TITLE
Nuclear material inventory estimation in solvent extraction contractors II

FINAL REPORT FOR THE PERIOD
September 1986 - September 1987

AUTHOR(S)
Adolphe Beyerlein

INSTITUTE
Clemson University, Clemson, South Carolina, U.S.A.

INTERNATIONAL ATOMIC ENERGY AGENCY
DATE November 1987
Nuclear Material Inventory
Estimation In Solvent
Extraction Contactors II

ADOLPH L. BEYERLEIN AND JOHN F. GELDARD

DEPARTMENT OF CHEMISTRY

CLEMSON UNIVERSITY
CLEMSON, SOUTH CAROLINA
Research Performed for the
International Atomic Energy Agency
Vienna
September, 1987
Contract No. 4441/TC
EXECUTIVE SUMMARY

Safeguards studies indicate that the effectiveness of near-real-time nuclear material accounting methods for nuclear fuel reprocessing facilities can be limited by nuclear material inventory variations in the contactors which are used to effect the separation and purification of uranium and plutonium from spent nuclear fuels. There are no direct on-line methods for measuring the contactor inventory. Consequently simple models for estimating the contactor inventory are being developed. In this report, investigations are described in three areas: (i) Improvements in the model that the authors have described previously for the steady state inventory estimation in mixer-settler contactors, (ii) extension of the model for steady state inventory estimation to transient inventory estimation for non-steady state conditions, and (iii) the development of a computer model CUSEP (Clemson University Solvent Extraction Program) for simulating the concentration profiles and nuclear material inventories in pulsed column contactors.

The model for contactors at steady state estimates the inventory from measured nuclear material concentrations in the feed streams according to the relations,

\[ H^0_\alpha = C^\alpha \lambda^\alpha, \]

\[ H^0_\alpha = C^\alpha \alpha \left( \frac{\lambda^\alpha}{\left[ 1 - 2r \left( C^U_\delta U + C^Pu_\delta Pu \right) / 8.71B \right]^2} \right), \]

where \( H^0_\alpha \) is the steady state inventory of nuclear material \( \alpha (\alpha = U \text{ or } Pu) \), \( C^\alpha \) is the feed stream concentration of \( \alpha \), \( B \) is the TB volume percent, and \( r \) is the aqueous feed stream to organic stream flow rate ratio. The first of the above equations is applicable to stripping contactors (\( \eta = s \)) or to plutonium in partitioning contactors (\( \eta = p \)). The second is applicable to A-type contactors (aqueous to organic extraction) or uranium in
partitioning contactors. The parameters $\Lambda_{\alpha}$, $\Gamma_{\alpha}$, $\lambda_{\alpha}$, and $\delta_{\alpha}$ are evaluated from flowsheet data for the contactor when it is put into service and at such times when the flowsheet is modified substantially. Once the parameters of the above equations are evaluated, the model is very easily applied.

Improvements in the above steady state model that are described in this report are the simplification of the methods for evaluating model parameters and development of methods for reducing the equations for a set of contactors coupled by flows to a single equation which estimates the total inventory of the set of contactors directly. The parameter evaluation was simplified by eliminating the distribution coefficients from the equations used for parameter calculation. The estimation of the distribution coefficients requires literature correlations given in terms of in situ acid and nuclear material concentrations within the contactor which are not available and must also be estimated. For A-type and partitioning contactors, the distribution coefficients were replaced with a parameter $\psi$ and the free TBP mole fraction. The parameter $\psi$ is a well defined function of the acid concentrations in the tanks feeding each purification cycle. The free TBP mole fraction can be expressed in terms of the nuclear material concentrations in the feed tanks and the flow rates. Both the acid and nuclear material concentrations in the feed tanks are available as measured data or nominal flowsheet data. For stripping contactors, the distribution coefficients were replaced with simple power law expressions, $(N_{a})^{\varepsilon}$ where $\varepsilon = 0.22$ for plutonium and $\varepsilon = 0.24$ for uranium. The quantity $(N_{a})$ is the total nitrate ion concentration estimated from feed stream acid and nuclear material concentrations.

In addition to simplifying the parameter evaluation in the model for inventory estimation, the separate equations for a set of contactors were reduced to a single equation to directly estimate the total inventory for the set of contactors. The latter simplification is often preferred over estimating the inventories for each contactor separately and then summing them. The equation for a set of contactors is assumed to have the following form,
where the notation (tot) designates the parameter applies to the set of contactors collectively. The $C_a^a$ is the nuclear material concentration in the tank feeding nuclear materials to the set of contactors. The above equation could be applied to the entire plant in which case $C_a^a$ is the nuclear material concentration in the tank feeding the initial purification cycle. When applying Equation (3) to an entire plant, one presumes that inventory variations originate with the stream feeding the initial purification cycle. Most variations that occur in normal operation will be of this type. Exceptions would be during an upset or rinseout-restart sequence where the operator may introduce changes at intermediate purification cycles as well as the first purification cycle. In such cases one would have to revert to estimates based on inventory equations for the single contactors.

The extension of the above described steady state model to the estimation of transient contactor inventories, $H^o_a$, for nonsteady state conditions is based upon the following exponential model for the single contactor,

$$ H^o_a = H^o_a - \Delta H^o_a \exp(-t/\tau), \quad (4) $$

where $H^o_a$ is the steady state inventory, $t$ is time, $\Delta H^o_a (= H^o_a - H^o_a')$ is the difference between the final steady state inventory and the initial inventory, $H^o_a'$ at $t = 0$. The time constant, $\tau$, is estimated from the steady state inventory with the relation,

$$ \tau = \frac{a H^o_a}{F a C_a}, \quad (5) $$
where the product $F^* C_a$ is the nuclear material throughput rate ($F^*$ and $C_a$ being the aqueous feed stream flow rate and feed stream concentration, respectively), $a$ is 0.8 for A-type contactors, 0.6 for partitioning contactors, 1.55 for stripping contactors, and 1.0 for a tank. The contactor $a$ values were obtained by fitting Equations (4) and (5) to a PUBG generated database for each contactor type with standard deviations being less than 7% of the steady state inventory. The $H^0$ and $\Delta H^0$ are estimated from the steady state model or a combination of the steady state model and Equation (4) applied to the preceding process.

The extension of Equation (4) to a system of contactors which are coupled by flows between them is based upon the following expression for an effective time constant, $\tau_{eff}$,

$$\tau_{eff} = \sum_i \tau_i,$$

where $\tau_i$ are the time constants of the individual tanks and contactors which are estimated from Equation (5). It is found that for smaller deviations from steady state, the transient inventory for a coupled system of contactors is accurately estimated from an exponential model (Equation (4)) by replacing $\tau$ with $\tau_{eff}$. For larger transient variations, such as would occur during a rinseout-restart sequence, significant deviations from an exponential model are observed in simulations of a reprocessing system of nine coupled contactors. The simulations are performed with a computer program using a modified PUBG as a subroutine. The inventories based upon computer simulations are well described by the modified exponential relation,

$$H_a = H^0_a - \Delta H^0_a (1 + 0.25 t - 0.55 t^2 + 0.12 t^3) \exp(-t),$$

where $t$ is $\tau/\tau_{eff}$.

The pulsed column computer model CUSEP (Clemson University Solvent Extraction Program) was developed and applied to exemplary contactors of all three types, A-type, stripping, and partitioning contactors. Concentration profiles and inventories calculated
from CUSEP are compared with measured data from pilot scale contactors containing uranium. Excellent agreement between measured and simulated data for both the concentration profile and inventories is obtained. These comparisons demonstrate that the program correctly predicts the concentration dispersion caused by pulsing and the dispersed phase holdup within the contactor. These are the two primary factors differentiating a pulsed column computer model from a mixer-settler computer model.

It is suggested that future research investigate (i) correction of the MUF (Material Unaccounted For) and CUMUF (Cumulative Material Unaccounted For) tests for mixer-settler contactor inventory using the simplified model developed in this work, (ii) development of a simple inventory estimation model for pulsed column contactors similar to that developed for mixer-settler contactors using CUSEP to provide necessary databases, and (iii) identify sources of bias appearing in the MUF and CUMUF tests using computer simulation techniques. Biases may occur in these tests because of measurement errors and their relation to the plant operation. These may be investigated using the computer program developed in this work (described in Appendix C) which simulates the plant operation. The program will need to be modified to also simulate concentration and volume measurement errors.
TABLE OF CONTENTS

EXECUTIVE SUMMARY i
TABLE OF CONTENTS vi
LIST OF TABLES viii
LIST OF FIGURES x
LIST OF SYMBOLS xi

I. Improved Steady State Model for Mixer-Settlers
   A. Introductory Comments 1
   B. More Utilizable Equations for the Parameters 2
   C. Application to a Reprocessing Facility 5
   D. Reductions in Form of the Inventory Estimation Equations 14
   E. Estimation of Contactor Inventory from Average Throughput 18

II. The Nonsteady State Model and Estimation of Contactor
    Inventories
   A. Introduction 22
   B. Development of the Nonsteady State Model 22
   C. The Application of the Inventory Estimation Models 31
   D. Correction of CUMUF for Contactor Inventory 37

III. Pulsed Column Computer Model : CUSEP
    A. Descriptions and Fundamental Theory 43
    B. Pulsed Column Theory 45
    C. Numerical Methods and Calculations 53

IV. Conclusions
   A. Summary 58
   B. Future Research 59

REFERENCES 62
APPENDICES 65

APPENDIX A. Derivation of More Utilizable Formulae for Parameters
   A. A-Type Contactors 66
   B. Partitioning Contactors 69
   C. Stripping Contactors 71

APPENDIX B. Inventory Equations for a Collection of Coupled
   Contactors
   A. Reduced Forms of the Inventory Equations 73
   B. Estimation of Contactor Inventories from Throughput 74

APPENDIX C. Simulation of a Reprocessing Facility
   A. Description of the Method and Computer Program 80
   B. Application to a Reprocessing Facility 81

(Continued on Next Page)
TABLE OF CONTENTS (Continued)

APPENDIX D. User's Guide for CUSEP
   A. CUSEP Program Listing ........................................ 89
   B. Organization and Subroutine Structure of CUSEP ............ 108
   C. The Arrangement and Format of Input to CUSEP ............. 111
   D. Glossary of Major Variables and Input Parameters ......... 115

APPENDIX E. Databases for Model Development ................... 119
LIST OF TABLES

Table

1. Nominal flowsheet data for the reprocessing plant diagrammed in Figure 1. 7
2. Inventories estimated from modified model equations of this work, model equations of earlier work, and PUBG calculations. 15
3. Plutonium contactor inventory for the plant of Figure 1 predicted by Equation (1.73). 19
4. Data on the reprocessing facility diagrammed in Figure 1 that are used for estimating the transient Pu inventory in the reprocessing area for a rinseout-restart sequence. 28
5. Tank solution concentrations and estimated contactor inventories during a rinseout-restart sequence of the reprocessing plant of Figure 1. 35
6. Data from 82-1 and 82-2 campaigns at the PNC-Tokai plant, which are given in Ref. 15 and 16, includes measured plutonium inventories (g), measured plutonium input into the reprocessing area, and measured plutonium output from the reprocessing area. 40

B1. Data used to calculate χ/a and resultant χ/a values for a typical reprocessing plant. 78
C1. Output from the computer simulation program. The inventories of each unit of the reprocessing plant sketched in Figure 1 are reported. 83

E1. Flowsheet data on A-type aqueous to organic extraction contactors used to generate a database with PUBG. The resultant PUBG inventories and fractional deviations of model calculations from PUBG inventories are also given. 120
E2. Flowsheet data on 1B contactors used to generate a database with PUBG. The resultant PUBG inventories for various phase ratios and fractional deviations of model calculations from PUBG inventories are also given. 122
E3. Flowsheet data on stripping contactors used to generate a database with PUBG and a comparison of resultant PUBG inventories with model calculations. 135
E4. Flowsheet data, steady state inventories, and standard deviations given as a fraction of the steady state inventories for comparison of time dependent model calculations with PUBG generated databases for startup of the A-type contactor. 138

(Continued on Next Page)
LIST OF TABLES (CONTINUED)

Table

E5. Flowsheet data, steady state inventories, and standard deviations given as a fraction of the steady state inventories for comparison of time dependent model calculations with PUBG generated databases for startup of the partitioning contactor. 139

E6. Flowsheet data, steady state inventories, and standard deviations given as a fraction of the steady state inventories for comparison of time dependent model calculations with PUBG generated databases for startup of the stripping contactor. 143
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>A simplified diagram illustrating the configuration of contactors and tanks of the PNC-Tokai nuclear fuel reprocessing plant.</td>
</tr>
<tr>
<td>2.</td>
<td>Approach to steady state for the restart of an A-type contactor.</td>
</tr>
<tr>
<td>3.</td>
<td>Approach to steady state for the restart of a partitioning contactor.</td>
</tr>
<tr>
<td>4.</td>
<td>Approach to steady state for the restart of a stripping contactor.</td>
</tr>
<tr>
<td>5.</td>
<td>The plutonium inventory predicted from the nonsteady model Equation (II.6) is compared with inventories from a computer simulation of the reprocessing plant of Figure 1.</td>
</tr>
<tr>
<td>6.</td>
<td>The uncorrected CUMUF for the 82-1 and 82-2 campaigns at the PNC-Tokai Plant (taken from Ref. 15).</td>
</tr>
<tr>
<td>7.</td>
<td>The CUMUF for the 82-1 and 82-2 campaigns at the PNC-Tokai Plant (Ref. 15) corrected for contactor inventories estimated by the inventory estimation model of this work.</td>
</tr>
<tr>
<td>8.</td>
<td>The corrected CUMUF of Ref. 15.</td>
</tr>
<tr>
<td>9.</td>
<td>Simplified drawing of a pulsed column contactor showing a continuous organic phase flowing from bottom to top and the aqueous dispersed phase flowing oppositely.</td>
</tr>
<tr>
<td>10.</td>
<td>The aqueous and organic concentration profiles of uranium in an A-type pulsed column.</td>
</tr>
<tr>
<td>11.</td>
<td>The aqueous concentration profile for plutonium in a partitioning contactor.</td>
</tr>
<tr>
<td>12.</td>
<td>The organic uranium concentration profile for the pulsed column contactor.</td>
</tr>
<tr>
<td>13.</td>
<td>The aqueous and organic concentration profiles in a pulsed column stripping contactor.</td>
</tr>
<tr>
<td>A1.</td>
<td>An illustration of the concentration profile for the organic phase of an A-type contactor.</td>
</tr>
<tr>
<td>C1.</td>
<td>The temporal response of a reprocessing facility with six plutonium contactors shaded by contactor.</td>
</tr>
</tbody>
</table>
LIST OF SYMBOLS

**Roman**

A
Mass transfer area between aqueous and organic phases.

\( a_i \)
Numerical constant obtained by least squares for the nonsteady state transient inventory estimation model.

B
Volume percent of TBP in the organic phase

\( C_\alpha^a \)
Concentration of \( \alpha (\alpha = U \text{ or Pu}) \) in an aqueous feed stream containing nuclear materials or an aqueous product stream.

\( C_\alpha^o \)
Concentration of \( \alpha (\alpha = U \text{ or Pu}) \) in an organic feed stream or product stream.

\( C_\alpha^a(x) \)
Aqueous phase concentration of \( U \text{ or Pu} \) in \( g/L \) at position \( x \) in a pulsed column.

\( C_\alpha^o(x) \)
Organic phase concentration of \( U \text{ or Pu} \) in \( g/L \) at position \( x \) in a pulsed column.

\( D_\alpha \)
Distribution coefficient of \( \alpha (\alpha = U \text{ or Pu}) \).

\( D_\alpha(x) \)
Distribution coefficient of \( \alpha \) in a pulsed column at position \( x \).

\( D(\sigma) \)
Dispersion coefficient for estimating the diffusional contribution to the longitudinal concentration dispersion in a pulsed column.

\( F_\alpha^a \)
Aqueous phase flow rate.

\( F_\alpha^o \)
Organic phase flow rate.

\( F^a_\alpha \)
Pulsed flow rate of the aqueous phase in a pulsed column.

\( F^o_\alpha \)
Pulsed flow rate of the organic phase in a pulsed column.

\( F^a_f \)
Flow rate of an aqueous feed stream.

\( F^o_f \)
Flow rate of an organic feed stream.

\( H_\alpha \)
Nuclear material inventory of \( \alpha = U \text{ or Pu} \).

\( H_\alpha^0 \)
The superscript \( ^0 \) designates steady state inventory.

[ ]
Square brackets designate molar concentrations.

\([H]_s\)
Acid concentration (M) in aqueous scrub stream.
LIST OF SYMBOLS (Continued)

$[H]_f$  Acid concentration (M) in the aqueous feed streams containing nuclear materials.

$[H]_r$  Acid concentration (M) in the aqueous feed streams containing reductant for partitioning.

$K_\alpha$  Functions of concentration that are calculated from literature correlations and yield the distribution coefficient for $\alpha = U$, Pu, or H via $D_\alpha = K_\alpha [\text{TBP}]^2$ where $[\text{TBP}]$ is the free TBP molarity. Free TBP is not complexed by acid or nuclear material.

$K$  Symbol without subscript $\alpha$ represents the mass transfer coefficient which determines the rate of mass transfer between phases.

$L_4$  Length of a mass transfer unit in a pulsed column.

$L_s$  Distance between sieve plates in a pulsed column.

$L_p$  Pulsing amplitude in units of length.

$N_a$  Total nitrate salting strength (also the total effective nitrate ion concentration).

$N_s$  Number of stages in the scrub bank (bank of stages beginning with the terminal stage where the scrub stream enters the contactor to the feed stage where nuclear materials enter the contactor).

$N_{Ex}$  Number of stages in the extraction bank (bank of stages beginning with the feed stage where nuclear materials enter the contactor to the terminal stage where the aqueous stream exits the contactor).

$R$  Residual TBP or fraction of TBP that is not complexed by nuclear material.

$r$  Aqueous to organic flow rate ratio within the contactor.

$r'$  The flow rate ratio of the aqueous stream feeding nuclear materials to the cycle containing the contactor of interest to the organic stream within the contactor of interest.

$r_a$  Ratio of the total flow rate of aqueous streams feeding reductant into a partitioning contactor to the flow rate of the aqueous stream feeding nuclear materials to the cycle containing the contactor.
LIST OF SYMBOLS (Continued)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>Absolute temperature.</td>
</tr>
<tr>
<td>t</td>
<td>Time.</td>
</tr>
<tr>
<td>V</td>
<td>Stage volume.</td>
</tr>
<tr>
<td>V_p</td>
<td>Pulsing amplitude in units of volume.</td>
</tr>
<tr>
<td>V^A(x)</td>
<td>Aqueous phase volume of a volume element Δx at position x in a pulsed column contactor.</td>
</tr>
<tr>
<td>V^O(x)</td>
<td>Organic phase volume of a volume element Δx at position x in a pulsed column contactor.</td>
</tr>
<tr>
<td>V_s</td>
<td>Volume of scrub bank (see N_s above for the definition of a scrub bank).</td>
</tr>
<tr>
<td>V_ex</td>
<td>Volume of extraction bank (see N_s above for the definition of an extraction bank).</td>
</tr>
<tr>
<td>X_t</td>
<td>Nuclear material throughput rate in metric tons per day.</td>
</tr>
</tbody>
</table>

Greek

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>As a subscript designates H, U, or Pu.</td>
</tr>
<tr>
<td>γ</td>
<td>Designates a parameter in the reduced Equation (1.68) for inventory estimation.</td>
</tr>
<tr>
<td>κ</td>
<td>Hydrodynamic function used for pulsed columns.</td>
</tr>
<tr>
<td>θ</td>
<td>Aqueous to organic phase volume ratio.</td>
</tr>
<tr>
<td>τ</td>
<td>Characteristic time constant for the modified exponential model of nonsteady state transient inventories.</td>
</tr>
<tr>
<td>ψ, ψ_1</td>
<td>Parameters dependent on acid concentration defined by Equations (1.4) and (1.5).</td>
</tr>
<tr>
<td>ω, ξ</td>
<td>Pulsing frequency and linear amplitude in a pulsed column.</td>
</tr>
<tr>
<td>Λ_S, Λ^D_U, λ_α, δ_α</td>
<td>Parameters dependent on nominal flow sheet data in the inventory estimation Equations (1.1) and (1.2).</td>
</tr>
<tr>
<td>f^3_A(x)</td>
<td>Rate at which nuclear materials are fed into a pulsed column at position x by an aqueous feed stream.</td>
</tr>
<tr>
<td>f^O_A(x)</td>
<td>Rate at which nuclear materials are fed into a pulse column at position x by an organic feed stream.</td>
</tr>
</tbody>
</table>
CHAPTER I

Improved Steady State Model for Mixer-Settlers

A. Introductory Comments

In a previous investigation,\textsuperscript{1,2} model equations were developed for estimating inventories in mixer-settler contactors at steady state. These equations are,

\begin{align}
H_\alpha^\sigma &= C_\alpha^\sigma L_\alpha^\sigma, \\
H_\alpha^\rho &= C_\alpha^\rho \left(\Gamma_\alpha^n + \frac{\lambda_\alpha}{[1 - 2^n(C_\alpha^\sigma U + C_\alpha^\delta Pu) / (8.71 B)]^2}\right),
\end{align}

where $H_\alpha^\sigma$ is the nuclear material inventory ($\alpha = U$ or $Pu$), $C_\alpha^\sigma$ is the nuclear material concentration in the aqueous stream feeding the cycle containing the contactor of interest, $B$ is the volume percent of TBP, and $r$ is the flow rate ratio of the aqueous stream feeding nuclear materials to the cycle containing the contactor of interest to the organic stream within the contactor of interest, and $\Gamma_\alpha$, $\lambda_\alpha$, $\Lambda_\alpha^n$, and $\delta_\alpha$ ($\eta = p$ or $s$ represents partitioning or stripping, respectively) are parameters. The measured data required as input for the above simplified model are the nuclear material concentrations $C_\alpha^\sigma$. The parameters are evaluated from nominal flow sheet data when the contactor is placed in service and on such occasions when the flow sheet is modified. Excepting for the introduction of the parameter $\delta_\alpha$, the above equations are identical in form to those derived in the original work.\textsuperscript{1,2}

Once the parameters of Equations (1.1) and (1.2) are evaluated, their routine application is quite convenient. The improvements reported herein are concerned with evaluation of the parameters. The original equations for evaluating these parameters contained distribution coefficients for the partitioning of nuclear materials between aqueous and organic phases. These must be estimated from literature correlations which are normally expressed in terms of the salting strength or ionic strength calculated from
acid and nuclear material concentrations within the contactor while it is operating. Such
in situ concentrations are not available and procedures must be devised to estimate them.
In this work the equations for the parameters have been reformulated in terms of acid and
nuclear material concentrations in the feed streams feeding each purification cycle which
are normally available as nominal flow sheet or measured data. These modified equations
are also much simpler in form than the original equations.\(^2\)

B. More Utilizable Equations for the Parameters

In Appendix A the modified equations for the parameters are developed by replacement
of the distribution coefficients, \(D_{\alpha}\), in the original equations using the relation,

\[
D_{\alpha} = \varepsilon_{\alpha} \psi R^2,
\]

where \(\psi\) is a function of the average acid concentrations introduced into the contactor feed
streams,

\[
\psi = \frac{0.00493 B^2 [H]^{1.57}}{(1 + 0.00662 [H]^4)} \left(1 + 0.104 [H]^{1.6}\right) \left(1 - \frac{\psi_1}{1 + \psi_1}\right),
\]

\[
\psi_1 = \frac{0.0197 B [H]^{1.82}}{1 + 0.0251 [H]^{4.5}}.
\]

The quantity \(R\) is the fraction of TBP (tri-n-butyl phosphate) not complexed by nuclear
materials,

\[
R = 1 - 2r'(C_{U}^{R} + C_{Pu}^{R})/(8.71 B),
\]

and the \(\varepsilon_{\alpha}\) are the temperature correction factors which for a nominal TBP volume
fraction of 30\% are,\(^3\)

\[
\varepsilon_{U} = 1.908 \exp(2500\alpha),
\]

\[
\varepsilon_{Pu} = 0.742 \exp(-200\alpha),
\]

\[
\tau = \frac{1}{T} - \frac{1}{298.16}.
\]
where $T$ is the absolute temperature. For most purposes it would be adequate to assume ambient temperature in which case $e_{ij} = 1.908$ and $e_{Pu} = 0.742$. The average acid molarities are given by,

$$[H] = 0.9 [H]_f + 0.1 [H]_s,$$

(1.10)

for A-type contactors,

$$[H] = 0.044 [H]_f / r + 0.1 [H]_r + 0.9 [H]_s,$$

(1.11)

for the scrub banks of partitioning contactors, and

$$[H] = 0.08 [H]_f / r + 0.1 [H]_r + 0.9 [H]_s,$$

(1.12)

for the extraction banks of partitioning contactors. The quantities $[H]_f$, $[H]_r$, and $[H]_s$ are acid molarities in the feed streams, reductant streams, and scrub streams, respectively, and $r$ is the aqueous to organic flow rate ratio in the contactor of interest.

