01</td>
<td>0</td>
<td>0.0</td>
<td>25.0</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>2.1317E-01</td>
<td>0</td>
<td>0.0</td>
<td>25.0</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
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<td>2.1317E-01</td>
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<td>0.0</td>
<td>25.0</td>
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</tr>
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<td>25.0</td>
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<td>0.0</td>
<td>25.0</td>
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<td>0.0</td>
<td>25.0</td>
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<td>25.0</td>
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<tr>
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<td>2.1317E-01</td>
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<td>25.0</td>
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</table>

### PHASE RATIOS AND FLOW RATIOS

<table>
<thead>
<tr>
<th>Stage No.</th>
<th>A/O Phase Ratio</th>
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</thead>
<tbody>
<tr>
<td>1 - 3</td>
<td>1.568E-01</td>
</tr>
<tr>
<td>4 - 11</td>
<td>6.460E-01</td>
</tr>
</tbody>
</table>

### STAGE FLOWS (SOLVENT-FREE VOLUMES)

<table>
<thead>
<tr>
<th>Stage Flow Vol.</th>
<th>Aqueous Phase</th>
<th>Recycle 2</th>
<th>Recycle 1</th>
<th>Total</th>
<th>Organic Phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td>Flow Out to Fill for Phase</td>
<td>Recycle 2</td>
<td>Recycle 1</td>
<td>Total</td>
<td>Phase</td>
</tr>
<tr>
<td>1</td>
<td>1.566E-01</td>
<td>2.076E-01</td>
<td>0.0</td>
<td>2.642E-01</td>
<td>1.566E-01</td>
</tr>
<tr>
<td>2</td>
<td>1.566E-01</td>
<td>2.076E-01</td>
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<tr>
<td>3</td>
<td>1.566E-01</td>
<td>2.076E-01</td>
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<tr>
<td>4</td>
<td>6.460E-01</td>
<td>1.156E-00</td>
<td>0.0</td>
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<td>6.460E-01</td>
</tr>
<tr>
<td>5</td>
<td>6.460E-01</td>
<td>1.156E-00</td>
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<tr>
<td>6</td>
<td>6.460E-01</td>
<td>1.156E-00</td>
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<tr>
<td>7</td>
<td>6.460E-01</td>
<td>1.156E-00</td>
<td>0.0</td>
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<tr>
<td>8</td>
<td>6.460E-01</td>
<td>1.156E-00</td>
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<tr>
<td>9</td>
<td>6.460E-01</td>
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<tr>
<td>10</td>
<td>6.460E-01</td>
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<td>1.156E-01</td>
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</tr>
<tr>
<td>11</td>
<td>6.460E-01</td>
<td>1.156E-00</td>
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</tbody>
</table>

### OVERALL FLOWS

<table>
<thead>
<tr>
<th>Stage Flow Vol.</th>
<th>Aqueous Phase</th>
<th>Recycle 2</th>
<th>Recycle 1</th>
<th>Total</th>
<th>Organic Phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td>Flow Out to Fill for Phase</td>
<td>Recycle 2</td>
<td>Recycle 1</td>
<td>Total</td>
<td>Phase</td>
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<td>1.795E-00</td>
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### Transient Behavior Results

#### Solute Concentrations in Effluent from Each Stage

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### ORGANIC PHASE

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99.90 PERCENT STEADY STATE AT OVERALL MATERIAL BALANCE
99.5 PERCENT OF STEADY STATE AFTER TIME INTERVAL 60
99.0 PERCENT OF STEADY STATE AFTER TIME INTERVAL 50
99.5 PERCENT OF STEADY STATE AFTER TIME INTERVAL 00

TOTAL G/L URANIUM IN: 6.77000E 01, OUT: 6.76908E 01
TOTAL G/L FLUORIDE IN: 4.43000E 01, OUT: 4.42566E 01
TOTAL MOLES HNO3 IN: 3.80031E 01, OUT: 3.80031E 01
### Calculations for a Solvent Extraction Process Having 3 Interacting Solutes

**Feed Stream Data**

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**Initial Profile**

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99.90 PERCENT STEADY STATE BY OVERALL MATERIAL BALANCE
90.0 PERCENT OF STEADY STATE AFTER TIME INTERVAL 10
95.0 PERCENT OF STEADY STATE AFTER TIME INTERVAL 11
99.0 PERCENT OF STEADY STATE AFTER TIME INTERVAL 16
99.5 PERCENT OF STEADY STATE AFTER TIME INTERVAL 16

TOTAL G/L CHROMIUM IN: 0.0, OUT: 0.0
TOTAL G/L PILOTIAUM IN: 1.59E02, OUT: 1.91E02
TOTAL MOLES HNO3 IN: 4.32E03, OUT: 4.31E03
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