In Appendix A it is shown that the parameters for the inventory estimation Equations (1.1) and (1.2) may be expressed in terms of $e$, $R$, and $\psi$ according to the equations,

$$\delta = 1 / \left[ 1 - \frac{V e \gamma}{(e e R)^2} \right],$$

(1.13)

$$\gamma = \frac{V e \delta}{1 + \gamma},$$

(1.14)

$$\lambda = \left( \frac{0.0971 + 0.8779}{s} \right) \Gamma / e_{Pu},$$

(1.15)

for uranium in A-type contactors,

$$\lambda = \left( \frac{0.0730 + 0.8208}{s} \right) \Gamma / e_{Pu},$$

(1.16)

for plutonium in A-type contactors, and

$$\lambda = \left( \frac{0.0871}{s} \right) \Gamma / e_{Pu},$$

(1.17)

for uranium in partitioning contactors,

$$\lambda = \left( \frac{0.0871}{s} \right) \Gamma / e_{Pu},$$

(1.18)
\begin{align}
\lambda^U &= \frac{Vr}{r(1 + \theta)} \left( \frac{\theta + 0.98N_a^{0.24} \exp(1260\theta)}{1 - 0.98N_a^{0.24} \exp(1260\theta)/r} \right), \\
\lambda^\text{Pu} &= \frac{Vr}{r(1 + \theta)} \left( \frac{\theta + 0.36N_a^{0.22} \exp(-1340\theta)}{1 - 0.36N_a^{0.22} \exp(-1340\theta)/r} \right),
\end{align}

(1.19)

(1.20)

where \( N_a \) is the total nitrate ion molarity calculated according to the relation,

\[ N_a = [H]_s + 2 \left( \frac{C_{\text{U}}^{N_a}/238 + C_{\text{Pu}}^{N_a}/239}{r} \right). \]

(1.21)

In the above relations, \( V_s \) is the volume of the scrub bank which includes the stage where the feed stream containing nuclear materials enters the contactor, \( V_{\text{Ex}} \) is the volume of the extraction bank which also includes the stage where the feed stream containing nuclear materials enters the contactor, \( \theta_s \) and \( \theta_{\text{Ex}} \) are the aqueous to organic phase volume ratios in the scrub and extraction banks, respectively, and \( \theta \) is the average aqueous to organic phase volume ratio in the entire contactor.

The numerical constants in the above equations were calculated by least squares methods using a PUBG database. The database and the detailed results of the least squares calculations are given in Tables E1 to E3 of Appendix E. The root mean square deviations of plutonium inventories estimated with model Equations (1.1) to (1.2) from the PUBG inventories are less than 6%. This is comparable to the root mean square deviations obtained in earlier work\(^1,2\) on the inventory estimation model and this implies that simplifications in the calculation of the model parameters were obtained without loss of accuracy. The root mean square deviations of uranium inventories from the PUBG generated inventories are less than 6% for A-type contactors. For uranium inventory estimates in partitioning and stripping type contactors the standard deviations were somewhat larger, being about 8%.

The quantities \( R \) and \( \psi \) separate the effect of acid concentrations and nuclear material concentrations on the model parameters for A-type and partitioning contactors. The effect
of acid is contained in \( \psi \) and the effect of nuclear materials is given by \( R \). Since explicit equations are given for both \( \psi \) and \( R \) (Equations (1.4) to (1.6)) the need to refer to literature distribution coefficient correlations is removed. In the next section of the Chapter, the improved utility of the equations is demonstrated by applying them to a representative reprocessing plant.

C. Application to a Reprocessing Facility

Exemplary Parameter Calculations

Figure 1 provides a simplified illustration of a nine contactor reprocessing facility with 200 metric tons annual throughput. In Table 1 are given nominal values of the operating parameters including flow rates and acid and nuclear material concentrations. The reprocessing facility and flow sheet are identical to those considered in the earlier work on inventory estimation using the simplified inventory estimation model.\(^{1,2}\) However, in this earlier effort, only the equations for the parameter calculation were given; the details of the parameter calculation were not provided because it involved the complex process of estimating the distribution coefficients from literature correlations. In this Section, the improved utility of the modified equations for parameter evaluation is demonstrated by presenting parameter calculations for three representative types (A-type, partitioning, and stripping) of contactors.

We begin the parameter calculation with the A-type contactor labeled contactor I in Figure 1. From Table 1, one can see that the feed stream and scrub stream acid concentrations are 3M, the nuclear material concentrations are 180 g/L of uranium and 1.2 g/L of plutonium, the feed stream flow rate (2.6 L/min) to organic stream flow rate (5.3 L/min) ratio \( (r) \) is 0.5, and the scrub stream flow rate (1.1 L/min) to organic stream flow rate ratio \( (r') \) is 0.2, and the scrub bank volume \( (V_s) \) is 932.5 L. The contactor temperature is assumed to be 30°C and the TBP concentration (B) is 30% by volume. For the assumed temperature, \( \tau = -5.53 \times 10^{-5} \) and the temperature correction...
First Purification Cycle

Second Purification Cycle

Plutonium Purification Cycle

Uranium Purification Cycle

Figure 1. A simplified diagram illustrating the configuration of contactors and tanks of the PNC-Tokai nuclear fuel reprocessing plant. Contactor designations are 1A, etc., for extraction contactors, 1E, etc., for stripping contactors, and 1B, etc., for partitioning contactors with the number of stages for each also shown. Large tanks are designated D1 through D3. Roman numerals are the PNC-Tokai numbering of the contactors. Arabic numerals show those parts of the plant that were included in the simulations.
**Table 1.**
Nominal flow sheet data for the reprocessing plant diagrammed in Figure 1.

\(T = 303\ \text{K and TBP is 30\%}\)

<table>
<thead>
<tr>
<th>Contactor No.</th>
<th>Scrub bank</th>
<th>Ext. bank</th>
<th>Stage</th>
<th>Scrub bank</th>
<th>Ext. bank</th>
<th>Volume</th>
<th>Phase volume ratio</th>
<th>Aqueous feed to purification cycle with contactor</th>
<th>Aq. scrub</th>
<th>Reduc tant stream</th>
<th>Organic</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Flow rate (L/min)</td>
<td>U (g/L)</td>
<td>Pu (g/L)</td>
<td>H(^+) (M)</td>
</tr>
<tr>
<td>I</td>
<td>932.5</td>
<td>-</td>
<td>-</td>
<td>0.83</td>
<td>-</td>
<td>4.5</td>
<td></td>
<td>2.6</td>
<td>180</td>
<td>1.2</td>
<td>3.0</td>
</tr>
<tr>
<td>II</td>
<td>-</td>
<td>-</td>
<td>111.2</td>
<td>1.16</td>
<td>-</td>
<td>0.5</td>
<td></td>
<td>2.6</td>
<td>180</td>
<td>1.2</td>
<td>3.0</td>
</tr>
<tr>
<td>III</td>
<td>1172.4</td>
<td>-</td>
<td>-</td>
<td>0.94</td>
<td>-</td>
<td>0.6</td>
<td></td>
<td>8.6</td>
<td>55</td>
<td>0.4</td>
<td>3.0</td>
</tr>
<tr>
<td>IV</td>
<td>1123.5</td>
<td>326.7</td>
<td>-</td>
<td>0.80</td>
<td>1.67</td>
<td>0.7</td>
<td></td>
<td>8.6</td>
<td>55</td>
<td>0.4</td>
<td>3.0</td>
</tr>
<tr>
<td>V</td>
<td>-</td>
<td>-</td>
<td>179.2</td>
<td>1.16</td>
<td>-</td>
<td>0.3</td>
<td></td>
<td>8.6</td>
<td>55</td>
<td>0.4</td>
<td>3.0</td>
</tr>
<tr>
<td>VI</td>
<td>1041.5</td>
<td>-</td>
<td>-</td>
<td>1.0</td>
<td>-</td>
<td>1.0</td>
<td></td>
<td>16.7</td>
<td>30</td>
<td>-</td>
<td>1.5</td>
</tr>
<tr>
<td>VII</td>
<td>-</td>
<td>-</td>
<td>152.0</td>
<td>1.16</td>
<td>-</td>
<td>1.0</td>
<td></td>
<td>16.7</td>
<td>30</td>
<td>-</td>
<td>1.5</td>
</tr>
<tr>
<td>VIII</td>
<td>129.4</td>
<td>-</td>
<td>-</td>
<td>0.44</td>
<td>-</td>
<td>2.7</td>
<td></td>
<td>3.9</td>
<td>1.2</td>
<td>1.2</td>
<td>4.0</td>
</tr>
<tr>
<td>IX</td>
<td>124.37</td>
<td>47.35</td>
<td>-</td>
<td>0.095</td>
<td>0.72</td>
<td>2.7</td>
<td></td>
<td>3.9</td>
<td>1.2</td>
<td>1.2</td>
<td>4.0</td>
</tr>
</tbody>
</table>
Factors (Equations (1.7) and (1.8)) become,

\[ \varepsilon_U = 1.908 \exp[-5.53 \times 10^{-5} (2500)] = 1.662 \text{,} \quad (1.22) \]

\[ \varepsilon_{Pu} = 0.742 \exp[-5.53 \times 10^{-5} (-200)] = 0.750 \text{.} \quad (1.23) \]

By substitution of \( r' = 0.5, \ C_j^3 + C_j^2 Pu = 181.2 \text{ g/L, and } B = 30 \) into Equation (1.6), one obtains for \( R \),

\[ R = \frac{2(0.5)(181.2)}{8.7(3.0)} = 0.3065 \text{.} \quad (1.24) \]

Using the above value of \( R \) and setting \([H] = 3\), we calculate \( \psi \) and \( \psi_1 \) from Equations (1.4) and (1.5),

\[ \psi_1 = \frac{0.0197 (3.0) [3.182 (0.3065)]}{1 + 0.0251 [3^4]} = 0.2959 \text{,} \quad (1.25) \]

\[ \psi = \frac{0.00493 (3.0)^2 [3.1.57 (1 + 0.104 [3])]}{1 + 0.00662 [3^4]} \left( \frac{1 - 0.2959}{1 + 0.2959} \right) = 20.050 \text{.} \quad (1.26) \]

From the calculated values of \( \varepsilon_{U}, \psi, \) and \( R \), the parameters may be calculated from Equations (1.13) to (1.19) yielding the following results,

\[ \delta_U = \frac{1}{1 - 0.2 / [(1.662)(20.05)(0.3065)^2]} = 1.068 \text{,} \quad (1.27) \]

\[ \delta_{Pu} = \frac{1}{1 - 0.2 / [(0.750)(20.05)(0.3065)^2]} = 1.165 \text{,} \quad (1.28) \]

\[ \Gamma_U = \frac{(932.5)(0.5)(1.068)}{(1 + 0.83)} = 272.1 \text{.} \quad (1.29) \]

\[ \Gamma_{Pu} = \frac{(932.5)(0.5)(1.165)}{(1 + 0.83)} = 296.8 \text{.} \quad (1.30) \]
\[ \lambda_U = \frac{[0.0971 + (0.877)(0.83)](272.1)}{(1.662)(20.05)} = 5.151 \quad (1.31) \]

\[ \lambda_{Pu} = \frac{[0.0730 + (0.820)(0.83)](296.8)}{(0.750)(20.05)} = 11.99 \quad (1.32) \]

The above results for \( \Gamma_U, \Gamma_{Pu}, \lambda_U, \) and \( \lambda_{Pu} \) agree extremely well with values (266, 289, 4.81, and 10.86, respectively) obtained previously for this same contactor.

The parameter evaluation for partitioning contactors is demonstrated by application of the parameter estimation equations to contactor IV of Figure 1. From Table 1, it is noted that the acid concentration feeding the cycle containing the contactor of interest ([H]_f) is 3.0 M, the scrub stream acid concentration ([H]_s) is 0.2 M, and the reductant stream acid concentrations ([H]_r) are 1.5 M. The aqueous to organic flow rate ratio (r) is 2.03/8.6 or 0.236 (See Table 1). These may be used to estimate acid concentrations associated with the scrub bank ([H]_Scrub) and extraction bank ([H]_Ex) from Equations (1.11) and (1.12),

\[ [H]_{Scrub} = 0.044(3) / 0.236 + 0.1(1.5) + 0.9(0.2) = 0.889 \text{ M} \quad (1.33) \]

\[ [H]_{Ex} = 0.08(3) / 0.236 + 0.1(1.5) + 0.9(0.2) = 1.347 \text{ M} \quad (1.34) \]

For the extraction bank, it is assumed that the amount of TBP complexed by nuclear material is negligible and R for the extraction bank (designated \( R_{Ex} \)) is unity. For the scrub bank R must be calculated from Equation (1.6) and the average uranium concentration, \( <C_U> \),

\[ <C_U> = C_U^a + r a C_R = 55 + 0.015(200) = 58 \text{ g/L} \quad (1.35) \]

where \( C_R (= 200 \text{ g/L}) \) is the total uranium concentration in the reductant stream and...
\( r_a = 0.015 \) is the ratio of the total flow rate of the aqueous streams feeding reductant into the partitioning contactor to the flow rate of the aqueous stream feeding nuclear materials to the cycle containing the partitioning contactor. Substitution of the above average value for the uranium concentration into Equation (1.6) yields the \( R \) value for the scrub bank,

\[
R_s = 1 - 2r^* Q_a / (8.71 B) = 1 - 2(1.0) (58) / (8.71 \times 30) = 0.556 . \tag{1.36}
\]

The above results for the acid concentration and \( R \) are substituted into Equation (1.5) to yield \( \psi \) values 0.261 and 0.927 for the scrub and extraction banks, respectively. The quantity \( \psi \) can now be calculated for the scrub banks and extraction banks using Equation (1.4),

\[
\psi_{\text{Scrub}} = \frac{0.00493 (3.0)^2 (0.889)^{1.57} \left[ 1 + 0.104 (0.889)^{1.6} \right]}{1 + 0.00662 (0.889)^4} \left( 1 - \frac{2r^*}{1.261} \right)
\]

\[
= 3.164 . \tag{1.37}
\]

\[
\psi_{\text{Ex}} = \frac{0.00493 (3.0)^2 (1.347)^{1.57} \left[ 1 + 0.104 (1.347)^{1.6} \right]}{1 + 0.00662 (1.347)^4} \left( 1 - \frac{2r^*}{1.927} \right)
\]

\[
= 4.200 . \tag{1.38}
\]

The temperature is assumed to be 30°C and the values for the temperature parameters \( e_u \) and \( e_{p_u} \) are 1.662 and 0.750, respectively (See Equations (1.22) and (1.23)). The volumes, \( V_s \) and \( V_{Ex} \), are 1123.5 and 326.7 L, respectively (See Table 1). The parameters for partitioning contactor IV of Figure 1 may now be calculated from Equations (1.13) and (1.18) at 30°C as shown below,

\[
\delta_u = \frac{1}{\{ 1 - 0.236 \left[ (1.662)(3.164)(0.556)^2 \right] \}} = 1.170 . \tag{1.39}
\]
\[ \Gamma_U = \frac{1123.5(1.0) (1.170)}{1 + 0.80} = 730.3 \]  
(1.40)

\[ \lambda_U = \frac{0.8 (730.3)}{1.662 (3.164) (0.556)^2 + 0.310}\left(1.59 - \frac{1.37}{1.662 (3.164) (0.556)^2}\right) = 96.05 \]  
(1.41)

\[ \Lambda^S_{Pu} = \frac{1.0(326.7)(1.67)}{0.236 (1 + 1.67)} \left[1 + 0.001 \left(5.83 + \frac{5.56}{1.67}\right) (0.750) (4.200)\right] = 891 \]  
(1.42)

Using the above calculated parameters, the following equations are obtained for the nuclear material inventory in partitioning contactor IV,

\[ H_U^0 = \Gamma_U \left(730 + \frac{96.1}{1 - 2.340\Gamma_U / (8.71 B)}\right) \]  
(1.43)

\[ H_{Pu}^0 = 891 C_{Pu}^a \]  
(1.44)

The calculation of parameters for stripping contactors is illustrated using nominal flow sheet data on Table 1 for Contactor II, i.e. \( C_U^3 = 180 \text{ g/L}, \ C_{Pu}^3 = 1.2 \text{ g/L}, \ [H]_s = 0.02, \ r = 6.2/5.5 = 1.13, \ r' = 2.6/5.5 = 0.47, \ \theta = 1.16, \text{ and } V = 111.2. \) Substitution of these data into Equations (1.19) to (1.20) yields,

\[ N_a = 0.02 + 2 (0.47)(180/238 + 1.2/239)/1.13 = 0.653 \]  
(1.45)

\[ \Lambda^S_U = \frac{0.47(111.2)(1.16 + 0.98 (0.653) 0.24 \exp\left(1260(-5.53 \times 10^{-5})\right))}{1.13(1 + 1.16) \left[1 - 0.98 (0.653) 0.24 \exp\left(1260(-5.53 \times 10^{-5})\right)\right]} = 158 \]  
(1.46)
\[ H_U^S = \frac{0.47(11.12) \left(1.16 + 0.36(0.653)\right) 0.22 \exp[-(1340) (0.53 \times 10^{-5})]} {1.13(1 + 1.16) \left(1 - 0.36(0.653) \exp[-(1340) (0.53 \times 10^{-5})]/1.13\right)} \]

\[ = 47.1. \]  

(1.47)

The inventory equations for Contactor II are,

\[ H_U = 158C_U^a, \]

(1.48)

\[ H_{Pu} = 47.1C_{Pu}^a. \]  

(1.49)

The above calculations are representative of what is involved in calculating the parameters of the inventory equations for the contactors of Figure 1. A summary of the inventory equations for all contactors follows.

**Contactor I**

\[ H_U^D = C_U^a \left( 272 + \frac{5.15}{[1 - 0.113(1.068C_U^a + 1.165C_{Pu}^a)/B]^2} \right), \]

(1.50)

\[ H_{Pu}^D = C_{Pu}^a \left( 297 + \frac{12.0}{[1 - 0.113(1.068C_U^a + 1.165C_{Pu}^a)/B]^2} \right). \]  

(1.51)

**Contactor II**

\[ H_U^D = 158C_U^a, \]

(1.52)

\[ H_{Pu}^D = 47.1C_{Pu}^a, \]  

(1.53)

**Contactor III**

\[ H_U^D = C_U^a \left( 860 + \frac{19.29}{[1 - 0.319(1.024C_U^a + 1.055C_{Pu}^a)/B]^2} \right), \]

(1.54)
\[ H^0_{Pu} = C^a_{Pu} \left( \frac{88.6 + 42.23}{1 - 0.319(1.024C^a + 1.055C^a_{Pu})/B} \right), \]  

(1.55)

Contactor IV

\[ H^0_U = (C^a + 0.015C^a_R) \left( 730 + \frac{96.1}{1 - 0.268(C^a + 0.015C^a_R)/B} \right), \]  

(1.56)

\[ H^0_{Pu} = 891 C^a_{Pu}, \]  

(1.57)

Contactor V

\[ H^0_U = 388 (C^a + 0.015C^a_R), \]  

(1.58)

Contactor VI

\[ H^0_U = C^a_U \left( 960 + \frac{118.3}{1 - 0.424C^a_U/B} \right), \]  

(1.59)

Contactor VII

\[ H^0_U = 435 C^a_U, \]  

(1.60)

Contactor VIII

\[ H^0_U = C^a_U \left( 689 + \frac{25.69}{1 - 1.55(1.135C^a_U + 1.358C^a_{Pu})/B} \right), \]  

(1.61)

\[ H^0_{Pu} = C^a_{Pu} \left( 824 + \frac{67.85}{1 - 1.55(1.135C^a_U + 1.358C^a_{Pu})/B} \right), \]  

(1.62)
Contactor IX

\[ H^0_U = \left( C_U^a + 0.015 C_R^a \right) \left( 3.70 + \frac{12.31}{\left[ 1 - 0.748 \left( C_U^a + 0.015 C_R^a \right) / S \right]^2} \right), \]

(1.63)

\[ H^0_{Pu} = 195 C_{Pu}^a . \]

(1.64)

In Table 2 the inventories estimated from the above equations for specified values of the nuclear material concentrations in the feed streams are compared with PUBG calculations and previous simplified model calculations. The agreement of the modified model estimates of this work with PUBG calculations is excellent for plutonium. The deviation of the estimate for the total uranium inventory from the PUBG estimate is about 6% (16 Kg) which should be compared with 1% (2.5 Kg) obtained in the earlier work. The larger deviation for the modified model results from the slightly lesser accuracy achieved for uranium inventories in the case of stripping and partitioning contactors as is judged from the comparison of standard deviations from PUBG databases (8% as compared with 5% for the original model). However in view of the simplification that is achieved without loss of accuracy for plutonium inventory estimates and the improved utilizability of the modified model, the somewhat lesser accuracy obtained for uranium inventory estimates is of no significance.

D. Reductions in Form of the Inventory Estimation Equations

The inventory equations can be reduced in number by writing them in a form to yield the inventories of separate purification cycles. This can be accomplished for a particular purification cycle by summing up the inventory equations for the separate contactors within the cycle. For the reprocessing plant of Figure 1 this yields the following three equations for the plutonium inventory,
Table 2

Inventories estimated from modified model equations of this work, model equations of earlier work (Ref. 1 and 2), and PUBG calculations.

<table>
<thead>
<tr>
<th>Contactor</th>
<th>$C_U^a$</th>
<th>$C_{Pu}^a$</th>
<th>$C_R^a$</th>
<th>U Inventory (Kg)</th>
<th>Pu Inventory (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>This Work</td>
<td>Ref. 1 &amp; 2</td>
</tr>
<tr>
<td>I</td>
<td>180</td>
<td>1.23</td>
<td>0.</td>
<td>61.6</td>
<td>60.2</td>
</tr>
<tr>
<td>II</td>
<td>180</td>
<td>1.23</td>
<td>0.</td>
<td>28.4</td>
<td>32.0</td>
</tr>
<tr>
<td>III</td>
<td>54.6</td>
<td>0.373</td>
<td>0.</td>
<td>53.5</td>
<td>56.2</td>
</tr>
<tr>
<td>IV</td>
<td>54.6</td>
<td>0.373</td>
<td>200.</td>
<td>65.5</td>
<td>70.9</td>
</tr>
<tr>
<td>V</td>
<td>54.6</td>
<td>0.373</td>
<td>0.</td>
<td>22.4</td>
<td>25.9</td>
</tr>
<tr>
<td>VI</td>
<td>30.9</td>
<td>0.0</td>
<td>0.</td>
<td>41.2</td>
<td>42.7</td>
</tr>
<tr>
<td>VII</td>
<td>30.9</td>
<td>0.0</td>
<td>0.</td>
<td>13.4</td>
<td>15.1</td>
</tr>
<tr>
<td>VIII</td>
<td>3.92</td>
<td>1.167</td>
<td>0.</td>
<td>2.9</td>
<td>2.9</td>
</tr>
<tr>
<td>IX</td>
<td>3.92</td>
<td>1.167</td>
<td>350.</td>
<td>3.6</td>
<td>3.4</td>
</tr>
</tbody>
</table>

Total Inventory 292.5 309.3 306.8 2741 2749 2711

Purification Cycle 1

$$H_{Pu}^0 = C_{Pu}^a \left( \frac{3.44 + \frac{12.0}{1 - 0.113(1.068C_U^a + 1.165C_{Pu}^a)/B}}{[1 - 0.113(1.068C_U^a + 1.165C_{Pu}^a)/B]^2} \right)$$ (1.65)

Purification Cycle 2

$$H_{Pu}^0 = C_{Pu}^a \left( \frac{1.777 + \frac{42.23}{1 - 0.319(1.024C_U^a + 1.055C_{Pu}^a)/B}}{[1 - 0.319(1.024C_U^a + 1.055C_{Pu}^a)/B]^2} \right)$$ (1.66)
The above reduction of the six plutonium contactor inventory equations to three equations, where each gives the total contactor inventory of a cycle, can be accomplished for any sequence of contactors coupled by flows. However, to obtain the simple form of the above three equations when more than one A-type contactor is in the sequence is more complex than merely summing up the equations for the separate contactors. In Appendix B a procedure is derived for reducing the separate contactor equations of any coupled set of contactors to a single equation of the form,

\[ H_{\alpha}^0(tot) = C^a_\alpha \left( \gamma_{\alpha}(tot) + \frac{\lambda_{\alpha}(tot)}{1 - \gamma(C^a_U + C^a_{Pu})/(8.71B)} \right)^2 \]  

where \( H_{\alpha}^0(tot) \) denotes the total contactor inventory (tot designates a composite quantity) of the set of coupled contactors under consideration, \( \gamma_{\alpha}(tot) \), \( \lambda_{\alpha}(tot) \), and \( \gamma \) are parameters, and \( C^a_\alpha \) are assumed to be the concentrations in the tanks feeding the initial contactor in the contactor sequence under consideration. The first parameter, \( \gamma_{\alpha}(tot) \), accounts for the first order contributions to the inventory from all contactors and the second term in the brackets accounts for the divergences in the inventory in the A-type contactors of the contactor sequence under consideration that take the entire uranium throughput (i.e. the divergence in the A-type contactor in the Pu purification cycle is neglected in this second term). In Appendix B we show that the parameters in the above equations are calculated from the relations,
The symbols contained by the parenthesis notation \((\cdot)_{\text{N}}\) have their usual meaning for a single contactor; the subscript \(N\) or \(M\) following the parenthesis designates the numeral (for example I, II, etc., in Figure 1) assigned to the contactor. The summation over \(M\) and \(M'\) designates a sum over the A-type contactors which contribute to the inventory of nuclear material \(\alpha\) and at the same time carry all of the uranium throughput (excludes the A-type contactor in the plutonium purification cycle). For example, these would be Contactors I and III for the plutonium inventory equations and Contactors I, III, and VI (see Figure 1) for the uranium inventory equations. The summation over \(N\) includes the remaining contactors (II, IV, VIII, and IX for Pu and II, IV, V, and VII to IX for U). Since Equations (I.69) to (I.71) are for parameter evaluation, the \((H^\alpha)_{\text{N}}\) or \((H^\alpha)_{\text{M}}\) may be calculated using nominal flow sheet values for \(C^\alpha\). However, once the parameters are evaluated, measured values of \(C^\alpha\) would be used in applying Equation (I.68).

In order to illustrate the application of Equations (I.68) through (I.71), they are employed to reduce the inventory estimation of the entire reprocessing plant of Figure 1 to a single equation. Using flow sheet values of Table 1 and the inventories of Table 2, the parameters are calculated from Equations (I.69) to (I.71). The results are substituted...

\[
\gamma = \frac{8.71B}{C^\alpha_{\text{U}} + C^\alpha_{\text{Pu}}} \left(1 - \frac{\sum_{M'} (G^\alpha_{\text{M'}})}{\sum_{M} [(H^\alpha_{\text{M}} - (C^\alpha_{\text{M'}})]}ight) \tag{1.71}
\]

\[
\Gamma_{\alpha \text{ (tot)}} = \frac{1}{C^\alpha_{\text{M}}} \left(\sum_{\text{N}} (H^\alpha_{\text{N}})_{\text{N}} + \sum_{\text{M}} (C^\alpha_{\text{M}} (H^\alpha_{\text{M}}))\right) \tag{1.69}
\]

\[
\lambda_{\alpha \text{ (tot)}} = \frac{1}{C^\alpha_{\text{M}}} \sum_{\text{M}} (G^\alpha_{\text{M}}) \tag{1.70}
\]
into Equation (1.68) to yield,

$$H^0_{U \text{ (tot)}} = C^a_U \left( 1452 + \frac{31.07}{[1 - 0.094 (C^a_U + C^a_{Pu})/B]^2} \right) \quad (1.72)$$

$$H^0_{Pu \text{ (tot)}} = C^a_{Pu} \left( 1975 + \frac{24.21}{[1 - 0.112 (C^a_U + C^a_{Pu})/B]^2} \right) \quad (1.73)$$

where $C^a_U$ and $C^a_{Pu}$ are the concentrations for the tanks feeding the initial purification cycle.

Reducing the contactor inventory for an entire plant to a single equation for each nuclear material is a very useful simplification. It presumes that the variations in the steady state contactor inventory are initiated at the first purification cycle, which is often the case. However, should the concentrations of all the tanks feeding the individual purification cycles be given, one might prefer to make use of the additional information by employing Equation (1.65) to (1.67) for the separate purification cycles, or Equations (1.50) to (1.64) for the separate contactors.

In Table 3 below, predictions of Equation (1.73) for plutonium are given. The effect of the divergent term in Equation (1.73) is quite evident from an examination of the data in Table 3 which shows that the increase in $H^0_{Pu \text{ (tot)}}$ is more pronounced than a strict proportionality to $C^a_{Pu}$ would predict.

E. Estimation of Contactor Inventory from Average Throughput

The total contactor inventory in a nuclear fuel reprocessing plant should to a first approximation be proportional to throughput. This should be the case, because there are limits to the choices of hydrodynamic residence time one may select in designing the contactors for a plant. If the throughput is made large by increasing the flow rate of the
Table 3

Plutonium contactor inventory for the Plant of Figure 1 predicted by Equation (1.73).

<table>
<thead>
<tr>
<th>$C_u^a$ (g/L)</th>
<th>$C_{Pu}^a$ (g/L)</th>
<th>$H_{Pu}^0$ (tot) (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>170</td>
<td>1.16</td>
<td>2506</td>
</tr>
<tr>
<td>180</td>
<td>1.23</td>
<td>2714</td>
</tr>
<tr>
<td>190</td>
<td>1.30</td>
<td>2953</td>
</tr>
<tr>
<td>200</td>
<td>1.37</td>
<td>3244</td>
</tr>
</tbody>
</table>

feed streams, the contactor size (and consequently its inventory) must be increased to keep the residence times within limits consistent with optimum contactor performance.

In Appendix B the following approximate formulae for contactor inventory, which assumes proportionality to throughput, are derived,

\[
H_{Pu}^0 = 6.0 X_t \Delta, \quad (1.74)
\]

\[
H_u^0 = 0.47 X_t, \quad (1.75)
\]

where $H_{Pu}^0$ is in kilograms, $H_u^0$ is in metric tons, $X_t$ is the throughput in metric tons per day, and $\Delta$ is the percentage of the throughput that is plutonium. The above formulae are based on a hydrodynamic residence time (defined as volume divided by total flow rate) of ten minutes per stage. This is approximately the residence time per stage for the mixer-settler contactors in the Tokai reprocessing plant.\(^7\)\(^8\)

Since concentration profiles in pulsed column contactors are similar in form to those in mixer-settler contactors,\(^9\) simplified expressions derived for mixer-settlers should be valid at least in form for pulsed column contactors. There will however be differences...
in the scales relating inventory to throughput which must be determined. Pulsed column contactors generally have smaller residence times than mixer-settlers, resulting in smaller contactor inventories. There has been a wide variation in the residence times reported for pulsed columns in pilot plant operations.\textsuperscript{10,11} Data reported on partitioning columns in a real plant\textsuperscript{12} would suggest that the longer residence times reported for pilot plants correspond more closely to those in real plants. These are about 30% as large as those reported for mixer-settler contactors in real plants.\textsuperscript{7,8} However, simulations of pulsed column operation, performed in this work using the computer program CUSEP (see Appendix D), show that the dispersion of the concentration profile is much greater in a pulsed column than in a mixer-settler which tends to increase the inventory by a factor of 1.5. Combining this factor with the shorter residence times in pulsed columns, one predicts a plant with pulsed columns to have about 45% of the contactor inventory of a plant with mixer-settler contactors. Incorporating the factor 0.45 into Equations (I.74) and (I.75), one obtains the following inventory equations for pulsed columns,

\begin{align*}
H_{Pu}^P &= 2.7X_1 \Delta , \\
H_{U}^P &= 0.21 X_1 .
\end{align*}

It is useful to apply Equations (I.74) and (I.75) to the reprocessing plant of Figure 1. This plant design reprocesses spent fuel that is 0.7% plutonium at a rate of 0.7 metric tons per day. The above model predicts the contactor inventory to be 2.9 Kg of plutonium and 0.329 metric tons of uranium which is in excellent agreement with the PUBG estimates of Table 2 (2.71 Kg of plutonium and 0.307 tons of uranium). The good agreement is perhaps not too surprising since the plant of Figure 1 has contactors with a ten minute residence time per stage which was the choice made for residence time in deriving Equations (I.74) and (I.75).
If one excludes the large variations in contactor inventory that may occur when A-type contactors are highly loaded with nuclear materials or the variations that occur during a rinseout-restart sequence, real mixer-settler contactor inventories are expected to be within 20% of the predictions of Equations (1.74) and (1.75). This error estimate is based on inventory variations for the variety of flow sheets that were studied in this work for A-type contactors, which contain most of the plutonium contactor inventory.

For large plants with a 4 ton per day throughput of nuclear fuel that is 0.7% plutonium, Equations (1.74) and (1.76) predict contactor inventories of 17 Kg of plutonium for a plant equipped with mixer-settler contactors and 8 Kg of plutonium for a plant equipped with pulsed column contactors. Since the pilot plant data on pulsed columns\(^{10,11}\) show substantial variations (over 50%) in residence times, the percentage deviations of real plant inventories from Equations (1.76) and (1.77) can be much larger than the percentage deviations from Equations (1.74) and (1.75) for plants with mixer-settler contactors. However the contactor inventories for a plant with pulsed columns are smaller than for a plant with mixer-settlers. Thus the absolute errors in the contactor inventory estimates for the two types of plants would be about the same.

The inventory equations based on throughput are simpler than those of the inventory estimation model discussed in Section A through D of this Chapter. They are also most useful when no flow sheet data are available. However equations based on throughput have large error estimates and they have the disadvantage of not being able to identify inventory variations due to variations in flow sheet parameters such as TBP concentration, feed stream concentrations, etc. Consequently correcting the MUF (Material Unaccounted For) and CUMUF (Cumulative Material Unaccounted For) tests for unmeasured inventory will require the more accurate inventory equations summarized in Sections C and D of this Chapter.
CHAPTER II

The Nonsteady State Model and Estimation of Contactor Inventories

A. Introduction

The inventory estimation equations just described in the previous Chapter provide accurate estimates as long as the system is operating near steady state. However circumstances will arise following large changes in the feed stream concentrations, during process upset, or during a rinseout-restart sequence where nonsteady state conditions can persist a long period. The variations in inventory that may occur during this period may be more significant than variations in the steady state inventories. Thus it is necessary to have a theory which estimates transient contactor inventories during nonsteady state periods to complement the steady state model described in the previous Chapter.

B. Development of the Nonsteady State Model

The simplest model for estimating transient inventories is an exponential model which may be expressed in the following manner,

\[ H_{\alpha} = H_{\alpha}^0 - (H_{\alpha}^0 - H_{\alpha}^\infty) \exp \left( -\frac{t}{\tau} \right), \]  

(II.1)

where \( H_{\alpha}^0 \) is the initial inventory at \( t = 0 \) (\( t \) being the time), \( H_{\alpha}^0 \) is the final steady state inventory at \( t = \infty \), and \( \tau \) is a time constant characterizing the transient behavior of the time dependent \( H_{\alpha} \). The initial time represents the time where the nonsteady state conditions were produced which initiated the subsequent transient behavior of the inventory. Equation (II.1) is applicable to the entire reprocessing facility or to any portion of it. We have found during the course of this work however that significant deviations from this equation occur for the entire reprocessing facility whose transient inventory begins to contain significant linear contributions in time (like a plug flow model) for a much longer period than an exponential model will approximate accurately.
However Equation (II.1) is accurate for a single contactor and the time constants derived from such a model provide the correct time scale for the transient behavior even for a large reprocessing facility. For this reason the exponential model is an excellent starting point for the development of a nonsteady state model for inventory estimation.

The quantitative basis for the model is that the time constant for a single contactor or tank, which is designated by \( i \), is given by,

\[
\tau_i = \frac{a_i \cdot H^0_i}{F \cdot \alpha_i} \quad (II.2)
\]

where \( a_i \) is a constant and \( F_i \) is the flow rate of the feed stream feeding nuclear materials to the contactor. The product \( F_i \cdot \alpha_i \) is the throughput rate of nuclear material \( \alpha \). The best way to understand the above formula is to apply it to a tank in which case \( a_i = 1 \) and at steady state the tank concentration is \( C_{\alpha} \). Thus the steady state tank inventory reduces to \( C_{\alpha} \cdot V \) where \( V \) is the tank volume and the formula for \( \tau_i \) of a tank reduces to,

\[
\tau_i = \frac{V}{F} \quad (II.3)
\]

One can immediately recognize the above as the classic formula for the residence time of a tank and it also is the exponential time constant for filling the tank with nuclear material \( \alpha \). Equation (II.2) is therefore merely an extension of the formula for the time constant of a tank with a uniform concentration to a contactor of nonuniform concentration. The validity of the formula for a tank presumes that the flow rate is constant or more practically that the flow rate variations are not significant. The same limitation on flow rate must be placed on Equation (II.2) for a contactor.

It is observed above that simple hydrodynamics requires that \( a_i = 1 \) for a tank. However for a contactor \( a_i \) must be determined empirically. This is accomplished by fitting Equation (II.1), using least squares, to PUBG generated databases for startup of contactors under a broad variety of conditions. For startup \( H_{\alpha}^0 = 0 \) thus Equation (II.1) reduces to,
The results of the least squares calculation yield \( a_t = 0.8 \) for A-type contactors, \( a_f = 0.6 \) for partitioning contactors, and \( a_s = 1.55 \) for stripping contactors. The flow sheet data defining the variety of conditions under which the PUBG databases were generated are given in Tables E4 to E6 of Appendix E. These tables give about 20 different flowsheets for each of the three contactor types. The database for each flowsheet contain about 20 inventories as a function of real time. Providing tabular presentations of each of these databases and the details of the least squares calculations would be a very voluminous presentation. As a compromise to such a presentation, only the standard deviations for each flow sheet condition and the steady state inventories are presented in Tables E4 to E6 and three representative databases are compared graphically with the model estimates in Figures 2 to 4.

The Figures show that the model tends to underestimate the inventories at intermediate times. Nevertheless the overall accuracy is very good as judged by the least squares standard deviations, which are less than 8% of the steady state inventory.

The estimation of the time constant for application of the transient theory to the coupled set of tanks and contactors in a reprocessing facility or a portion of the reprocessing area, is accomplished with the equation,

\[
\tau = \sum_{i} \tau_i, \quad (II.5)
\]

where the \( \tau_i \) are the time constants estimated from Equation (II.2) for the various units (tanks and contactors) in the reprocessing facility or the portion of the facility of interest for a particular calculation. If Equation (II.5) is applied to a portion of the reprocessing area the various units must be sequentially coupled, i.e. no two units can be coupled via an intervening tank or contactor that does not belong to the portion of the facility under consideration. In principle, the above time constants may be substituted into Equation...
along with the appropriate total steady state inventory and \( H_a^0 \) of the coupled system in order to estimate the time dependent inventory. The accuracy of this procedure was checked by developing a program that is described in Appendix C which can simulate the operation of the coupled set of contactors and tanks for the entire reprocessing plant or a portion of it under consideration. This program uses a subroutine that is a form of PUBG \(^5\) which has been modified to take input feed streams having time dependent concentrations and flow rates in order to account for the coupling among the contactors.

In Figure 5 are illustrated the simulated results for the inventory of a reprocessing plant sketched in Figure 1 and whose flow sheet conditions are given in Table I. The simulations are for a rinseout-restart sequence in which the feed stream feeding nuclear materials to the first purification cycle is replaced with an aqueous acid solution containing no nuclear materials in order to begin the rinseout. After 12 hours the feed stream flow of nuclear materials is restarted.

As Figure 5 shows both the rinseout and restart are strongly linear except at longer times. We have found that the following modified exponential expression accounts for this transient behavior very well,

\[
H_a(c) = H_a^0(c) - [H_a^0(c) - H_a^0(0)] \left[ 1 + 0.25 \tau - 0.55 \tau^2 + 0.12 \tau^3 \right] \exp(-\tau),
\]

where,

\[
\tau = \frac{1}{\alpha},
\]

represents a reduced time. The notation (c) indicates the corresponding inventory will be a composite inventory of tanks and contactors rather than a purely contactor inventory. The predictions of Equations (II.6) are also given in Figure 5 for purposes of comparing with the simulated results. The data for calculating \( \tau (= 10.42 \text{ hr}) \) from Equations (II.2) and (II.5) are given in Table 4. The Table shows that the calculations presented in Figure 5 were obtained assuming that the two feed tanks feeding the second purification cycle and

\[
(II.7)
\]
Figure 2. Approach to steady state for the restart of an A-type contactor. Data generated by PUBG is designated by points and the model calculation (Eq (II.4)) is the smooth curve. (Refer to dataset 9 of Table E4)

Figure 3. Approach to steady state for the restart of a partitioning contactor. Data generated by PUBG is designated by points and the model calculation (Eq (II.4)) is the smooth curve. (Refer to dataset 1 of Table E5)
Figure 4. Approach to steady state for the restart of a stripping contactor. Data generated by PUBG is designated by points and the model calculation (Eq (II.4)) is the smooth curve. (Refer to dataset 16 of Table E6)

Figure 5. The plutonium inventory predicted from the nonsteady model Equation (II.6), — , is compared with the computer simulation, • •, of the rinse-out-restart for the reprocessing plant of Figure 1.
Table 4

Data on the reprocessing facility diagrammed in Figure 1 that are used for estimating the transient Pu inventory in the reprocessing area for a rinseout-restart sequence

<table>
<thead>
<tr>
<th>Unit</th>
<th>Flow Rate (L/hr)</th>
<th>Throughput (g/hr)</th>
<th>Steady State Pu Inventory (Real Plant)</th>
<th>Volume (L)</th>
<th>( a_t )</th>
<th>( \tau_t ) (hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contactor I</td>
<td>- -</td>
<td>192</td>
<td>523</td>
<td>- -</td>
<td>0.8</td>
<td>2.18</td>
</tr>
<tr>
<td>Contactor II</td>
<td>- -</td>
<td>192</td>
<td>62</td>
<td>- -</td>
<td>1.55</td>
<td>0.50</td>
</tr>
<tr>
<td>Buffer Tank D1</td>
<td>516</td>
<td>192</td>
<td>722</td>
<td>10 1900</td>
<td>1.0</td>
<td>0.02</td>
</tr>
<tr>
<td>Contactor III</td>
<td>- -</td>
<td>192</td>
<td>400</td>
<td>- -</td>
<td>0.8</td>
<td>1.67</td>
</tr>
<tr>
<td>Contactor IV</td>
<td>- -</td>
<td>192</td>
<td>324</td>
<td>- -</td>
<td>0.6</td>
<td>1.01</td>
</tr>
<tr>
<td>Buffer Tank D2</td>
<td>162</td>
<td>192</td>
<td>526</td>
<td>10 470</td>
<td>1.0</td>
<td>0.06</td>
</tr>
<tr>
<td>Contactor V</td>
<td>- -</td>
<td>192</td>
<td>1043</td>
<td>- -</td>
<td>0.8</td>
<td>4.35</td>
</tr>
<tr>
<td>Contactor VI</td>
<td>- -</td>
<td>192</td>
<td>200</td>
<td>- -</td>
<td>0.6</td>
<td>0.63</td>
</tr>
<tr>
<td>Total</td>
<td>- -</td>
<td>-</td>
<td>3800</td>
<td>- -</td>
<td>10.42</td>
<td>16.92</td>
</tr>
</tbody>
</table>
plutonium purification cycle, respectively, are small being about 10 liters. This was done to speed up the computer simulations which require large amounts of computer time. This choice does not reflect a limitation of the model (Equation (II.6)) which is easily applied to any configuration of tanks and contactors irrespective of size. Data are also given in Table 4 for realistic tank sizes and the corresponding $\tau$ is 16.92 hr. In order that the rinseout proceeds to the same extent for the more realistic choice of feed tank sizes as that illustrated in Figure 5, its time duration must be the same as that in Figure 5 when expressed in reduced time units. For the more realistic tank sizes, this corresponds to 19.5 hours.

Equation (II.6) yields the composite inventory of all contactors and buffer tanks in the coupled system under consideration. However most often the buffer tank inventory is measured and in such instances, one would only want to estimate the contactor inventory. One normally cannot apply Equation (II.6) directly to the total contactor inventory of the reprocessing plant because the calculation of the time constant $\tau$, by Equation (II.5) requires that the system be sequentially coupled, i.e. no two contactors can be coupled via an intervening buffer tank which will not be the case in a real plant. However contactor inventory can be estimated using Equation (II.6) and the following relations,

\[ H_{\alpha} = H_{\alpha}(c) - H_{\alpha}(D1) - H_{\alpha}(D2) \]  
\[ H_{\alpha}(D1) = H_{\alpha}(2) - H_{\alpha}(1) \]  
\[ H_{\alpha}(D2) = H_{\alpha}(4) - H_{\alpha}(3) \]

where $D1$ refers to the buffer tank between the first and second purification cycles, $D2$ refers to the buffer tank between the second and final purification cycles, $H_{\alpha}(1)$ is the inventory in the first purification cycle, $H_{\alpha}(2)$ is the inventory in the first purification cycle and $D1$ buffer, $H_{\alpha}(3)$ is the inventory in the first and second purification cycles and $D1$ buffer tank, and $H_{\alpha}(4)$ is the inventory in the first and second purification cycles and the $D1$ and $D2$ buffer tanks. The inventories $H_{\alpha}(i)$ ($i = 1$ to 4) are for sequentially coupled systems as defined above and their inventories may be calculated with Equations...
The above evaluation of the contactor inventory (Equations (II.8) to (II.10)) is complicated and not very desirable. A more utilizable equation, which is identical in form to Equation (II.6), can be obtained for nonsteady state contactor inventory, if $H_a(c)$, $H_a'(c)$, and $H_a''(c)$ are replaced by contactor inventories ($H_a$, $H_a'$, and $H_a''$, respectively), i.e.,

$$H_a = H_a' - (H_a' - H_a) \left[ 1 + 0.25 T - 0.55 T^2 + 0.12 T^3 \right] \exp(-T). \quad (II.11)$$

The $T$ used to calculated $T$ from Equation (II.11) still is the time constant of the entire sequentially coupled system (the tanks and the contactors) just as in Equation (II.6). Contactor inventory estimates based on Equation (II.11) are accurate to within 5% if the total buffer tank inventory is less than the total contactor inventory. This accuracy judgement is based on comparisons of estimates from Equation (II.11) with estimates from the more fundamental Equations (II.6) to (II.10). Equation (II.11) becomes less accurate if the buffer tank inventory becomes larger than the contactor inventory, because the time dependence of the system begins to be determined by the buffer tanks. For the latter cases the separate purification cycles may be assumed to be nearly at steady state relative to the buffer tanks, and the total contactor inventory may be estimated as the sum of the contactor inventories of the separate purification cycles calculated from the Equations (I.65) to (I.67).

The strong nonexponential behavior that was observed for coupled sets of tanks and contactors was not anticipated, however some later reflection indicated it is to be expected. Solving differential equations for the transient holdup in a coupled set of tanks yields a similar nonexponential behavior. One notes that Equations (II.6) and (II.11) attempt to emphasize linear behavior which can to some extent be accomplished by removing the contribution of $1/2 T^2$ to the exponential (i.e. the quadratic term in a Taylor's series expansion of $\exp(-T)$) leaving the linear term in $T$, as the more dominant contributor. This is accomplished with the $0.55 T^2$ in the parenthesis of Equation (II.6), the $0.55$ implying there must be some overcompensation. The terms $0.25 T$ and $0.12 T^3$ are
additional terms determined empirically. The former further enhances the linear behavior and the latter provides the compensation that is needed to explain the curvature contribution to $H_a(c)$ that is present in Figure 5 at longer times.

C. The Application of the Inventory Estimation Models

Criteria for Application of Nonsteady State Models

The inputs to the nonsteady state models (Equations (11.6) or (11.11)) are time and the steady state inventories. The latter may be estimated from Equations (1.50) to (1.73). Thus once the problem of estimating steady state inventories has been solved the problem of estimating nonsteady state inventories has also been solved. From this statement one might at first conclude that applying the more general nonsteady state theory, which includes steady state as a special case, is preferable to applying steady state theory. The incorporation of time into the nonsteady state model does however complicate its application and for a majority of the nuclear material accounting applications of inventory estimation theory, the steady state theory is sufficiently accurate. Therefore criteria are desirable for using nonsteady state theory that will keep its application at a minimum and yet assure accurate inventory estimates for all other cases where steady state theory is applied.

In view of the above considerations criteria for application of nonsteady state theory have been established numerically, using the requirement that the contactor inventory estimates must have an accuracy that is within 10% of the steady state contactor inventory. These criteria are best stated by considering two general classes or types of applications of the theory. We will designate as Class A those cases where the concentration of the stream feeding the first purification cycle is provided, but no measured concentrations of intermediate buffer tanks are given. For this class two criteria have been established for application of nonsteady state theory: (I) the inventory
variations resulting from the nonsteady state condition may be larger than 10% of the steady state inventory (i.e. \( |H_a - H^0_a| / H^0_a > 0.10 \)) and (2) the time following the perturbation that caused the nonsteady state condition is less than twice the characteristic time (2\(\tau\)) of the entire reprocessing system.

The second class, which will be designated Class B, refers to those cases where the measured nuclear concentrations of all tanks are provided. These cases are more common because nuclear material accounting procedures for safeguards purposes require measured tank inventories which are obtained from measured tank solution concentrations and volumes. The situations falling into Class A are special cases that may occur at isolated times where for some reason no inventories of intermediate buffer tanks were measured but nevertheless after later considerations estimated inventories are desired.

For the cases falling into Class B three criteria have been established for application of nonsteady state theory: (I) the inventory variations resulting from the nonsteady state conditions are larger than 40% of the steady state inventory (i.e. \( |H_a - H^0_a| / H^0_a > 0.40 \)), (2) the time following the perturbation causing the nonsteady state condition is less than twice the characteristic time (2\(\tau\)) of the entire system, and (3) the buffer tank inventory is less than the contactor inventory. If any one of the above three conditions do not hold, the contactor inventory may estimated as the sum of the contactor inventories of the separate purification cycles calculated from steady state theory (Equations (1.65) to (1.67)) and the measured concentrations of the tank solutions feeding each purification cycle. The latter inventory estimates, where conditions (I) to (3) are not met, are accurate because the separate purification cycles approach steady state so rapidly (5 times as fast as the overall system) that they are effectively at steady state relative to the tank solution concentrations.

The criteria for Class B imply nonsteady state theory only needs to be applied if there are very large deviations from steady state conditions. This situation occurs because the time dependent buffer tank concentrations which are input into the alternative estimate
adequately account for nonsteady state behavior if the deviations from steady state are not too large. The conditions where nonsteady state theory would need to be applied to cases of Class B do not occur frequently in practice. Nevertheless two situations are of special interest; (i) a rinseout-restart sequence and (ii) the introduction of a new feed solution resulting from the dissolution of a new batch of spent fuel with a very different plutonium content from the previous batch. The application of the nonsteady state theory to a rinseout-restart sequence will be dealt with in greater detail in the following paragraphs.

**Methods for Application of Inventory Estimation Models**

Before discussing any specific applications of nonsteady state theory it is instructive to follow through a general sequence for applying Equations (II.6) or (II.11). In discussing this sequence we will for simplicity designate inventory as \( H_a \) without the specific designation \( H_a(c) \) to differentiate composite inventory of Equation (II.6) from contactor inventory in Equation (II.11) as was done in Chapter II. The initial time or \( t = 0 \) for applying these equations is defined as the time when the change in nuclear material throughput that resulted in a nonsteady state condition occurred. Equations (II.6) or (II.11) are applicable to this case if the new nuclear material throughput rate is held constant for a certain time, \( t \). The input, \( H^\circ_a \), to Equations (II.6) and (II.11) are the steady state nuclear material inventories that would be achieved if the new nuclear material throughput persisted for a long time \( (t \to \infty) \). These are calculated from the appropriate steady state equations (Equations (I.50) to (I.73)) and tank solution concentrations. The input, \( H^\circ_t \), to the nonsteady state theory is the initial inventory present at \( t = 0 \). This value represents an initial condition and must be calculated from conditions that existed prior to the perturbation at \( t = 0 \), which could be a steady state or nonsteady state condition. The simplest initial condition is startup where \( H^\circ_t = 0 \). This is a likely condition one might wish to use for beginning a nonsteady state calculation. The \( H^\circ_t \) and the calculated value of \( H^\circ_t \) are used to estimate \( H_a \) for any time, \( t \), using Equation (II.6) or
(II.11) until a change in nuclear material throughput occurs. The change in conditions brought about by a change in throughput must be accounted for by modifying the calculation. This is accomplished by essentially restarting the calculation. The time when the change in throughput occurred is reset to zero and the inventory calculated for that time will be \( H_{\alpha}' \) for the new calculation. The \( H_{\alpha}' \) is recalculated to correspond to the new throughput conditions. With these new inputs, \( H_{\alpha} \) can be calculated for times following the change in throughput. This process can be continued for a whole sequence of throughput perturbations on the system thereby generating inventory estimates for all times.

We will next demonstrate the application of the above described sequence of calculations to the plutonium concentration data given in Table 5. The concentration data in the table for the feed solution to the first purification cycle are selected to be representative of those which could occur for a rinseout-restart sequence in the reprocessing plant of Figure 1. The first two rows of Table 5 contain data for the 36 hours prior to the rinseout where the system is operating at steady state. The rinseout-restart takes place over a four day period, beginning at the time, 36 hours, and extending to the time, 132 hours.

Since the system is at steady state from 0 to 36 hours, only inventory estimates based on steady theory are given in Table 5 for this period. The data in row 4 of the Table are obtained at 48 hours which is 12 hours after the rinseout began. It is useful to illustrate how the nonsteady state inventory for this time is calculated. We begin by noting that the final steady state inventory for the rinseout is zero (\( H_{\alpha}^0 = 0 \)) and the initial inventory \( H_{\alpha}^0 \) at the time the rinseout began is assumed to be steady state value (2648 grams) obtained at 24 hours. The reduced time, \( \tilde{t} \), is calculated as follows,

\[
\tilde{t} = \frac{t}{\tau} = \frac{12}{16.92} = 0.71 ,
\]

where 16.92 hours is the characteristic time, \( \tau \), taken from Table 4. Substitution of these values for \( H_{\alpha}^0, H_{\alpha}^0 \) and \( \tilde{t} \) into Equation (II.11) yields the following calculation,
\[ H_{Pu} = 2648 \left[ 1 + 0.25(0.71) - 0.55(0.71)^2 + 0.12(0.71)^3 \right] \exp(-0.71) \]

= 1228, \hspace{1cm} (II.13)

where the calculated value, 1228 grams, corresponds to that given in Table 5. At 84 hours the system is still under the rinseout conditions. Thus the value for \( H_{Pu} \) remains at zero and \( H_{Pu} \) can be estimated by exactly the same calculation as is illustrated above by Equation (II.13). The only change would be the value for \( T \) which must now be 2.84 in order to correspond to 48 hours after the rinseout began. This calculation yields the inventory of 3.5 grams given in Table 5. This value is very small and means the rinseout is virtually complete.

Table 5

<table>
<thead>
<tr>
<th>No.</th>
<th>Time (hrs.)</th>
<th>Concentration of feed to the initial cycle (g/L)</th>
<th>Nonsteady State Inventory (g)</th>
<th>Steady State Inventory (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>1.23</td>
<td>2714</td>
<td>2714</td>
</tr>
<tr>
<td>2</td>
<td>24</td>
<td>1.20</td>
<td>2648</td>
<td>2648</td>
</tr>
<tr>
<td>3</td>
<td>36</td>
<td>0.0</td>
<td>Rinseout begins</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>48</td>
<td>0.0</td>
<td>1228</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>84</td>
<td>0.0</td>
<td>3.5</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
<td>84</td>
<td>1.20</td>
<td>Restart begins</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>108</td>
<td>1.20</td>
<td>2271</td>
<td>2648</td>
</tr>
<tr>
<td>8</td>
<td>132</td>
<td>1.40</td>
<td>2973</td>
<td>3090</td>
</tr>
</tbody>
</table>

35
With the completion of the rinseout after 84 hours, the system is again restarted. At
108 hours which is 24 hours after restart, the tank concentrations are measured. In
order to calculate nonsteady state inventories for this time, the time when the restart
began (84 hours) is set to zero and $H_{Pu}'$ is the inventory that is estimated for that time
(3.5 grams). The final steady state inventory must be calculated from the concentra-
tion of the tank solution feeding the first cycle (1.20 g/L) using the steady state equation for
the entire reprocessing system (Equation (I.73)) as follows,

$$
H_{Pu}^0 = 1.20 \left\{ 1975 + \frac{24.21}{1 - 0.112(180 + 1.20)/30} \right\} = 2648 \quad \text{(11.14)}
$$

The above equation assumes the nominal flow sheet value for the uranium concentra-
tion of 180. g/L given in Table I and a TBP volume fraction of 30%. Using the above values,
2648 and 3.5 grams, for $H_{Pu}'$ and $H_{Pu}'$, respectively, and Equation (II.ii) for $H_{Pu}$, one
obtains the following result,

$$
H_{Pu} = 2648 - (2648 - 3.5) \left[ 1 + 0.25(1.42) - 0.55(1.42)^2 
+ 0.12(1.42)^3 \right] \exp(-1.42) = 2271 \quad \text{(11.15)}
$$

where $\bar{T} = 24/16.91 = 1.42$ is used.

One observes that at 132 hours the tank concentration feeding the first purification
cycle is 1.40 g/L which differs slightly from the 1.20 g/L measured at the previous time,
108 hours. In applying nonsteady state theory it is suggested to assume this change in Pu
throughput occurred at beginning of the time interval, 108 to 132 hours, and reset the
time at 108 hours to zero. The $H_{Pu}'$ is taken to be the estimated inventory at 108 hours
(2271 grams) using Equation (I.73), and concentration of the tank feeding the first
purification cycle at 132 hours (1.40 g/L). This produces the following nonsteady state
calculation for the inventory at 132 hours,

$$
H_{Pu} = 3090 - (3090 - 2271) \left[ 1 + 0.25(1.42) - 0.55(1.42)^2 
+ 0.12(1.42)^3 \right] \exp(-1.42) = 2973 \quad \text{(11.16)}
$$
where $\tau = 1.42$ is used.

The above sample calculations demonstrate the application of nonsteady state theory for a variety of cases. By criteria we have established however, the nonsteady state calculation is not more accurate than an alternative steady state calculation for all the cases in Table 5. The most obvious examples are the nonsteady state calculations at 84 hours and 132 hours which are 48 hours into rinseout and 48 hours (2.8\tau) into restart, respectively. Since the time is greater than 2\tau (See criteria 2 case B), the nonsteady state values differ negligibly from the steady state calculations as can be verified by examination of Table 5. The value 2271 grams at 108 hours differs significantly from the steady state value (2648 grams), but since it is within 40\% of the steady state value (See Criteria (I) Case B) it would not differ significantly (less than 10\%) from a value that assumes steady state for the separate purification cycles. This leaves only the nonsteady state value, 1228 grams, at 84 hours (12 hours into rinseout or 0.71\tau) as being significantly more accurate than alternative estimates assuming steady state.

D. Correction of CUMUF for Contactor Inventory

Since the purpose of simple methods for estimating contactor inventory is the correction of near-real time dynamical accounting methods for the unmeasured inventory, in this Section a demonstration is given on using these estimates to correct the CUMUF test. The MUF is given by,

$$ MUF_{i} = BH_{i} + I_{i} - O_{i} - EH_{i} $$  \hspace{1cm} (II.17)

where $BH_{i}$ is the inventory for the reprocessing facility measured at the beginning of a time interval ($t_{i+1} - t_{i}$), the $I_{i}$ and $O_{i}$ are the nuclear material input and nuclear material removed from the facility, respectively, during this same time interval, and $EH_{i}$ is the measured nuclear material inventory at the end of the time interval. One should note the relation between $EH_{i}$ for the time interval beginning at $t_{i}$ and the beginning inventory $BH_{i+1}$ for the time interval beginning at $t_{i+1}$.
The CUMUF for time $t$ is given by,

$$\text{CUMUF} = \sum_{0 \leq i \leq t} \text{MUF}_i.$$  

(Normalized the contactor inventory is neglected in the measurement of $B_{H_i}$ and $E_{H_i}$. Correction of MUF and CUMUF for contactor inventory is obtained by replacing $E_{H_i}$ and $B_{H_i}$ in Equation (11.17) with $(B_{H_i})_C$ and $(E_{H_i})_C$ defined as follows,

$$(B_{H_i})_C = B_{H_i} + H_i,$$

$$E_{H_i} = E_{H_i} + H_i + 1.$$

where $H_i$ and $H_{i+1}$ are the contactor inventories estimated from the inventory equations described in this Chapter and Chapter 1.

In order to demonstrate the correction of CUMUF test for contactor inventory, the data measured in the 82-1 and 82-2 campaign for field testing near-real-time accountancy at the PNC-Tokai reprocessing plant are employed. These data were employed because both corrected and uncorrected CUMUF tests have already been reported for the data. The concentrations of the tanks feeding each purification cycle that were used to estimate the unmeasured inventory corrections are the same as those used to estimate the tank inventories and were available as unpublished data.

The time constant data for the PNC-Tokai reprocessing plant corresponds to that given in Table 4 for a real plant. One sees from this table that the time constant, $\tau$, for the entire reprocessing area is 16.92 hours. Since the measured data were collected over 5 to 10 day intervals, the times for performing a nonsteady state inventory estimate are much greater than $2\tau$. Consequently, by criteria established in the previous Section of this Chapter, steady state estimates of the contactor inventory are sufficiently accurate. Since the feed concentrations to each cycle were available to the authors, the contactor inventories were estimated for each purification cycle using the steady state Equations (1.65) to (1.67). These calculations use the nominal values for the uranium concentration.
of the streams feeding each cycle (180, 55 and 4 g/L, respectively; see Table 1). The TBP is 30% by volume (B = 30).

The calculated contactor inventories showed substantial variation from one time interval to another. Since these variations could represent short term fluctuations in the concentrations used to estimate the contactor inventories, we used instead of \( H_i \), \(<H_i>\) defined as,

\[
<H_i> = \frac{H_{i-1} + H_i}{2},
\]

(II.22)
to correct BH and EH according Equations (II.20) and (II.21) if the time interval \( t_i - t_{i-1} \) was less than 10 days. The above smoothing procedure prevents the correction from introducing the fluctuations in calculated \( H_i \) into CUMUF, but does not affect the trends or average magnitude of CUMUF.

The results for MUF and CUMUF are given in Table 6. The uncorrected CUMUF, and the CUMUF corrected in this work are given in Figures 6 and 7, respectively. Figure 8 shows the corrected CUMUF of Miura et. al. These workers assume a contactor plutonium inventory of 3.2 Kg, which is a best value determined by assuming that the contactor inventory remained constant during the measurement campaigns. Differences between the corrected CUMUF of this work and the earlier work are attributable to the variation in the steady state contactor inventory used in this work which ranged from about 1.0 to 4.0 Kg. The time intervals where rinseout and a subsequent restart occur are identified in the caption of Figure 6 for the uncorrected CUMUF. Note that the restarts are accompanied by a positive CUMUF which represents the building up of inventory within the contactor. In the corrected CUMUF the contactor inventory is accounted for which has the effect of eliminating the positive values.

We see in the corrected CUMUF of Figure 7 there is a gradual onset of negative bias starting with the first time interval. After the first rinseout the negative bias appears to level out to a constant value. This negative bias was generally most pronounced at the completion of a rinseout where the CUMUF values are not altered by correction for
Table 6.

Data from the 82-1 and 82-2 campaigns at the PNC-Tokai Plant, which is given in Ref. 15 and 16, includes measured plutonium inventories (g), measured plutonium input into the reprocessing area, and measured plutonium output from the reprocessing area. Also included are the smoothed contactor inventory, corrected inventories, corrected MUF, and corrected CUMUF.

<table>
<thead>
<tr>
<th>No.</th>
<th>(BH&lt;sub&gt;i&lt;/sub&gt;)&lt;sub&gt;c&lt;/sub&gt;</th>
<th>I&lt;sub&gt;i&lt;/sub&gt;</th>
<th>Q&lt;sub&gt;i&lt;/sub&gt;</th>
<th>EH&lt;sub&gt;i&lt;/sub&gt;</th>
<th>&lt;i&gt;H&lt;/i&gt;</th>
<th>(EH&lt;sub&gt;i&lt;/sub&gt;)&lt;sub&gt;c&lt;/sub&gt;</th>
<th>MUF</th>
<th>CUMUF</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1508</td>
<td>0</td>
<td>0</td>
<td>1508</td>
<td>0</td>
<td>1508</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1508</td>
<td>9105</td>
<td>0</td>
<td>9672</td>
<td>900</td>
<td>10572</td>
<td>41</td>
<td>41</td>
</tr>
<tr>
<td>3</td>
<td>10572</td>
<td>19597</td>
<td>16967</td>
<td>11485</td>
<td>1823</td>
<td>13308</td>
<td>-106</td>
<td>-65</td>
</tr>
<tr>
<td>4</td>
<td>13308</td>
<td>11765</td>
<td>12000</td>
<td>11092</td>
<td>1846</td>
<td>12938</td>
<td>135</td>
<td>70</td>
</tr>
<tr>
<td>5</td>
<td>12938</td>
<td>25411</td>
<td>24335</td>
<td>12834</td>
<td>1968</td>
<td>14802</td>
<td>-768</td>
<td>-718</td>
</tr>
<tr>
<td>6</td>
<td>14802</td>
<td>19458</td>
<td>18327</td>
<td>14257</td>
<td>2441</td>
<td>16698</td>
<td>-765</td>
<td>-1483</td>
</tr>
<tr>
<td>7</td>
<td>16698</td>
<td>14183</td>
<td>15903</td>
<td>12254</td>
<td>2357</td>
<td>14611</td>
<td>367</td>
<td>-1116</td>
</tr>
<tr>
<td>8</td>
<td>14611</td>
<td>9916</td>
<td>12685</td>
<td>10968</td>
<td>1586</td>
<td>12554</td>
<td>-712</td>
<td>-1828</td>
</tr>
<tr>
<td>9</td>
<td>12554</td>
<td>6452</td>
<td>4359</td>
<td>13075</td>
<td>1639</td>
<td>14714</td>
<td>-67</td>
<td>-1895</td>
</tr>
<tr>
<td>10</td>
<td>14714</td>
<td>5204</td>
<td>17562</td>
<td>1043</td>
<td>9</td>
<td>7052</td>
<td>1304</td>
<td>-591</td>
</tr>
<tr>
<td>11</td>
<td>7052</td>
<td>4862</td>
<td>0</td>
<td>5354</td>
<td>1019</td>
<td>6373</td>
<td>-459</td>
<td>-1050</td>
</tr>
<tr>
<td>12</td>
<td>6373</td>
<td>5674</td>
<td>0</td>
<td>10669</td>
<td>1902</td>
<td>12771</td>
<td>-724</td>
<td>-1774</td>
</tr>
<tr>
<td>13</td>
<td>12771</td>
<td>26499</td>
<td>23999</td>
<td>12347</td>
<td>3086</td>
<td>15434</td>
<td>-162</td>
<td>-1936</td>
</tr>
<tr>
<td>14</td>
<td>15434</td>
<td>13287</td>
<td>11167</td>
<td>13750</td>
<td>2938</td>
<td>16688</td>
<td>865</td>
<td>-1071</td>
</tr>
<tr>
<td>15</td>
<td>16688</td>
<td>9840</td>
<td>11703</td>
<td>13942</td>
<td>2774</td>
<td>16716</td>
<td>-1891</td>
<td>-2962</td>
</tr>
<tr>
<td>16</td>
<td>16716</td>
<td>4083</td>
<td>11578</td>
<td>8221</td>
<td>1540</td>
<td>9761</td>
<td>-540</td>
<td>-3502</td>
</tr>
<tr>
<td>17</td>
<td>9761</td>
<td>0</td>
<td>7237</td>
<td>3598</td>
<td>11</td>
<td>3609</td>
<td>-1085</td>
<td>-4587</td>
</tr>
<tr>
<td>18</td>
<td>3609</td>
<td>0</td>
<td>0</td>
<td>3753</td>
<td>0</td>
<td>3753</td>
<td>-144</td>
<td>-4731</td>
</tr>
<tr>
<td>19</td>
<td>3753</td>
<td>8045</td>
<td>0</td>
<td>8301</td>
<td>827</td>
<td>9128</td>
<td>2670</td>
<td>-2061</td>
</tr>
<tr>
<td>20</td>
<td>9128</td>
<td>11425</td>
<td>4176</td>
<td>13450</td>
<td>1935</td>
<td>15385</td>
<td>992</td>
<td>-1069</td>
</tr>
<tr>
<td>21</td>
<td>15385</td>
<td>15218</td>
<td>12164</td>
<td>16687</td>
<td>2449</td>
<td>19136</td>
<td>-697</td>
<td>-1766</td>
</tr>
<tr>
<td>22</td>
<td>19136</td>
<td>15973</td>
<td>17200</td>
<td>155553</td>
<td>2967</td>
<td>18520</td>
<td>-617</td>
<td>-2383</td>
</tr>
<tr>
<td>23</td>
<td>18520</td>
<td>18598</td>
<td>16254</td>
<td>19352</td>
<td>3510</td>
<td>22862</td>
<td>-2007</td>
<td>-4390</td>
</tr>
<tr>
<td>24</td>
<td>22862</td>
<td>16044</td>
<td>17747</td>
<td>14188</td>
<td>3492</td>
<td>17680</td>
<td>3479</td>
<td>-911</td>
</tr>
<tr>
<td>25</td>
<td>17680</td>
<td>13418</td>
<td>12519</td>
<td>16788</td>
<td>4003</td>
<td>20791</td>
<td>-2212</td>
<td>-3123</td>
</tr>
<tr>
<td>26</td>
<td>20791</td>
<td>12716</td>
<td>17809</td>
<td>10696</td>
<td>3483</td>
<td>14179</td>
<td>1719</td>
<td>-1404</td>
</tr>
<tr>
<td>27</td>
<td>14179</td>
<td>12820</td>
<td>12339</td>
<td>11900</td>
<td>2523</td>
<td>14423</td>
<td>237</td>
<td>-1167</td>
</tr>
<tr>
<td>28</td>
<td>14423</td>
<td>20489</td>
<td>19141</td>
<td>14354</td>
<td>2689</td>
<td>17043</td>
<td>-1272</td>
<td>-2439</td>
</tr>
<tr>
<td>29</td>
<td>17043</td>
<td>6485</td>
<td>23058</td>
<td>1524</td>
<td>113</td>
<td>1637</td>
<td>-1167</td>
<td>3606</td>
</tr>
<tr>
<td>30</td>
<td>1637</td>
<td>0</td>
<td>1789</td>
<td>0</td>
<td>1789</td>
<td>-152</td>
<td>-3758</td>
<td></td>
</tr>
</tbody>
</table>
Figure 6. The uncorrected CUMUF for the 82-1 and 82-2 campaigns at the PNC-Tokai Plant (taken from Ref. 15). Startups occur at dataset numbers 0, 10, and 18.

Figure 7. The CUMUF for the 82-1 and 82-2 campaigns at the PNC-Tokai plant (Ref. 15) corrected for contactor inventories estimated by the inventory estimation model of this work. Startups occur at dataset numbers 0, 10, and 18.
Figure 8. The corrected CUMUF of Reference 15. The correction assumes a contactor inventory of 3.2 Kg of plutonium. Startups occur at dataset numbers 0, 10, and 18.

unmeasured inventory.

In conclusion we wish to focus attention on the range of contactor inventories (1.0 to 4.0 Kg) estimated for normal steady state operation. In this connection it should be noted that at the beginning of the 82-1 campaign (No’s 1 to 6 in the Figure), before bias has had a chance to set in, the positive uncorrected CUMUF values (Figure 6) of approximately 2 Kg are almost exactly compensated for in the corrected CUMUF of this work (Figure 7). This lends support to our inventory estimation method as a means of correcting CUMUF. It also indicates that at the beginning of the 82 campaigns the contactor inventories (about 2 Kg) were much lower than previously expected based on selections of the best constant value for the contactor inventory. These results lend more support to the conclusions of Miura et. al.\textsuperscript{15,16} on the need to correct the CUMUF test for contactor inventory.
CHAPTER III
Pulsed Column Computer Model: CUSEP

A. Descriptions and Fundamental Theory

Pulsed columns are cylindrical and arranged vertically as shown in Figure 9. The aqueous scrub stream enters at the top of the column while the organic stream enters at the bottom. Feed streams containing nuclear materials enter at some intermediate point of the contactor much like for mixer-settler contactors. The entire liquid column is pressure pulsed from below. The pulsing forces the liquid through sieve plates positioned at various points down the length of the contactor which results in the droplet dispersion of the phase of lower volume. Depending on the application, the dispersed phase may be either the organic or the aqueous phase.

There are similarities between pulsed columns and mixer-settlers, namely their concentration profiles are very similar. Consequently mixer-settler programs such as SEPHIS\textsuperscript{17} and PUBG\textsuperscript{13} are used with some success in simulating pulsed column behavior. However, there are design differences between mixer-settlers and pulsed columns which make a mixer-settler computer model unsatisfactory for simulation of pulsed column behavior in some important respects. In particular (i) the aqueous to organic phase ratio must be calculated in pulsed column computer models whereas it is input into mixer-settler computer models, and (ii) a mixer-settler computer model cannot account for the dispersion in the concentration profile that results from the pulsing. The phase volume ratio referred to in (i) does not affect the simulation of the concentration profile but it is necessary for estimation of contactor inventory which is the primary quantity of interest. In the next Section the theory used to develop the pulsed column simulation program CUSEP (Clemson University Solvent Extraction Program) is described.
Figure 9. Simplified drawing of a pulsed column contactor showing a continuous organic phase flowing from bottom to top and the aqueous dispersed phase flowing oppositely.
B. Pulsed Column Theory

The pulsed column has no discrete stage structure. Consequently the nuclear material concentrations are given as a function of a continuous variable, x, which represents a vertical position in the column as illustrated in Figure 9. However in order to develop a computer model, one must discretize the mass balance equations describing the pulsed column operation. One may then write the mass balance equations in much the same way as for mixer-settler contactors with some modifications,

\[
\frac{\partial [V^O(x)C^O(x)]}{\partial t} = - F^O_{\alpha} \frac{\partial C^O(x)}{\partial x} + F^O_{\alpha} \frac{\partial C^O(x+\Delta x)}{\partial x} + \phi^O_{\alpha}(x) \\
- KA[C^O_{\alpha}(x) - D \frac{\partial (x)C^O_{\alpha}(x)}{\partial x} + D^{(d)} \frac{\partial^2 C^O_{\alpha}(x)}{\partial x^2}], \tag{III.1}
\]

\[
\frac{\partial [V^a(x)C^a(x)]}{\partial t} = - F^a_{\alpha} \frac{\partial C^a(x)}{\partial x} + F^a_{\alpha} \frac{\partial C^a(x-\Delta x)}{\partial x} + \phi^a_{\alpha}(x) \\
+ KA[C^O_{\alpha}(x) - D \frac{\partial (x)C^a_{\alpha}(x)}{\partial x} + R^a_{\alpha}] \tag{III.2}
\]

The symbol, x, enclosed in parenthesis indicates that the associated dependent variable is a function of the vertical position in the column. The linear interval \(\Delta x\) (see Figure 9) also defines a volume element located at position x. The symbols \(V^O(x)\) and \(V^a(x)\) represent the volume of the aqueous and organic phase within the element \(\Delta x\). The symbols K and A represent the mass transfer coefficient and mass transfer area, respectively. Their product, \(KA\), determines the rate of transfer of nuclear material between the aqueous and organic phases. The above equations presume the organic phase is the continuous phase in that Equation (III.1) contains the diffusional term \(D^a_{\alpha} \frac{\partial^2 C^a_{\alpha}(x)}{\partial x^2}\). This term accounts for longitudinal dispersion of the concentrations by diffusional processes. In this research it was found that the diffusional term has a negligible effect on the concentration dispersion compared to the convective remixing.
caused by the pulsing. Consequently it is only significant in the limit of a zero pulsing rate and is neglected in the computer model CUSEP.

The pulsed flow rates of the aqueous and organic streams within the column are given by,

\[ F^a_\omega = F^a + V^a_p \left( \frac{\omega}{\omega} \right) \cos(\omega t + \frac{\phi}{\tau}) \]  

\[ F^o_\omega = F^o + V^o_p \left( \frac{\omega}{\omega} \right) \cos(\omega t + \frac{\phi}{\tau}) \]  

where \( F^a \) and \( F^o \) are the aqueous and organic flow rates, respectively, with no pulsing, \( \phi \) is a phasing constant which is normally set to zero, \( \omega \) is the pulsing frequency in radians per minute, \( V^a_p \) is the pulse amplitude in volume units, and \( V^a/V_T \) and \( V^o/V_T \) are the volume fractions of the aqueous and organic phases, respectively.

The symbols \( \phi^a_\alpha(x) \) and \( \phi^o_\alpha(x) \) are the rates of transfer of nuclear material by organic and aqueous feed streams, respectively, into the element \( \Delta x \). These rates are given by,

\[ \phi^o_\alpha(x) = \frac{F^o_\alpha c^o_f(x)}{F^o_\alpha} \]  

\[ \phi^a_\alpha(x) = \frac{F^o_\alpha c^a_f(x)}{F^o_\alpha} \]  

where \( F^o_\alpha \) and \( F^a_\alpha \) are feed stream flow rates and \( c^o_f(x) \) and \( c^a_f(x) \) are feed stream concentrations. The symbol \( R^o_\alpha \) represents the rate of production of nuclear material \( \alpha \) by chemical reaction.

The distribution coefficients within an element \( \Delta x \) are calculated from the relations,

\[ D_{U(VI)}(x) = K_{U(VI)}[TBP]^2 \]  

\[ D_{Pu(V)}(x) = K_{Pu(V)}[TBP]^2 \]  

\[ D_{Pu(IV)} = 0.01138 D_{Pu(V)}(x) \]  

\[ D_H(x) = K_H([TBP] + [TBP]^2) \]  

\[ D_{U(IV)}(x) = K_{U(IV)}[TBP]^2 \]
where $K_U$, $K_{Pu}$, and $K_H$ are calculated from the literature correlations,\(^4\),

\[
K_U' = 3.7N_a^{1.57} + 1.4N_a^{3.9} + 0.011N_a^{7.3},
\]

\[
K_U = K_U' [0.2 + 0.55(0.01B)^{1.25} + 0.0074N_a^{2}],
\]

\[
K_{U(IV)} = K_{U(IV)}' (0.0541 + 0.000658N_a^{2}),
\]

\[
K_{U(VI)} = K_{U(VI)}' [4(0.01B)^{-0.17} - 3] \exp(2500\tau),
\]

\[
K_{Pu(IV)} = K_{Pu(IV)}' [4(0.01B)^{-0.17} - 3] \exp(-200\tau),
\]

\[
K_H = K_H' [1 - 0.54 \exp(-0.15B)] \exp(340\tau),
\]

\[
\tau = \frac{1}{T} \cdot \frac{1}{298.16},
\]

where $T$ is the absolute temperature. The quantity $N_a$ is the modified nitrate salting strength and is given by the relation,\(^6\)

\[
N_a = [H]_a + 2[U(VI)]_a + (4 - 2\delta)[Pu(IV)]_a
+ 3[Pu(III)]_a + (4 - 3\chi)[U(IV)]_a,
\]

\[
\delta = \begin{cases} 
1, & \text{if U(VI) is present or} \\
0, & \text{if no U(VI) is present,}
\end{cases}
\]

\[
\chi = [Pu(IV)]_a / ([U(VI)]_a + [Pu(IV)]_a,)
\]

where $[ ]_a$ represents the aqueous phase molarity. The free TBP molarity is obtained by solving the equation,

\[
[TBP] = [TBP]_T - 2D_{U(VI)}[U(VI)]_a - 2D_{Pu(IV)}[Pu(IV)]_a
- 2D_{U(IV)}[U(IV)]_a - K_H[H]_a[TBP] + 2[TBP]^2,
\]

\[47\]
In the program CUSEP the solution of the above equation is obtained numerically using Newton's method.

The reactions involved in partitioning to produce a separation of uranium and plutonium are the reduction of plutonium by either U(IV) or hydroxylamine nitrate (HAN),

\[ U^{4+} + 2Pu^{4+} + 2H_2O \rightarrow UO_2^{2+} + 2Pu^{3+} + 4H^+ , \quad (III.23) \]

\[ \text{HAN} + Pu^{4+} \rightarrow Pu^{3+} + H^+ + H_2O + \text{other products}. \quad (III.24) \]

If U(IV) is used as the reductant, one must consider the oxidation of U(IV) to U(VI),

\[ U^{4+} + NO_3^- + H_2O \rightarrow UO_2^{2+} + H^+ + HNO_2^- \quad (III.25) \]

If the reductant is HAN then the following rate expression\(^{19}\) must be substituted into the mass balance Equation (III.2),

\[
P_{Pu(III)} = \frac{K [\text{HAN}]_a^2 [\text{Pu(IV)}]_a^2}{[H]^4 [\text{Pu(II)}]_a^2 (K_d + [NO_3^-]_a)^2} \quad (III.26)\]

The removal of HAN must be accounted for since its concentration appears in the above rate expression. The constant K has a value of 0.029 M\(^5\)/sec at 30°C and an activation energy of 31 Kcal. The constant K\(_d\) in the above Equation has a value of 0.33 in molarity units. When using U(IV), the rates of the reactions are as follows,\(^{8,18,19}\)

\[
R_{Pu(II)} = -R_{Pu(IV)} = 170 \frac{[\text{U(IV)}]_a [\text{Pu(IV)}]_a}{[H]^2} \quad (III.27)
\]
The term $K'[U(IV)]_a[NO_3^-]_a$ represents the rate of oxidation of U(IV) by nitric acid. The rate parameter $K'$ depends on the presence of hydrazine stabilizer and is input into the program. Normally a value of 0.001 in units of mol$^{-1}$min$^{-1}$ is used. When using CUSEP to simulate partitioning, the volume input must be in units of liters and the flow rate input must be in units of liters per minute because all rate constants are expressed in these units. The effects of the chemical reactions on H$^+$, HAN, and NO$^-$ are accounted for according to the stoichiometry given in Equations (III.23) to (III.25).

The temperature in each element $\Delta x$ is calculated assuming a steady state formula,

$$T(x) = \frac{C_{pa} F_0 T(x-\Delta x) + C_{po} F_0 T(x+\Delta x) + C_{pa} F_0 T_{1, f} + C_{po} F_0 T_{1, f}}{C_{pa} F_0 + C_{po} F_0 + C_{pa} F_0 + C_{po} F_0}.$$  \hspace{1cm} (III.29)

The specific heats in the above Equation are given by the formulae,$^{20}$

$$C_{pa} = 1 \text{ Cal/gram},$$  \hspace{1cm} (III.30)

$$C_{po} = 0.321 + 7.8 \times 10^{-4} \text{ B}.$$  \hspace{1cm} (III.31)

The steady state assumption enhances the achievement of a steady state temperature along the length of the column. Since temperature is not important in determining nonsteady state column behavior, the calculational advantages of Equation (III.29) outweigh other considerations.

The discussion thus far is common to all investigations that have been performed on pulsed columns.$^{12,21}$ However the various investigative approaches differ on how to account for convective remixing.$^{12}$ The reason for difficulties is that this is not accounted for within the framework of the basic mass balance Equations (III.1) and (III.2). Convective remixing effects are accounted for by momentum balance equations.
which determine the convective velocities within the contactor. The diffusion term in Equation (III.1) is of the wrong form and magnitude to explain the very dominant remixing effects that are observed. One can arrive at this conclusion analytically by examining the diffusion term, but we have also established this by a number of numerical calculations on pulsed columns in which we have included it in Equations (III.1) or (III.2). It is very likely for this reason that pulsed column computer models often predict contactor concentrations and inventories that are much larger than those measured experimentally.

The model for accounting for convective remixing should in principle be a very simple one, since its primary effect is to promote greater longitudinal concentration uniformity along the column. The length of a column segment that can be regarded as uniform should therefore be characteristic of convective remixing. Since it is caused by convective velocity, it should, as a first approximation, be a linear function of convective velocity of the following type,

$$L_p = L_p + b\xi.$$  \hspace{1cm} (III.32)

where $\xi$ is the pulse amplitude in units of length (cm) and $b$ is a numerical factor. The equation defines what will be referred to as a mass transfer unit or a mass transfer length. The quantity $L_p$ is the distance between the sieve plates. The reason for inclusion of $L_p$ is because it is expected that the disturbance to convective flow near the sieve plates will always produce remixing in the regions between the sieve plates. In order to incorporate Equation (III.32) into the mass balance Equations (III.1) and (III.2), the $\Delta x$ is selected to be equal to $L_p$, i.e.,

$$\Delta x = L_p.$$  \hspace{1cm} (III.33)

By integrating the mass balance equations and matching the concentration profiles with measured uranium concentration profiles in the A-type contactors of Reference 21, we find for the constant $b$,

$$b = 0.046.$$  \hspace{1cm} (III.34)
where flow rates are given in cc/min and $L_I$ and $L_J$ are in cm. By using Equation (III.32) with the above choice of $b$, the measured concentration profiles are predicted to within 5% by integrating the mass balance Equations (III.1) and (III.2) for a variety of contactor conditions.

For mixer-settler contactors the assumption of mass transfer equilibrium between aqueous and organic phases yielded results in reasonably good agreement with measurements.\textsuperscript{1} In the case of pulsed column contactors, one finds that this is probably again the case for A-type contactors, but it appears that for stripping contactors significant deviations from mass transfer equilibrium may occur. Consequently one needs to account for the mass transfer rate between the phases in terms of the mass transfer coefficient $K$ and the mass transfer area $A$. The total interfacial area between the phases within a mass transfer unit is the area of the droplets of the dispersed phase multiplied by the number of droplets, $N_d$, of diameter $d$,

$$A = N_d \pi d^2.$$  \hfill (III.35)

Within a mass transfer unit whose volume is designated $V_I$, the number of droplets is given by,

$$N_d = \frac{6V_I \theta_d}{\pi d^3 (1 + \theta_d)}.$$  \hfill (III.36)

where $\theta_d$ is the volume fraction of the dispersed phase. Thus the mass transfer area $A$ within the volume $V_I$ (or element $\Delta x$) may be expressed by the formula,

$$\frac{A}{V_I} = \frac{6\theta_d}{d(1 + \theta_d)}.$$  \hfill (III.37)

For the evaluation of $\theta_d$ and $d$, the formulae of Miyauchi and Oya\textsuperscript{22} were used. For the organic-water extraction systems used in nuclear reprocessing these formulae reduce to,
\[
\theta_d = \begin{cases} 
6.32 (F^d)^{2/3} & \kappa > 0.21 \\
0.66 (F^d)^{2/3} & \kappa < 0.21 
\end{cases} \quad (\text{III.38})
\]

\[
d = 0.041 \left( \frac{\omega^5}{l_p^1/3} \right)^{-1/2} \quad (\text{III.39})
\]

\[
\kappa = 0.066 \frac{\omega^5}{(B\ell_p)^{1/3}} \quad (\text{III.40})
\]

\[
\beta = \frac{m^2}{(1 - m)(1 - m^2)} \quad (\text{III.41})
\]

where \( m \) is the fraction of sieve plate area that is free hole area and \( F^d \) is the dispersed phase flow rate. In order to calculate the numerical prefactor of 0.066 in the expression for \( \kappa \), viscosity, density, and surface tension data on dodecane and water from J. Timmermans\textsuperscript{23} were used. The predictions of Equation (III.38) for the dispersed phase volume fraction are in excellent agreement with the experimental data of Reference 10.

At this point no value or expression has been obtained for the mass transfer coefficient \( K \) and so it remains input into the computer program. This does not present an immediate difficulty because its value is only critical to simulating stripping contactors which contain only a small fraction of the total plutonium inventory (about 10%). Eventually a value will be determined for \( K \) by more comparisons of measured concentration profiles with calculated values.

The inventory for nuclear material \( \alpha \) is calculated according to the formula,

\[
H^\alpha_P = \frac{V}{1 + \theta_d} \sum_{x} \left[ C_{\alpha}^C(x) + C_{\alpha}^d(x) \theta_d \right], \quad (\text{III.42})
\]

where the summation is taken over all mass transfer units and the superscripts c and d refer to continuous and dispersed phases, respectively. The \( \theta_d \) is calculated from Equation (III.38).

52
C. **Numerical Methods and Calculations**

Appendix D contains a User's Manual for CUSEP, which provides all details needed to apply it. In this Section some details on the numerical methods used in CUSEP are given which are also relevant to using it. The numerical solution of the differential Equations (III.1) and (III.2) is obtained using fourth order Runge-Kutta integration. Since this is the only set of equations one needs to solve for the concentrations, CUSEP is structurally simpler than its counterpart for mixer-settler contactors, PUBG, which has separate mixer mass balance equations and settler mass balance equations to be solved. Nevertheless the pulsed column contactors present a much more difficult calculation because the pulsed flow rate is so rapid that its short time scale dominates all other considerations in selecting the time step for integration. Thus the time step in CUSEP is about one tenth that used in PUBG, where the time step is determined by unpulsed flow rates. The result is that the computational times for CUSEP is roughly a factor of ten longer than for PUBG. This is not as serious a disadvantage as it at first appears, because modern main frame computers are three to four times faster than those of five years ago. Also many modern main frame machines are equipped with array processors and VAST software (for vector processing) which would reduce the computational time by at least another factor of three.

Instabilities in the integration process usually occurs because too large a time step was selected. This normally results in the calculation of a negative value for one of the concentrations, \( C_\alpha (x) \) or \( C_\beta (x) \). Should this occur in CUSEP, the absolute value for the concentration is compared with a standard chosen by the user. If the value is smaller than the standard, the program sets the concentration to zero and continues the calculation. This process is called clipping. If the absolute value for the concentration is larger than the standard, the time step is reduced by half and the concentration is recalculated. This process is repeated until satisfactory values for the concentrations are obtained. The Runge-Kutta time step is then returned to its original value and the calculation is allowed to proceed.

53
In a calculation where high accuracy is desired the standard should be set sufficiently small to avoid clipping. If computer time is an important consideration a standard of larger magnitude may be selected. In the next Section, the CUSEP calculations are applied to typical contactors of each type and comparisons with measured data are made.

In Figures 10 through 13 are presented plots of concentration profiles calculated with CUSEP. The uranium concentration profiles for A-type contactors of Figure 10 are calculated for two pulsed flow rates in order to illustrate the more dispersive effect the higher pulse flow rate has on the concentration profile. The calculated inventory for the higher pulsed flow rate, 583 g, agrees well with the measured value of 560 g.\textsuperscript{10}

Figure 11 and 12 contain the predicted organic uranium and aqueous plutonium concentration profiles for a partitioning contactor. No measured data were available to the authors on partitioning pulsed column contactors so that this is only a demonstration calculation.

The uranium concentration profile for the stripping contactor presented in Figure 13 was obtained under two conditions, one for mass transfer equilibrium and the other for significant deviations from mass transfer equilibrium (\(K = 0.8 \text{ dm} \) and \(A = 40 \text{ dm}^2\)). The latter concentration profile agrees well with the experimental data\textsuperscript{21} indicating that deviations from mass transfer equilibrium occur in stripping contactors. These deviations apparently did not occur in the A-type contactors.
Figure 10. The aqueous and organic concentration profiles of uranium in an A-type pulsed column. The aqueous feed contains 273.3 g/L U and 2.44 M acid (flow rate 0.165 L/min). The scrub stream acid is 2.97 M (flow rate 0.08 L/min) and the TBP is 15% (flow rate 1.05 L/min). The column diameter is 5.0 cm and the pulse amplitude is 2.0 cm. In (A), the pulse frequency is 40 cycles per min and in (B) 83 cycles per min.
Figure 11. The aqueous concentration profile for plutonium in a partitioning contactor. The organic feed stream contains 2.0 g/L Pu, 10.0 g/L U, and 0.10 M acid (flow rate 1.05 L/min). The scrub is 0.2 M acid (flow rate 0.08 L/min) and the reductant stream contains 40.0 g/L U(IV), 20.0 g/L U(VI), and 1.5 M acid (flow rate 0.165 L/min). The column diameter is 5.0 cm, the pulse amplitude is 2.0 cm, and the pulse frequency is 83 cpm.

Figure 12. The organic uranium concentration profile for the pulsed column contactor. The input data is the same as for Figure 11 above. The aqueous profile is included to show how the pulse disperses material through the column.
Figure 13. The aqueous and organic concentration profiles in a stripping contactor. The organic stream contains 42.2 g/L U and 0.12 M acid (flow rate 1.05 L/min). The aqueous stream contains 0.001 M acid (flow rate 1.30 L/min). The column has a diameter of 7.5 cm, the pulse amplitude is 2 cm, and in both (A) and (B) the pulse frequency is 57 cycles per minute. In (A), material transfer between the phases occurs at the equilibrium limit, whereas in (B) there is a deviation from equilibrium. The mass transfer area, \( A \), is 40 square decimeters and the mass transfer coefficient, \( K \), is 0.75 decimeters per minute.
CHAPTER IV

Conclusions

A. Summary

The utilisability of the model for estimating steady state inventories in mixer-settler contactors has been significantly improved. First the equations for calculating the parameters for the model have been simplified by expressing them in terms of feed stream acid and nuclear material concentrations which are readily available as measured data or nominal flow sheet data. The original expressions contained distribution coefficients which are usually expressed in terms of in situ concentrations within the contactor. The second improvement is the development of reduced forms of the equations which may be used to directly estimate the total contactor inventory within a particular purification cycle or even the entire plant rather than obtain them as a sum of estimates on single contactors. These improvements have been obtained with little or no loss of accuracy which is about 5% for plutonium inventory estimates as judged by deviations from PUBG calculations.

A modified exponential model for estimation of transient inventories under nonsteady state conditions is presented which is based on formulae for characteristic time constants for single contactors and tanks. The time constant for a set of coupled contactors and tanks is obtained as a sum of time constants for the single contactors and tanks. The only input into the model are the steady state inventories estimated from the steady state model. In order to account for the nonexponential contributions to the transient behavior that occur in coupled systems, a modified exponential model is employed. For an application to a representative reprocessing plant, the model inventories agree within 10% with inventories calculated from a computer simulation of a rinseout-restart sequence for the plant.
A computer model (CUSEP) has been developed for simulating the operation of pulsed column contactors. The model has been applied to representative contactors of each type. The model predicts concentration profiles and inventories that are in excellent agreement (to within 10%) with reported experimental data\textsuperscript{10,21} for uranium extraction in A-type contactors. The agreement with measured data on uranium extraction in stripping type contactors is less good, but nevertheless satisfactory when one considers stripping type contactors contain only a small fraction of the plutonium inventory. There is no measured concentration profile data available on partitioning pulsed column contactors, but a demonstration calculation appeared to give reasonable results. The good agreement between model predictions and measured concentration profiles indicates that the model correctly predicts the concentration dispersion in the column that is caused by pulsing. The agreement between the predicted and measured nuclear material inventories demonstrates that the dispersed phase volume holdup is accurately predicted. The need to predict the disperse phase volume is unique to pulsed columns because the phase volume ratio is input into mixer-settler computer models such as PUBG.

B. Future Research

Future research efforts should include: (i) development of a simple inventory estimation model for pulsed column contactors analogous to that developed in this work for mixer-settler contactors, (ii) perform additional investigations of the correction of MUF and CUMUF tests using the model developed for estimating mixer-settler contactor inventory, (iii) identify sources of bias appearing in the MUF and CUMUF tests using computer simulation techniques. The computer simulation methods referred to in (iii) would use programs developed in this work which are described in Appendix C.

The development of inventory estimation models analogous to those just developed for mixer-settler contactors are also needed for pulsed column contactors, if the correction of CUMUF tests for unmeasured inventory is to become a universal procedure for near-
real-time accounting. The pulsed column is perhaps preferred for plants with a high nuclear material throughput. There were obstacles to performing such investigations prior to this work, because there were no pulsed column simulation programs which could be used very effectively to provide the databases for the development of an inventory estimation model. The difficulty with earlier pulsed column computer models is that they underestimated the concentration dispersion caused by convective remixing produced by the pulsing. This problem was solved with the computer model CUSEP, which can provide the necessary databases for development of an inventory estimation model.

Additional studies on the correction of MUF and CUMUF tests for contactor inventory may affect their interpretation. The most unexpected result obtained with the correction of the 82-1 and 82-2 campaign data for the PNC-Tokai plant are the larger than expected range of contactor inventories (1.0 to 4.0 Kg) that contribute to the uncorrected CUMUF. The lower value of this range is much lower than any contactor inventory estimate made previously for purposes of correcting the measured data obtained from these campaigns. The small inventories (on the average 1.8 Kg) occurred at the beginning of the 82-1 campaign and they are quite reasonable when one notes that they explain the positive values (about 2 Kg) of the uncorrected CUMUF at the beginning of this campaign.

Although as indicated above investigations on MUF and CUMUF tests are very desirable to identify sources bias that complicate their interpretation, the number of such investigations one can conduct is limited by the availability of measured data. Consequently future research should consider simulating data on which MUF and CUMUF tests can be conducted. Sources of bias that may arise from purely random measurement errors could be studied very effectively using simulated data. Such a bias would arise because the input and output concentrations and inventories may be measured with different accuracy and the effects which are reflected in their values may occur over different time spans. For example the input plutonium concentration to the first cycle may suddenly change in value over a very short time interval with the introduction of a
new solution into the feed tank. However this variation will be dissipated in the contactors and its effect will appear over a much longer time span in the product stream. Even random errors in the product concentration and random variations in the flow rates may result in a bias in the integrated output when combined with the input whose variation occurred over a very short time span. Should such a bias occur, it will depend on the magnitude of the measurement error, frequency of the measurement, and the nature of the reprocessing system with respect to how it dissipates variations in the input streams. These dependencies would be difficult to study experimentally, but are quite easily varied in a computer simulation of the process and the measurement of its parameters. A computer program which could be used quite effectively for this type of investigation was developed in this work and is described in Appendix C.
REFERENCES


REFERENCES (Continued from Previous Page)


REFERENCES (Continued from Previous Page)


APPENDIX A

Derivation of More Utilizable Formulas for Parameters

A. A-Type Contactors

The fundamental relation for the inventory $H_{\alpha}^0 (\alpha = U \text{ or } Pu)$ which is the basis for the simplified model of A-Type contactors is the following,

$$H_{\alpha}^0 = \frac{V_s c_{\alpha}^0}{(1 + \theta)(1 - n/D_{\alpha}^0)} \left(1 + \sum_{n=1}^{m} \frac{a_n + b_n}{(D_{\alpha}^0)}\right), \quad (A.1)$$

where $a_n$ and $b_{n}$ are constants independent of the flowsheet or contactor. The superscript 0 indicates that Equation (A.1) is formulated in terms distribution coefficients for the organic product stream which exits from Stage 1 (See Figure A1). In order to better understand the concentration profile for the organic phase of an A-type contactor, Figure A1 provides an illustration:

Figure A1. An illustration of the concentration profile for the organic phase of an A-type contactor. The higher concentration of nuclear material in the feed stage produces the smaller "free" TBP concentration, $[\text{TBP}]_f$, and a smaller distribution coefficient, $D_{\alpha}$, in that stage as compared with the corresponding values, $[\text{TBP}]_1^0$ and $D_{1}^0$, respectively, in stage 1.
describe the divergent behavior of the inventory in the A-type contactors, we have reformulated Equation (A.1) in terms of distribution coefficients in the feed stage where the "free" TBP (TBP not complexed by acid or nuclear material) is smaller than in the stage where the organic product stream exits (See Figure A1). Since the distribution coefficients are proportional to the square of the "free" TBP concentration, the distribution coefficients in the feed stage are significantly smaller than those in Stage 1 where the organic product stream exits. With this reformulation, least squares calculations using a PUBG database (See Table E1 of Appendix E) show the inventory is well approximated by retaining only the first term in Equation (A.1), i.e.,

\[
H_\alpha^0 = \frac{v_c a^0}{(1 + \theta)(1 - \gamma/D^0)} \left( 1 + \frac{a + b e}{D^0_D} \right).
\]  

\[\text{(A.2)}\]

The procedure for reformulating the expression for \(H_\alpha^0\) beginning with Equation (A.2) is to write the distribution coefficients as the product of three factors,

\[
D_\alpha = \varepsilon_\alpha \psi R^2,
\]  

\[\text{(A.3)}\]

\[
D_\alpha^0 = \varepsilon_\alpha \psi (R_0)^2.
\]  

\[\text{(A.4)}\]

where \(R\) and \(R_0\) represent the mole fractions of TBP not complexed by uranium or plutonium, in the feed stage and in stage 1, respectively, i.e.,

\[
R_0 = 1 - \frac{2r(C^a_\alpha U + C^a_\alpha Pu)}{8.71 B},
\]  

\[\text{(A.5)}\]

\[
R = 1 - \frac{2r(C^\delta_\alpha U + C^\delta_\alpha Pu)}{8.71 B},
\]  

\[\text{(A.6)}\]

\[
\varepsilon_\alpha = \frac{1}{[1 - \gamma/(\varepsilon_\alpha \psi (R_0)^2)]}.
\]  

\[\text{(A.7)}\]

The \(\varepsilon_\alpha\) are temperature correction factors which are obtained from Ref. 4.
\[ \varepsilon_U = 1.908 \exp(2500 \tau) \]  \quad (A.8)

\[ \varepsilon_{P_U} = 0.742 \exp(-200 \tau) \]  \quad (A.9)

\[ \tau = \frac{1}{T} - \frac{1}{298.16} \]  \quad (A.10)

The factors \( \delta_\alpha \) are obtained from our previous work\(^1\) and they correct the organic exit stream concentrations so that they correspond to the concentrations in the feed stage (See Equation (II.14) of Ref. 1).

The above reformulation effectively replaces the distribution coefficient with the empirical factor \( \psi \) and its success depends upon being able to obtain empirical correlations for this quantity that are much simpler than the literature correlations\(^4\) for the original distribution coefficients. The following relation has been employed for \( \psi \),

\[
\psi = 0.00493 B^2 \frac{1.57}{[H]} (1 + 0.104 \frac{[H]}{[H]^4}) \left( \frac{1 - \psi_1}{1 + \psi_1} \right), \quad (A.11)
\]

\[
\psi_1 = \frac{0.0197 B^2 \frac{1.82}{[H]^{4.5}}}{1 + 0.0251 [H]^{4.5}}, \quad (A.12)
\]

The form of \( \psi \) is suggested by the expansion of the “free” TBP molarity in Ref. 1 (See Equation (III.40) of Ref. 1), the relation of the distribution coefficient to the “free” TBP molarity (See Equation (II.24) and (II.25) of Ref. 1), and Richardson’s correlations for the distribution coefficient.\(^4\) The numerical constants in Equations (A.11) and (A.12) were obtained by a least squares calculation in which Equation (A.3) was fitted to distribution coefficients calculated from literature correlations.

Once a well defined expression for \( \psi \) was obtained the distribution coefficient in the inventory expression (Eq. (A.2)) was replaced with the corresponding expressions on the right hand side of Equations (A.3) and (A.4),

\[
\frac{v^2}{\alpha} = \frac{\frac{V C^2 \frac{r}{s}}{\alpha}}{(1 + \theta) \left[ 1 - \frac{\psi R^2}{\alpha} \right]} \left( 1 + \frac{a + b \theta}{\psi R^2} \right). \quad (A.13)
\]
The above equation was then fitted to the PUBG database of Table E1 with the results for plutonium being $a = -0.0730$, $b = 0.8200$ with a standard deviation of 6%. For uranium, the results are $a = -0.0971$, $b = 0.8768$ with a standard deviation of 4%. In the above least squares calculation, the following equation for acid was used,

\[
[H] = 0.91 [H]_s + 0.09[H]_f .
\] (A.14)

With Equation (A.14) we have formulated the problem in terms of the scrub stream acid and feed stream acid concentrations, which are available as measured data or nominal flow sheet data.

By identifying Equation (A.13) with the parametric form of the inventory equation,

\[
\frac{\lambda}{\alpha} = C\left( \frac{r e^{\delta e}}{\alpha} \right) \left( \frac{\lambda}{\alpha} \right) \left( \frac{1 - 2r'(C_{U}^{\delta U} + C_{Pu}^{\delta Pu})/(8.71 B)^2}{1 - 2r'(C_{U}^{\delta U} + C_{Pu}^{\delta Pu})/(8.71 B)^2} \right) .
\] (A.15)

the final expressions for the remaining parameters of the A-type contactor inventory equations are obtained,

\[
\frac{\lambda}{\alpha} = \frac{(a + b\theta)r}{\alpha} .
\] (A.16)

\[
\frac{\lambda}{\alpha} = \frac{(a + b\theta)r}{\alpha} .
\] (A.17)

B. Partitioning Contactors

The following equations are the starting point for developing inventory relations for partitioning type contactors,

\[
H^{0}_{Pu} = \frac{r' r C_{Pu}^{\delta} V_{Ex}^{\theta Ex}}{r (1 + \theta Ex)} \left[ 1 + \left( \frac{a + b\theta}{\theta Ex} \right) D_{Pu}^{0} \right] ,
\] (A.18)

\[
H^{0}_{U} = \frac{r' <C_{U}^{\delta}> V_{s}}{1 + \theta S} \left( \frac{a + b\theta}{\theta S} \right) ,
\] (A.19)

where $\alpha, \beta, a, b$ are parameters to be determined, $D_{Pu}^{0}$ refers to the distribution
coefficient of reduced plutonium (Pu(III)). The average uranium concentration \(< C_U >\), which includes averaging over the uranium in the organic feed stream and in the reductant streams, is given by Equation (1.35). As in the case of A-type contactors, the distribution coefficients in the above equations are replaced according to Equation (A.3), yielding the results,

\[
H^0_{Pu} = \frac{r' C_{Pu}^a V_{Ex} \theta_{Ex}}{r (1 + \theta_{Ex})} \left[ 1 + \left( \alpha + \frac{\beta}{\theta_{Ex}} \right) \left( 0.01138 \varepsilon_{Pu} \psi R^2 \right) \right], \quad (A.20)
\]

\[
H^0_U = \frac{r' C_{U}^a V_{Ex} \theta_{Ex}}{(1 + \theta_{Ex})} \left[ 1 + \frac{a + b \theta_{Ex}}{\varepsilon_{U} \psi R^2} \right], \quad (A.21)
\]

where the relation between Pu(IV) and Pu(III) distribution coefficients has been used,\(^6\)

\[
D^0_{Pu} = 0.01138 D_{Pu} \quad (A.22)
\]

The numerical parameters in Equations (A.20) and (A.21) were calculated by a least squares calculations using the PUBG database in Table E2 of Appendix E and the following relations for \([H]\) and \(R\),

\[
[H] = \begin{cases} 
0.08 \frac{[H]_f}{r} + 0.1 [H]_r + 0.9 [H]_s & \text{for plutonium} \\
0.044 \frac{[H]_f}{r} + 0.1 [H]_r + 0.9 [H]_s & \text{for uranium} 
\end{cases} \quad (A.23)
\]

\[
R = \begin{cases} 
1 & \text{for plutonium} \\
1 - 2r' C_{U}^a \delta_{U} / (8.71 B) & \text{for uranium} 
\end{cases} \quad (A.24)
\]

The results for plutonium are \(\alpha = 0.512\) and \(\beta = 0.489\) with a standard deviation of 5%. For uranium \(a = 0\) and the following expressions were required for \(b\) and \(R^0\),

\[
b = 1.59 - \frac{1.367}{\varepsilon_{U} \psi R^2} + \frac{0.3109}{(\varepsilon_{U} \psi R^2)^2} \quad (A.25)
\]

\[
R^0 = 1 - 2r' C_{U}^a / (8.71 B) \quad (A.26)
\]
in order to obtain a standard deviation of 8%. The identification of the inventory Equations (A.20) and (A.21) with the parametric form of the inventory equations,

\[ H_{Pu}^0 = C_{Pu}^0 A_{Pu}^0, \quad (A.27) \]

\[ H_{U}^0 = <C_U^0> \left( \Gamma_U^0 + \frac{\lambda_U}{1 - 2r'C_U^0 \delta_U^0 / (8.71 B)^2} \right), \quad (A.28) \]

yields the following results for the parameters,

\[ A_{Pu}^0 = \frac{r' V_{Ex}^0}{r (1 + \theta_{Ex}^0)} \left[ 1 + 0.001 \left( 5.83 + \frac{5.56}{\theta_{Ex}^0} \right) e_{Pu}^0 \right], \quad (A.29) \]

\[ \Gamma_U^0 = \frac{V_{s} r' \delta_U^0}{1 + \theta_{s}^0}, \quad (A.30) \]

\[ \lambda_U^0 = \frac{\theta \Gamma_U^0}{\varepsilon_{U}^0} \left( 1.59 - \frac{1.37}{\varepsilon_{U}^0 \gamma R_{02}^2} + \frac{0.31}{(\varepsilon_{U}^0 \gamma R_{02}^2)^2} \right), \quad (A.31) \]

The results of the least squares calculations have been incorporated into the above equations.

C. Stripping Contactors

For stripping contactors the approximate simplified equation is used as a starting point (See Eq. (II.72) of Ref. 1),

\[ H_{Pu}^0 = \frac{r' C_{Pu}^0 V(D + \theta)}{r (1 + \theta) (1 - D / r)} \quad (A.32) \]

Since there was a significant coupling between the acid and nuclear material contributions to \( H_U^0 \), the distribution coefficient was replaced with a function of total effective nitrate.
ion concentration which is related to both the acid and nuclear material concentrations by the relation,

\[ N_a = [H_s] + 2r \cdot (C^{a}_U / 238 + C^{a}_Pu / 239) / r . \tag{A.33} \]

The following functional dependence was assumed as a replacement for \( D_\alpha \):

\[ \frac{D_\alpha}{\alpha} = C N^\alpha \exp(E_\alpha / \alpha) . \tag{A.34} \]

Replacement of \( D_\alpha \) in Equation (A.32) with expression on the right hand side of Eq. (A.34) yields,

\[ \frac{H^0_{Pu}}{r} = \frac{r \cdot C_{Pu} \cdot \frac{\exp(\theta + C N^\alpha \exp(E_\alpha / \alpha))}{\exp(\theta + C N^\alpha \exp(E_\alpha / \alpha))} / \alpha}{r (1 + \theta)(1 - C N^\alpha \exp(E_\alpha / \alpha) / \alpha)} . \tag{A.35} \]

The numerical constants \( C, \varepsilon, \) and \( E_\alpha \) were calculated by a least squares calculation using a PUBG database given in Table E3. The results for plutonium are: \( C = 0.36, \varepsilon = 0.22, \) and \( E_{Pu} = -1340 \) and for uranium the results are: \( C = 0.98, \varepsilon = 0.24, \) and \( E_{U} = 1260. \) The root mean square deviations for the least squares are 4% and 8% for plutonium and uranium, respectively.

Substitution of the least squares results into Equation (A.35) and identifying the coefficient to \( C_\alpha^a \) with \( \Lambda^S_\alpha \), one obtains the results for the parameters,

\[ \Lambda^S_{Pu} = \frac{V_{r^*}}{r(1 + \theta)} \left( \frac{\theta + 0.36 N_a^{0.22} \exp(-1340 \cdot \tau)}{1 - 0.36 N_a^{0.22} \exp(-1340 \cdot \tau) / \tau} \right) . \tag{A.37} \]

\[ \Lambda^S_{Pu} = \frac{V_{r^*}}{r(1 + \theta)} \left( \frac{\theta + 0.36 N_a^{0.22} \exp(-1340 \cdot \tau)}{1 - 0.36 N_a^{0.22} \exp(-1340 \cdot \tau) / \tau} \right) . \tag{A.37} \]
APPENDIX B

Inventory Equations for a Collection of Coupled Contactors

A. Reduced Forms of the Inventory Equations

Inventory equations for a set of coupled contactors are said to be reduced when the single contactor equations are summed to one equation for the entire system of contactors. For A-type contactors this produces sums of the form,

\[ dX = \sum_{M} \frac{C_{aM} \lambda_{aM}}{1 - 2\gamma' M (C_{UM} + C'_{PuM})/\delta_{UM}} [8.71 B]^{2} \quad (B.1) \]

where in the denominator of the second term it is assumed that \( \delta_{PM}/\delta_{UM} \) is unity. The first summation may be summed to a single effective parameter. However one would like to include in this parameter the contributions of all other contactors that can be treated in terms of a single effective parameter, which produces the result,

\[ C_{a} \Gamma_{a} (\text{tot}) = \sum_{N} H_{aN}^{o} + \sum_{M} C_{aM} \Gamma_{aM} \quad (B.2) \]

where \( C_{a}^{o} \) is the concentration of the stream that feeds nuclear materials to the first contactor in the flow sequence and \( C_{aM}^{o} \) are concentrations of intermediate streams that feed the single contactors labeled M. The summation over N includes all contactors that are not included in the summation over M. Equation (B.2) defines the parameter \( \Gamma_{a} (\text{tot}) \) and demonstrates the origin of Equation (1.69).

In order to reduce the second term, the following approximate relations are assumed,

\[ \frac{a}{(1 - b)^{2}} = \sum_{M} \frac{a_{M}}{(1 - b_{M})^{2}} \quad (B.3) \]

\[ a = C_{a} \lambda_{a} (\text{tot}) \quad (B.4) \]

\[ b = \gamma (C_{U} + C_{Pu}) / (8.71B) \quad (B.5) \]
\[ a_M = \sum_M a_M \]  \hspace{1cm} (B.6)

\[ b_M = 2r_M (C_{UM}^a + C_{PuM}^a) \delta_{UM}/(8.71B) \]  \hspace{1cm} (B.7)

It is to be noted from Equation (1.2) and above equations that,

\[ \frac{a_M}{(1 - b_M)^2} = H^0_{\alpha M} - C_{\alpha M}^a \Gamma_{\alpha M'} \]  \hspace{1cm} (B.8)

In order to obtain the best reduction, \( a \) is selected be,

\[ a = \sum_M a_M \]  \hspace{1cm} (B.9)

in which case one can immediately solve for \( b \),

\[ b = 1 - \sqrt{\frac{\sum_M a_M}{\sum_{M'} (a_M')^2}} \]  \hspace{1cm} (B.10)

By making the substitutions of Equations (B.5) to (B.7) into Equation (B.10), one obtains,

\[ \gamma (C_{\alpha M}^a + C_{\alpha M}^a) / (8.71 B) = 1 - \sqrt{\frac{\sum_M C_{\alpha M}^a \lambda_{\alpha M}}{\sum_{M'} (H^0_{\alpha M'} - C_{\alpha M'}^a \Gamma_{\alpha M'})}} \]  \hspace{1cm} (B.11)

By solving the above for \( \gamma \), the desired result (Eq. (1.71)) is obtained. The desired result for \( \lambda_{\alpha}^{(tot)} \), Equation (1.70), is readily obtained from a combination Equations (B.4), (B.6), and (B.9).

B. Estimation of Contactor Inventories from Throughput

In a first approximation, the total contactor inventory in a nuclear fuel reprocessing plant should be proportional to the throughput with a proportionality that is best
developed by relating the scale or size of the plant to the hydrodynamic residence time for the contactors.

We begin our derivation by recalling the relation of the steady state contactor inventory to the effective time constant (\( \tau \)) used to estimate the transient inventory, namely,

\[
\tau = \frac{aH_0^0}{F^aC^a}, \quad (B.12)
\]

where the product \((F^aC^a)\) represents the throughput rate. The above relation can be rearranged to the following form,

\[
H_0^0 = F^aC^a \tau / a, \quad (B.13)
\]

which suggests that it is useful for estimating steady state inventories \(H_0^0\). We have found empirically using PUBG calculations that the ratio of \( \tau \) to the hydrodynamic residence time, \( \tau_H \), can be represented by the relations,

**A-Type Contactors**

<table>
<thead>
<tr>
<th>Type</th>
<th>( \tau / \tau_H )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pu</td>
<td>1.287 - 0.196 [H]</td>
</tr>
<tr>
<td>U</td>
<td>0.720 - 0.067 [H]</td>
</tr>
</tbody>
</table>

**Stripping Contactors**

<table>
<thead>
<tr>
<th>Type</th>
<th>( \tau / \tau_H )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pu</td>
<td>2.061 exp[-(1552)( \tau )]</td>
</tr>
<tr>
<td>U</td>
<td>10.034 exp[(2500)( \tau )]</td>
</tr>
</tbody>
</table>

**Partitioning Contactors**

<table>
<thead>
<tr>
<th>Type</th>
<th>( \tau / \tau_H )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pu</td>
<td>1</td>
</tr>
<tr>
<td>U</td>
<td>0.720 - 0.067 [H]</td>
</tr>
</tbody>
</table>

where

\[
\tau = \frac{1}{T - \frac{1}{298.16}}, \quad \text{(B.20)}
\]

\[
\tau_H = \frac{\text{Volume}}{\text{Total Flow Rate}}. \quad \text{(B.21)}
\]
T is the absolute temperature and [H] is the acid molarity for the aqueous scrub stream. The $\tau_H$ for the A-type contactors is the hydrodynamic residence time for the scrub bank and for stripping it is the residence time for a single stage. For Pu in partitioning contactors, $\tau_H$ refers to the extraction bank and for uranium in partitioning contactors it refers to the scrub bank. The root mean square deviations from Equations (B.14) and (B.15) are 10% and from Equations (B.16) and (B.17) are 25%. The latter larger standard deviation will not affect the error estimates in the total contactor inventory significantly because the inventory in stripping contactors is only a small fraction of the total contactor inventory.

The hydrodynamic residence time per stage for the contactors in the Tokai reprocessing plant is about 10 minutes. Therefore for stripping contactors we assume $\tau_H = 10$ minutes. For A-type contactors the residence time per stage is 10 minutes in the extraction bank which is the bank where it would have its smaller value because of the higher total flow rates in that bank. We have developed a formula which expresses the desired scrub bank residence time in terms of the 10 minute per stage residence time in the extraction bank and the feed stream to organic stream flow rate ratio, $r'$, which is,

$$
\tau_H = \frac{(3 + 3r' + r'^2) 10N_s}{(1 + r')^2}
$$

where $N_s$ is the number of stages in the scrub bank. For the extraction bank in partitioning contactors, $\tau_H$ is 65 minutes based on data from the Tokai plant. The product of $\tau_H$ and $\tau/\tau_H$ yields the desired formula for $\tau$. These formulae are summarized below.

**A-Type Contactors**

Pu:

$$
Pu: \tau = \frac{10N_s (1.287 - 0.196[H])(3 + 3r' + r'^2)}{(1 + r')^2}
$$

(B.23)
\[
\tau = \frac{10N_s (0.720 - 0.067[H]) (3 + 3' + r'^2)}{(1 + r')^2}, \quad (B.24)
\]

**Stripping Contactors**

Pu: \( \tau = 20.61 \exp[-(1562)\tau] \), \quad (B.25)

U: \( \tau = 100.34 \exp[(2500)\tau] \), \quad (B.26)

**Partitioning Contactors**

Pu: \( \tau = 60 \), \quad (B.27)

U: \( \tau = \frac{10N_s (0.720 - 0.067[H]) (3 + 3' + r'^2)}{(1 + r')^2} \), \quad (B.28)

where \( \tau \) is defined by Equation (B.20). The values of \( \tau \) given by Equations (B.23) to (B.28) may be used to estimate contactor inventories from Equation (B.13).

In Table B1 are given the acid concentrations \([H]\), and the \( r' \) and \( a \) values used to calculate \( \tau/a \) from Equations (B.23) to (B.28) for a typical reprocessing plant. The acid concentration for the initial cycle is assumed to be 3M and \( r' \) is assumed to be 1/2, which are very typical values for a reprocessing plant with a feed stream to the initial purification cycle containing 180 g/L of nuclear material. The values of \( r' \) in the remaining cycles are estimated by assuming that aqueous to organic flow rate ratios in stripping contactors are 1.2 and that the Pu concentration in the Pu product stream is about 10 g/L. The acid concentrations to the A-type contactors in the final purification cycles are assumed to be 1M which is also typical of most reprocessing facilities. The number of stages in the scrub bank, \( N_s \), is assumed to be 8 for A-type contactors in the first two purification cycles and in the plutonium purification cycle. For the uranium purification cycle, it is assumed to be 6. The sum of all the values of \( \tau/a \) in the last two columns of Table B1 multiplied by the throughput yields the following expressions for
Table B1

Data used to calculate $\tau/a$ and resultant $\tau/a$ values
for a typical reprocessing plant

<table>
<thead>
<tr>
<th>Purification Cycle</th>
<th>Contactor Type</th>
<th>$\tau$</th>
<th>$a$</th>
<th>$\tau$/$\tau_H$</th>
<th>$\tau_H$(Min)</th>
<th>$\tau/a$ (Min)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$U$</td>
<td>$Pu$</td>
<td>$U$</td>
</tr>
<tr>
<td>1</td>
<td>A-type</td>
<td>3.0</td>
<td>2.0</td>
<td>0.60</td>
<td>0.52</td>
<td>0.70</td>
</tr>
<tr>
<td></td>
<td>Stripping</td>
<td>-</td>
<td>-</td>
<td>1.55</td>
<td>10.03</td>
<td>2.06</td>
</tr>
<tr>
<td>2</td>
<td>A-type</td>
<td>3.0</td>
<td>0.8</td>
<td>0.60</td>
<td>0.52</td>
<td>0.70</td>
</tr>
<tr>
<td></td>
<td>Partitioning</td>
<td>0.2</td>
<td>1.3</td>
<td>0.88</td>
<td>0.71</td>
<td>1.00</td>
</tr>
<tr>
<td></td>
<td>Stripping</td>
<td>-</td>
<td>-</td>
<td>1.55</td>
<td>10.03</td>
<td>-</td>
</tr>
<tr>
<td>U</td>
<td>A-type</td>
<td>1.0</td>
<td>0.6</td>
<td>0.60</td>
<td>0.65</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Stripping</td>
<td>-</td>
<td>-</td>
<td>1.55</td>
<td>10.03</td>
<td>-</td>
</tr>
<tr>
<td>Pu</td>
<td>A-type</td>
<td>1.0</td>
<td>0.12</td>
<td>0.60</td>
<td>-</td>
<td>1.09</td>
</tr>
<tr>
<td></td>
<td>Partitioning</td>
<td>0.2</td>
<td>1.0</td>
<td>0.88</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

s - Superscript refers to scrub bank

e - Superscript refers to extraction bank

* - The $a$ values are preliminary estimates obtained prior to completion of the work yielding the best $a$ values given in Chapter II.B of this report. Incorporation of for best $a$ values would not produce significant changes in the results for $\tau/a$. 
uranium and plutonium inventory for a plant with mixer-settler contactors,

\[ H_{Pu}^0 = 9.61 X'_t \Delta, \quad (B.29) \]
\[ H_{U}^0 = 670 X'_t, \quad (B.30) \]

where \( X'_t \) is the throughput in mass per minute (mass units are arbitrary at this point, being identical for \( H_{U}^0 \) and \( X'_t \)) and \( \Delta \) is the percentage of throughput that is plutonium.

Conversion of throughput units to metric tons per day yields the following relations,

\[ H_{Pu}^0 = 6.0 X_t \Delta, \quad (B.31) \]
\[ H_{U}^0 = 0.47 X_t, \quad (B.32) \]

where \( H_{Pu}^0 \) is in kilograms, \( X_t \) is the throughput in metric tons per day, and \( H_{U}^0 \) is in metric tons.
APPENDIX C

Simulation of a Reprocessing Facility

A. Description of the Method and Computer Program

The simulation of a reprocessing facility must take into account the coupling between the various units (tanks and contactors) of the facility. The input stream into the initial purification cycle determines the throughput for the facility and the product streams of contactors within the facility will provide the feed for the next contactor in the sequence. Other streams that feed the contactors at intermediate positions in the sequence affect the process and total inventory but contain no nuclear materials and therefore do not affect the throughput and have little effect on the coupling between the various units of the facility.

Since the computer must simulate both contactors and tanks there are two basic processes that it must perform. These are (i) simulate the entry of a product stream from a contactor into a tank and the dilutions of the tank concentrations with an acid adjustment stream or an organic stream, and (ii) simulate the contactor operation for a feed with a time dependent concentration determined by the time dependence of the product stream for the preceding contactor in the flow sequence. The coupling between the contactors implied by (ii) means that the overall mass balance equations between all units are coupled and integration of these equations will provide all the tank concentrations, concentration profiles, and inventories. The integration of the equations for the ith tank over a time interval \((t_2 - t_1)\) is based on the following integration formula,

\[
C_{\alpha i}(t_2) = C_{\alpha i}(t_1) \exp \left[ -(t_2 - t_1)/\tau_1 \right] + \exp \left[ -t_2/\tau_i \right] \int_{t_1}^{t_2} \frac{\Phi_{\alpha}}{V_i} \exp \left[ t/\tau_i \right] dt, \quad (C.1)
\]

\[
\tau_1 = \frac{V_i}{F_i}, \quad (C.2)
\]
\[ \Phi = \sum_j F_j C_{a_j}(t), \]  

(C.3)

where \( V_j \) is the tank volume, \( F_j \) is the total flow rate through the tank, \( C_{a_j}(t) \) are tank concentrations at time \( t \), and the summation over \( j \) represents a summation over all feed streams introducing nuclear material \( \alpha \) into the tank. The integration of the contactor equations is accomplished with a subroutine that is a modified form of PUBG. The modification makes the PUBG subroutine capable of accepting time dependent feed stream concentrations. In normal applications to single contactors these are assumed to be constant.

The input into the program is the flow sequence of the configuration of tanks and contactors and flow sheet data on all streams feeding the reprocessing system (would not include streams feeding a contactor that are internal to the reprocessing system, such as a feed stream to a contactor which is a product stream from a previous contactor). The program can accept as input any arbitrary configuration of tanks and contactors. From these input data, all tank concentrations and concentration profiles of each contactor (i.e. concentration of every stage) are calculated as a function of time. Normally, a different time is required to reach steady state for each unit. Consequently, the appropriate time step size selected for integrating the mass balance equations is also different. The user may select the appropriate step size for each unit independently. The program automatically adjusts the smaller steps to make the larger ones integral multiples of them so that the integration may be synchronized with respect to time.

B. Application to a Reprocessing Facility

The program was applied to the restart of the reprocessing plant of Figure 1. The flow sheet data required for input was taken from Table 1. The initial condition for the calculation was that all streams were started with no nuclear materials present and then the nuclear materials were suddenly introduced into the feed of the first cycle at concentrations 180 g/L U and 1.23 g/L Pu. This feed concentration and flow rate were
held constant throughout the simulation.

Since the program calculates all concentration profiles and inventories as a function of time, it generates a huge amount of data and it is a logistics problem to handle and retrieve the data one desires. In this application, we retrieved the inventories of each unit as a function of time. In order to illustrate how the output is displayed, a portion of it is included in Table C1. The units are identified by an arabic numeral. The function of each unit may be identified from Figure 1, in which they are also labeled by the same arabic numeral. The final steady state Pu inventory is 2656 g which is in good agreement with the previously calculated result of 2711 g. The results of Table C1 include both tanks and contactors, but for the purposes of this calculation the tank sizes were made small (10 L) so that their contributions to the total inventory are negligible. In Figure C1 a three dimensional plot of the transient behavior of the inventories of the six contactors containing plutonium is displayed.
Table C1. Output from the computer simulation program. The inventories of each unit of the reprocessing plant sketched in Figure 1 and total inventories at 10 minute intervals for time period 0 to 600 minutes and near steady state (over 2400 min) are reported.

<table>
<thead>
<tr>
<th>UNIT</th>
<th>10.0MIN</th>
<th>20.0MIN</th>
<th>30.0MIN</th>
<th>40.0MIN</th>
<th>50.0MIN</th>
<th>60.0MIN</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO.</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
</tr>
<tr>
<td>1</td>
<td>4.03E+01</td>
<td>7.65E+01</td>
<td>1.12E+02</td>
<td>1.48E+02</td>
<td>1.82E+02</td>
<td>2.15E+02</td>
</tr>
<tr>
<td>2</td>
<td>1.12E+00</td>
<td>5.71E+00</td>
<td>2.13E+01</td>
<td>7.99E+00</td>
<td>2.69E+00</td>
<td>1.24E+00</td>
</tr>
<tr>
<td>3</td>
<td>0.00E+00</td>
<td>2.00E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>4</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>5</td>
<td>4.34E-00</td>
<td>5.94E-00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>6</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>7</td>
<td>5.94E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>8</td>
<td>2.00E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>9</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>10</td>
<td>4.34E-00</td>
<td>5.94E-00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>11</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>12</td>
<td>5.94E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>13</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>14</td>
<td>4.34E-00</td>
<td>5.94E-00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>15</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
<td>1.12E+00</td>
</tr>
<tr>
<td>16</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>17</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>18</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>19</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>TOTAL</td>
<td>4.03E+01</td>
<td>7.65E+01</td>
<td>1.12E+02</td>
<td>1.48E+02</td>
<td>1.82E+02</td>
<td>2.15E+02</td>
</tr>
</tbody>
</table>
Table C1 (Continued)

<table>
<thead>
<tr>
<th>UNIT</th>
<th>200.0MIN.</th>
<th>210.0MIN.</th>
<th>220.0MIN.</th>
<th>230.0MIN.</th>
<th>240.0MIN.</th>
</tr>
</thead>
<tbody>
<tr>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
</tr>
<tr>
<td>1</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>2</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>3</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>4</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>5</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>6</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>7</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>8</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>9</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>10</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>11</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>12</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>13</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>14</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>15</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>16</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>17</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>18</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
<tr>
<td>19</td>
<td>4.15E+02</td>
<td>4.24E+02</td>
<td>4.32E+02</td>
<td>4.41E+02</td>
<td>4.49E+02</td>
</tr>
</tbody>
</table>

TOTAL 6.76E+02 7.13E+02 7.46E+02 7.79E+02 8.13E+02

COMPLETE SYSTEM INVENTORY AS A FUNCTION OF TIME

<table>
<thead>
<tr>
<th>UNIT</th>
<th>250.0MIN.</th>
<th>260.0MIN.</th>
<th>270.0MIN.</th>
<th>280.0MIN.</th>
<th>290.0MIN.</th>
<th>300.0MIN.</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO.</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
</tr>
<tr>
<td>1</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>2</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>3</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>4</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>5</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>6</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>7</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>8</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>9</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>10</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>11</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>12</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>13</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>14</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>15</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>16</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>17</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>18</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
<tr>
<td>19</td>
<td>4.57E+02</td>
<td>4.64E+02</td>
<td>4.71E+02</td>
<td>4.78E+02</td>
<td>4.85E+02</td>
<td>4.92E+02</td>
</tr>
</tbody>
</table>

TOTAL 8.61E+02 9.34E+02 9.46E+02 9.62E+02 1.01E+03 1.04E+03

84
Table C1 (Continued)

<table>
<thead>
<tr>
<th>UNIT</th>
<th>310.0MXN</th>
<th>320.0MXN</th>
<th>330.0MXN</th>
<th>340.0MXN</th>
<th>350.0MXN</th>
<th>360.0MXN</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO.</td>
<td>1.085E+03</td>
<td>1.171E+03</td>
<td>1.151E+03</td>
<td>1.185E+03</td>
<td>1.219E+03</td>
<td>1.255E+03</td>
</tr>
</tbody>
</table>

TOTAL SYSTEM INVENTORY AS A FUNCTION OF TIME

UNIT 370.0MXN. 380.0MXN. 390.0MXN. 400.0MXN. 410.0MXN. 420.0MXN.
NO. PU PU PU PU PU PU
1 5.040E-02 5.040E-02 5.085E-02 5.100E-02 5.120E-02 5.137E+02
2 5.176E-02 5.090E-02 5.528E-00 5.560E-00 5.444E-00 5.498E-00
3 5.016E-01 5.044E-01 5.076E-01 5.090E-01 5.092E-01 5.082E-01
4 1.398E-16 1.398E-16 2.346E-16 3.159E-16 4.052E-16 5.147E-16
5 3.419E-00 3.348E-00 3.465E+00 3.483E+00 3.502E+00 3.519E+00
6 3.026E-02 3.072E-02 3.112E+00 3.152E+00 3.194E+00 3.235E+00
7 3.847E-02 3.936E-02 3.963E+00 3.992E+00 4.021E+00 4.050E+00
8 2.997E-02 2.984E-02 3.172E+00 3.266E+00 3.362E+00 3.468E+00
9 2.821E-02 2.812E-02 2.755E+00 2.787E+00 2.829E+00 2.882E+00
10 7.966E-08 6.846E-08 5.928E-08 5.138E-08 4.468E-08 3.900E-08
11 7.874E-09 6.863E-09 5.239E-09 3.889E-09 2.462E-09 1.797E-09
12 1.447E-08 1.305E-08 1.170E-08 1.046E-08 9.345E-09 8.327E-09
13 1.127E-09 1.067E-09 9.501E-09 8.468E-09 7.517E-09 6.574E-09
14 1.014E-07 1.088E-07 1.166E-07 1.032E-07 9.468E-08 8.507E-08
15 1.313E-21 1.621E-21 1.946E-21 2.346E-21 2.782E-21 3.247E-21
17 1.063E-02 1.221E+02 1.601E+02 1.791E+02 1.872E+02 2.002E+02
18 7.079E-02 9.749E-02 1.070E+00 1.156E+00 1.234E+00 1.307E+00
19 6.758E-02 9.392E-02 1.176E+00 1.305E+00 1.427E+00 1.549E+00
20 1.287E-03 1.322E+03 1.356E+03 1.391E+03 1.425E+03 1.460E+03

TOTAL COMPLETE SYSTEM INVENTORY AS A FUNCTION OF TIME

UNIT 430.0MXN. 440.0MXN. 450.0MXN. 460.0MXN. 470.0MXN. 480.0MXN.
NO. PU PU PU PU PU PU
1 5.165E-02 5.184E-02 5.178E-02 5.190E-02 5.200E-02 5.219E-02
2 5.310E-02 5.362E-00 5.560E-00 5.602E-00 5.636E-00 5.663E-00
3 5.974E-01 5.998E-01 6.014E-01 6.032E-01 6.049E-01 6.065E-01
5 3.536E-00 3.552E+00 3.564E+00 3.566E+00 3.569E+00 3.571E+00
7 3.447E-02 3.465E-02 3.480E-02 3.495E-02 3.510E-02 3.525E-02
8 3.441E-02 3.449E-02 3.455E-02 3.459E-02 3.464E-02 3.469E-02
9 3.617E-08 3.004E-08 2.650E-08 2.345E-08 2.082E-08 1.856E-08
10 7.492E-09 8.164E-09 9.620E-09 1.127E-08 1.307E-08 1.513E-08
11 7.410E-07 6.458E+00 5.840E+00 5.214E+00 4.564E+00 4.016E+00
12 7.412E-09 5.128E-09 3.868E-09 2.628E-09 1.877E-09 1.451E-09
13 5.914E-09 6.014E-09 6.082E-09 6.147E-09 6.206E-09 6.260E-09

85
<table>
<thead>
<tr>
<th>NO.</th>
<th>UNIT</th>
<th>TOTAL</th>
<th>COMPLETE SYSTEM INVENTORY AS A FUNCTION OF TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>3.76E+21</td>
<td>4.29E+21</td>
<td>4.67E+21</td>
</tr>
<tr>
<td>16</td>
<td>5.76E+21</td>
<td>6.23E+21</td>
<td>4.67E+21</td>
</tr>
<tr>
<td>17</td>
<td>2.23E+22</td>
<td>2.64E+22</td>
<td>2.67E+22</td>
</tr>
<tr>
<td>18</td>
<td>2.70E+22</td>
<td>3.22E+22</td>
<td>3.05E+22</td>
</tr>
<tr>
<td>19</td>
<td>3.72E+22</td>
<td>4.69E+22</td>
<td>5.84E+22</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>TOTAL</td>
<td>1.49E+03</td>
<td>1.83E+03</td>
<td>1.56E+03</td>
</tr>
</tbody>
</table>

Table C1 (Continued)
### Table C1 (Continued)

#### Complete System Inventory as a Function of Time

<table>
<thead>
<tr>
<th>UNIT</th>
<th>2410.0MIN.</th>
<th>2420.0MIN.</th>
<th>2430.0MIN.</th>
<th>2440.0MIN.</th>
<th>2450.0MIN.</th>
<th>2460.0MIN.</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO.</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
</tr>
<tr>
<td>1</td>
<td>5.230E+02</td>
<td>5.230E+02</td>
<td>5.230E+02</td>
<td>5.230E+02</td>
<td>5.230E+02</td>
<td>5.230E+02</td>
</tr>
<tr>
<td>2</td>
<td>5.805E+00</td>
<td>5.805E+00</td>
<td>5.805E+00</td>
<td>5.805E+00</td>
<td>5.805E+00</td>
<td>5.805E+00</td>
</tr>
<tr>
<td>3</td>
<td>6.146E+01</td>
<td>6.146E+01</td>
<td>6.146E+01</td>
<td>6.146E+01</td>
<td>6.146E+01</td>
<td>6.146E+01</td>
</tr>
<tr>
<td>5</td>
<td>3.750E+00</td>
<td>3.750E+00</td>
<td>3.750E+00</td>
<td>3.750E+00</td>
<td>3.750E+00</td>
<td>3.750E+00</td>
</tr>
<tr>
<td>6</td>
<td>4.005E+02</td>
<td>4.005E+02</td>
<td>4.005E+02</td>
<td>4.005E+02</td>
<td>4.005E+02</td>
<td>4.005E+02</td>
</tr>
<tr>
<td>7</td>
<td>4.334E+00</td>
<td>4.334E+00</td>
<td>4.334E+00</td>
<td>4.334E+00</td>
<td>4.334E+00</td>
<td>4.334E+00</td>
</tr>
<tr>
<td>8</td>
<td>3.424E+02</td>
<td>3.424E+02</td>
<td>3.424E+02</td>
<td>3.424E+02</td>
<td>3.424E+02</td>
<td>3.424E+02</td>
</tr>
<tr>
<td>10</td>
<td>1.873E-10</td>
<td>1.873E-10</td>
<td>1.873E-10</td>
<td>1.873E-10</td>
<td>1.873E-10</td>
<td>1.873E-10</td>
</tr>
<tr>
<td>12</td>
<td>1.906E-09</td>
<td>1.906E-09</td>
<td>1.906E-09</td>
<td>1.906E-09</td>
<td>1.906E-09</td>
<td>1.906E-09</td>
</tr>
<tr>
<td>13</td>
<td>1.119E-11</td>
<td>1.119E-11</td>
<td>1.119E-11</td>
<td>1.119E-11</td>
<td>1.119E-11</td>
<td>1.119E-11</td>
</tr>
<tr>
<td>14</td>
<td>1.231E-10</td>
<td>1.231E-10</td>
<td>1.231E-10</td>
<td>1.231E-10</td>
<td>1.231E-10</td>
<td>1.231E-10</td>
</tr>
<tr>
<td>15</td>
<td>1.096E-09</td>
<td>1.096E-09</td>
<td>1.096E-09</td>
<td>1.096E-09</td>
<td>1.096E-09</td>
<td>1.096E-09</td>
</tr>
<tr>
<td>16</td>
<td>1.158E+01</td>
<td>1.158E+01</td>
<td>1.158E+01</td>
<td>1.158E+01</td>
<td>1.158E+01</td>
<td>1.158E+01</td>
</tr>
<tr>
<td>17</td>
<td>1.043E+05</td>
<td>1.043E+05</td>
<td>1.043E+05</td>
<td>1.043E+05</td>
<td>1.043E+05</td>
<td>1.043E+05</td>
</tr>
<tr>
<td>18</td>
<td>7.926E+01</td>
<td>7.926E+01</td>
<td>7.926E+01</td>
<td>7.926E+01</td>
<td>7.926E+01</td>
<td>7.926E+01</td>
</tr>
<tr>
<td>19</td>
<td>1.996E+02</td>
<td>1.996E+02</td>
<td>1.996E+02</td>
<td>1.996E+02</td>
<td>1.996E+02</td>
<td>1.996E+02</td>
</tr>
<tr>
<td>TOTAL</td>
<td>2.656E+03</td>
<td>2.656E+03</td>
<td>2.656E+03</td>
<td>2.656E+03</td>
<td>2.656E+03</td>
<td>2.656E+03</td>
</tr>
</tbody>
</table>

---

### Table C1 (Continued)

<table>
<thead>
<tr>
<th>UNIT</th>
<th>2470.0MIN.</th>
<th>2490.0MIN.</th>
<th>2510.0MIN.</th>
<th>2520.0MIN.</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO.</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
<td>PU</td>
</tr>
<tr>
<td>1</td>
<td>5.230E+02</td>
<td>5.230E+02</td>
<td>5.230E+02</td>
<td>5.230E+02</td>
</tr>
<tr>
<td>2</td>
<td>5.805E+00</td>
<td>5.805E+00</td>
<td>5.805E+00</td>
<td>5.805E+00</td>
</tr>
<tr>
<td>3</td>
<td>6.146E+01</td>
<td>6.146E+01</td>
<td>6.146E+01</td>
<td>6.146E+01</td>
</tr>
<tr>
<td>5</td>
<td>3.750E+00</td>
<td>3.750E+00</td>
<td>3.750E+00</td>
<td>3.750E+00</td>
</tr>
<tr>
<td>6</td>
<td>4.005E+02</td>
<td>4.005E+02</td>
<td>4.005E+02</td>
<td>4.005E+02</td>
</tr>
<tr>
<td>7</td>
<td>4.334E+00</td>
<td>4.334E+00</td>
<td>4.334E+00</td>
<td>4.334E+00</td>
</tr>
<tr>
<td>8</td>
<td>3.424E+02</td>
<td>3.424E+02</td>
<td>3.424E+02</td>
<td>3.424E+02</td>
</tr>
<tr>
<td>9</td>
<td>2.261E-11</td>
<td>2.261E-11</td>
<td>2.261E-11</td>
<td>2.261E-11</td>
</tr>
<tr>
<td>10</td>
<td>1.873E-10</td>
<td>1.873E-10</td>
<td>1.873E-10</td>
<td>1.873E-10</td>
</tr>
<tr>
<td>11</td>
<td>1.170E-11</td>
<td>1.170E-11</td>
<td>1.170E-11</td>
<td>1.170E-11</td>
</tr>
<tr>
<td>12</td>
<td>1.906E-09</td>
<td>1.906E-09</td>
<td>1.906E-09</td>
<td>1.906E-09</td>
</tr>
<tr>
<td>13</td>
<td>1.119E-11</td>
<td>1.119E-11</td>
<td>1.119E-11</td>
<td>1.119E-11</td>
</tr>
<tr>
<td>14</td>
<td>1.231E-10</td>
<td>1.231E-10</td>
<td>1.231E-10</td>
<td>1.231E-10</td>
</tr>
<tr>
<td>15</td>
<td>1.096E-09</td>
<td>1.096E-09</td>
<td>1.096E-09</td>
<td>1.096E-09</td>
</tr>
<tr>
<td>16</td>
<td>1.158E+01</td>
<td>1.158E+01</td>
<td>1.158E+01</td>
<td>1.158E+01</td>
</tr>
<tr>
<td>17</td>
<td>1.043E+05</td>
<td>1.043E+05</td>
<td>1.043E+05</td>
<td>1.043E+05</td>
</tr>
<tr>
<td>18</td>
<td>7.926E+01</td>
<td>7.926E+01</td>
<td>7.926E+01</td>
<td>7.926E+01</td>
</tr>
<tr>
<td>19</td>
<td>1.996E+02</td>
<td>1.996E+02</td>
<td>1.996E+02</td>
<td>1.996E+02</td>
</tr>
<tr>
<td>TOTAL</td>
<td>2.656E+03</td>
<td>2.656E+03</td>
<td>2.656E+03</td>
<td>2.656E+03</td>
</tr>
</tbody>
</table>

---

87
Figure C1. The temporal response of a reprocessing facility with six plutonium contactors shaded by contactor. Roman numerals correspond to those used to label contactors in Figure 1.
APPENDIX D

A User's Guide for CUSEP

A. CUSEP Program Listing

COMMON/UTO/  I
COMMON/UT1/  CON(6),TEMPD,TEMPF,TEMPC,SPH
COMMON/UT2/  TRB8,TRK,PCNT
COMMON/UT3/  NRDXX,NAA,NOR
COMMON/BLOCKO/  AFLOPC(102),OFLOPC(102),AQPCFL(102),ORPCFL(102)
COMMON/BLOCK1/  ARY(6),STOICH(6)
COMMON/BLOCK2/  AQ(6),OR(6)
COMMON/BLOCK4/  CONVA,CONVO,TEMP
COMMON/BLOCK5/  CX(6),SX(6),DAD(6),CMA(6),CMO(6),SAT(6),SOT(6)
COMMON/BLOCK6/  XASJ(6,102),X0SJ(6,102)
COMMON/BLOCK7/  LAQM(102),LORM(102),NAQM(102),NORM(102)
COMMON/ALL/  NTOP,NPROUT,NQSEP,NQ0P,ICNT
COMMON/COEFS/  PFX1,PFX2,PFX3,PFX4
COMMON/FEEDS/  XAFX(6,102),XOFX(6,102),AFLEX(102),OFLEX(102)
COMMON/FEEDT/  TAFX(102),TOFX(102)
COMMON/MOLWT/  GMW(6)
COMMON/MTRANS/  AREA(102),TRNSCO(6,102)
COMMON/PULSE/  ENDIAM,CLDIAM,PLSAMP,PLFREQ,PFLOW
COMMON/RATE/  NFX(6),NX(6)
COMMON/TBP/  TLRNCE,CTBP,PCNTBP,TBPM(102)
COMMON/TMPC/  NCOM1,NCOM2,NCOM3,NCOM4,NTEM
COMMON/TMPS/  ATS(102),OTS(102),TEMPA1,TEMPA2,TEMPO1,TEMPO2
COMMON/TIMES/  H,HHI,HLO,HPRINT,TAU,PRTIME,ZEIT,PZET,PRZEIT,PRNTME
COMMON/VOLS/  ASVOL(102),OSVOL(102),TSVOL(102),VQOR(102)
DIMENSION ASX(6),COEF(4),COEFS(4),OSX(6),PHIA(6,102),PHIO(6,102),
            PHTA(102),PHTO(102),PHVA(102),PHVO(102),QA(6,102),QAN(6,102),
            QO(6,102),QON(6,102),QTA(102),QTO(102),QA1(102),QVO(102),
            XBAQ(6,102),XBOQ(6,102),HGT(102),CAQ(6),COR(6)
REAL*8  TITLE(10,10)
REC6=1.0/6.0
TV0PI=6.283185E+00
100
    COEF(1)=0.0
    COEF(2)=0.5
    COEF(3)=0.5
    COEF(4)=1.0
    COEFS(1)=1.0
    COEFS(2)=2.0
    COEFS(3)=2.0
    COEFS(4)=1.0
    GMW(1)=1.008
    GMW(2)=238.0
    GMW(3)=239.0
    GMW(4)=239.0
    GMW(5)=238.0
    GMW(6)=62.0
    STOICH(2)=2.0
    STOICH(3)=2.0
    CX(1)=2.016
    CX(2)=1.190E+02
    CX(3)=2.380E+02
    CX(4)=2.380E+02

89
CX(5)=-1.190E+02
CX(6)=6.200E+01
SX(1)=0.0
SX(2)=238.0
SX(3)=0.0
SX(4)=0.0
SX(5)=-238.0
SX(6)=0.0
NPX(1)=-2
NPX(2)=0
NPX(3)=+1
NPX(4)=0
NPX(5)=+1
NPX(6)=0
NAX(1)=0
NAX(2)=0
NAX(3)=0
NAX(4)=0
NAX(5)=1
NAX(6)=1
DO 10 J=4,6
STOICH(J)=0.0
10 CONTINUE
HLO=0.0

C H  THE TIME INCREMENT TO BE USED IN THE RUNGA-KUTTA INTEGRATION.
C THE VALUE OF H MAY BE CHANGED DURING THE COURSE OF THE
C CALCULATION TO PREVENT NEGATIVE CONCENTRATIONS FROM BEING
C GENERATED, BUT REVERTS TO THE ORIGINAL VALUE FOR THE NEXT
C INTEGRATION PERIOD. THE NEW VALUE IS PRINTED EACH TIME
C THAT IT IS CHANGED.
C HHI  THE TIME AT WHICH THE CALCULATION IS TO STOP. IF STEADY
C STATE IS REACHED BEFORE HHI, THE CALCULATION STOPS AND
C PRINTS THE PROFILE OF CONCENTRATIONS AND THE TIME.
C HPRINT  THE TIME BETWEEN THE PRINTING OF CONCENTRATION PROFILES.
C TRASE  PERMISSIBLE LEVEL OF CLIPPING IN THE RUNGA-KUTTA INTEGRATION.
C TAU  THE VALUE OF THE RATE CONSTANT FOR 'AUTOOXIDATION' OF U+4
C TO U+6. THE RATE LAW IS ASSUMED TO BE FIRST ORDER IN THE TOTAL
C NITRATE ION CONCENTRATION AND IN THE U+4 CONCENTRATION.
C TEMPD  THE DEFAULT TEMPERATURE OF THE SYSTEM. IF A FEED STREAM
C TEMPERATURE DIFFERS FROM TEMPD, FUNCTION TMIX WILL BE
C CALLED TO ACCOUNT FOR HEAT EXCHANGE THROUGHOUT THE SYSTEM.
C NMS  THE NUMBER OF MIXER-SETTLER BANKS IN THE CONTACTOR.
C NTITLE  THE NUMBER OF TITLE CARDS TO BE READ IN AND PRINTED AS THE
C INTRODUCTION TO THE OUTPUT OF EACH PROBLEM. THE NUMBER
C MUST NOT EXCEED 10.
C NQSEP  THE COMPUTATIONAL OPTION TO BE USED IN THE CALCULATION.
C IF NQSEP=1, DEVIATIONS FROM MASS TRANSFER EQUILIBRIA ARE
C ASSUMED, AND MASS TRANSFER AREAS AND COEFFICIENTS MUST BE
C INPUT. IF NQSEP=0, EQUILIBRIUM MASS TRANSFER IS ASSUMED, THE
EQUILIBRIUM CONSTANTS BEING CALCULATED INTERNALLY IN
SUBROUTINE DISCO.

THE INPUT FORMAT *** 6 E10.3, 314 ***
READ(1,9000,END=77) H,HHI,HPRINT,TBASE,TAU,TEMPD
9000 FORMAT(6E10.3)
IF(H.EQ.0.0) GO TO 79
READ(1,9900) NMS,NTITLE,NQSEP
9900 FORMAT(14)
NMS1=NMS+1
NMS2=NMS+2

NTITLE TITLE CARDS ARE READ IN. THE MAXIMUM NUMBER IS 10.
WRITE (3,1901)
1901 FORMAT( '///:///)
DO 11 J=1,NTITLE
READ(1,1000) (TITLE(J,K),K=1,10)
1000 FORMAT(10A8)
WRITE (3,1001) (TITLE(J,K),K=1,10)
11 CONTINUE

NPX(1)=-4
NPX(2)=0
NPX(3)=+2
NPX(4)=-2
NPX(5)=+2
NPX(6)=-2
CX(1)=2.016
CX(2)=0.0
CX(3)=-2.39E+2
CX(4)=+2.39E+2
CX(5)=-3.404E+1
CX(6)=+1.24E+2

CONTINUE
ZEIT=0.0
PZEIT=0.0
PRZEIT=0.0
IF(NQOP.EQ.0) GO TO 20
WRITE (3,1008)
1008 FORMAT('-',40X,'INPUT DATA FOR THE MASS TRANSFER AREAS',
, 'AND COEFFICIENTS')
WRITE (3,1009)
1009 FORMAT('-',21X,'STAGE I TRANSFER I',26X,'MASS TRANSFER ',
, 'COEFFICIENT')
WRITE (3,1010)
1010 FORMAT('-',15X,'NO. I AREA I NITRIC ACID I URANIUM I',
, ' PU(IV) I PU(III) I REDUCTANT I NITRATE ION')
WRITE (3,1011)
1011 FORMAT(27X,7 (' I ',10X))
15 READ(1,9001) I,J,QQQ
9001 FORMAT(2I3,4X,E10.3)
DO 16 I=1,J
KP = K + 1
AREA(KP) = QQQ
16 CONTINUE
IF (J .EQ. NMS) GO TO 17
GO TO 15
17 READ(1,9002) I, J, (CON(K), K = 1, 6)
9002 FORMAT(2I3,4X,6E10.3)
DO 19 K = I, J
KP = K + 1
QQQ = AREA(KP)
WRITE (3,1014) K, QQQ, (CON(III), III = 1, 6)
1014 FORMAT(22X,I3,2X,7(' ',1PE10.3))
DO 18 III = 1, 6
TRNSCO(III, KP) = CON(III)
18 CONTINUE
19 CONTINUE
IF (J .EQ. NMS) GO TO 20
GO TO 17
20 READ(1,9003) PCNTBP, TLRNCE, STDV1, STDV2
9003 FORMAT(4F10.0)
STDV1 = STDV1 * 1.0E-02
STDV2 = STDV2 * 1.0E-02
C CALL FTIME(ISEED)
TLRNCE = TLRNCE * 1.0E-02
CTBP = PCNTBP
CTBP = CTBP * 1.0E-02
SPH = 0.321 + 0.078 * CTBP
F = CTBP * 3.65145
READ(1, 9901) PLSAMP, PLFREQ, CLDIAM, ENDIAM 9901 FORMAT(4F10.0)
PLFREQ = PLFREQ * TWOPI
VOLFAC = 1.0E-03
PLSVOL = 7.854E-01 * CLDIAM**2 * PLSAMP * PLFREQ * VOLFAC
CALL READVL(HGT, VAQR)
ENDSEC = 7.854E-01 * ENDIAM**2 * VOLFAC
CNTSEC = 7.854E-01 * CLDIAM**2 * VOLFAC
TSVOL(2) = HGT(2) * ENDSEC
TSVOL(NMS1) = HGT(NMS1) * ENDSEC
DO 22 I = 3, NMS
TSVOL(I) = HGT(I) * CNTSEC
22 CONTINUE
C FEED STREAM DATA
C INITIALIZE ALL FEEDSTREAM FLOW RATES AND CONCENTRATIONS
DO 36 I = 1, 6
AQ(I) = 0.0
QR(I) = 0.0
ARY(I) = 0.0
36 CONTINUE
DO 38 I = 1, NMS2
DO 37 J = 1, 6
XAFX(J, I) = 0.0
XBAQ(J, I) = 0.0
XOFX(J, I) = 0.0
XBOR(J, I) = 0.0
XASJ(J, I) = 0.0
XOSJ(J, I) = 0.0
CONTINUE
AFLEX(I)=0.0
OFLEX(I)=0.0
AQPCFL(I)=0.0
ORPCFL(I)=0.0
AFLOPC(I)=0.0
OFLOPC(I)=0.0
ATS(I)=TEMPD
OTS(I)=TEMPD
LAQM(I)=1
NAQM(I)=0
LORM(I)=1
NORM(I)=0
TBPM(I)=F
TAFX(I)=0.0
TOFX(I)=0.0
CONTINUE
NAQ=0
NOR=0
NCOM=0
PRTIME=0.0
C SUBROUTINE FEEDST IS CALLED. THE NECESSARY INPUT DATA MUST BE
SUPPLIED. DETAILS OF FORMAT ARE GIVEN IN THE SUBROUTINE.
CALL FEEDST
IF(NOR.EQ.1.OR.NAQ.EQ.1) GO TO 41
GO TO 49
DO 48 I=2,NMS1
NOR=NORM(I)
NAQ=NAQM(I)
IF(NAQ.NE.1) GO TO 44
TEMP=TAFX(I)
DO 42 J=1,NCOM
AQ(J)=XAFX(J,I)/GMW(J)
42 CONTINUE
TCONC=-1.0
CALL MOLVOL(TCONC,NOR,NAQ)
AFLEX(I)=AFLEX(I)/CONVA
DO 43 J=1,NCOM
AAA=AQ(J)*CONVA*GMW(J)
XAFX(J,I)=AAA
XBAQ(J,I)=AAA
43 CONTINUE
IF(NOR.NE.1) GO TO 47
TEMP=TOFX(I)
DO 45 J=1,NCOM
OR(J)=XOFX(J,I)/GMW(J)
45 CONTINUE
TCONC=-1.0
CALL MOLVOL(TCONC,NOR,NAQ)
OFLEX(I)=OFLEX(I)/CONVO
DO 46 J=1,NCOM
AAA=OR(J)*CONVO*GMW(J)
XOFX(J,I)=AAA
XBOR(J,I)=AAA
46 CONTINUE
47 CONTINUE
48 CONTINUE
49 CONTINUE
CALL FLOWS
DO 53 I=2,NMS1
QQQ=AFLEX(I)
AAA=AFLOPC(I-1)
ZZZ=XASJ(1,1-I)*AAA+XAFX(1,1)*QQQ
XASJ(1,1)=ZZZ/(QQQ+AAA)
53 CONTINUE
PRNTME=HLO+HHI
WRITE (3,1023)
1023 FORMAT(’-’,53X,’TABLE OF TIMES AND CONSTANTS’) WRITE (3,1024)
1024 FORMAT(’ ’,36X,’ ’)
WRITE (3,1025) HLO
1025 FORMAT(’ ’,35X,’ START TIME ’,1PE10.3,’ ’)
WRITE (3,1026) PRNTME
1026 FORMAT(’ ’,35X,’ STOP TIME ’,1PE10.3,’ ’)
WRITE (3,1027) H
1027 FORMAT(’ ’,35X,’ RUNGE-KUTTA INTEGRATION TIME ’,1PE10.3,’ ’)
WRITE (3,1028) HPRINT
1028 FORMAT(’ ’,35X,’ PROFILE PRINT TIME ’,1PE10.3,’ ’)
WRITE (3,1029) PRTIME
1029 FORMAT(’ ’,35X,’ PROFILE GENERATION TIME (CARDS OR DISK) ’,1PE10.3,’ ’)
WRITE (3,1030) TBASE
1030 FORMAT(’ ’,35X,’ RUNGE-KUTTA TIME CONSTANT ’,1PE10.3,’ ’)
AAA=TLRNCE*1.0E+02
WRITE (3,1130) AAA
1130 FORMAT(’ ’,35X,’ TOLERANCE FOR CONVERGENCE TESTS ’,1PE10.3,’ ’)
WRITE (3,1137) PLSAMP
1137 FORMAT(’ ’,35X,’ PULSE AMPLITUDE IN CM ’,1PE10.3,’ ’)
WRITE (3,1138) PLFREQ
1138 FORMAT(’ ’,35X,’ PULSE FREQUENCY IN CYCLES PER MINUTE ’,1PE10.3,’ ’)
WRITE (3,1139) CLDIAM
1139 FORMAT(’ ’,35X,’ PULSED COLUMN DIAMETER IN CM ’,1PE10.3,’ ’)
IF(NRDXN.EQ.1) GO TO 60
IF(TAU.GT.0.0) GO TO 59
WRITE (3,1031)
GO TO 60
59 WRITE (3,1032) TAU
1031 FORMAT(’ ’,35X,’ REDUCTANT IS HYDROXYLAMINE’,31X,’ ’)
1032 FORMAT(’ ’,35X,’ U+4 -> U+6 OXIDATION RATE CONSTANT ’,1PE10.3,’ ’)
60 IF(STDDEV1.EQ.0.0) GO TO 601
WRITE(3,1033)
AAA=STDDV1*1.0E+02
WRITE(3,1034) AAA

601 IF(STDDV2.EQ.0.0) GO TO 602
WRITE(3,1033)
AAA=STDDV2*1.0E+02
WRITE(3,1035) AAA

602 WRITE (3,1036)
1033 FORMAT(' ',35X,' I STANDARD DEVIATION FOR FLUCTUATIONS',19X,
' I')
1034 FORMAT(' ',35X,' I IN THE AQUEOUS FEED STREAMS ............ ',
'.1PE10.3, ' I')
1035 FORMAT(' ',35X,' I IN THE ORGANIC FEED STREAMS ............ ',
'.1PE10.3, ' I')
1036 FORMAT(' ',36X,' I')

CALL PRINTS
ICNT=1
IF(NPRFIN.EQ.1) ICNT=2
AQPCFL(NMS1)=AFLOPC(NMS1)
ORPCFLC 2)=0FL0PC(2)
TRK=H
NQREV=NQOP

62 NMIX=0
IF(NQREV.EQ.1) NMIX=1
PTIME=ZEIT*PLOTS
PFLOW=PLSVOL*COS(PTIME)
DO 64 I=2,NMS1
DO 63 J=1,NCOM
PHIA(J,I)=0.0
PHIO(J,I)=0.0
QA(J,I)=0.0
Q0(J,I)=0.0
CONTINUE
QVA(I)=0.0
QVO(I)=0.0
PHVA(I)=0.0
PHVO(I)=0.0
QTA(I)=0.0
QTO(I)=0.0
PHTA(I)=0.0
PHTO(I)=0.0
CONTINUE
DO 65 K=2,NMS
KP=K+1
AQPVEL=ASVOL(K)*PFLOW/TSVOL(K)
ORPVEL=PFLOW-AQPVEL
AQFLOW=AFLOPC(K)+AQPVEL
AAA=ABS(AQFLOW)
AQPCFL(K)=AAA
LAQM(K)=AAA/AQFLOW
ORFLOW=OFLOPC(KP)-ORPVEL
QQQ=ABS(ORFLOW)
ORPCFL(KP)=QQQ
LORM(KP)=QQQ/ORFLOW
CONTINUE

95
NCHECK=0
NTEM=0
NDIR=1

I=1
DO 72 J14=1,4
COEFI=COEFS(J14)
COEFJ=COEF(J14)
DO 691 ISTG=1,NMS
I=I+NDIR
IP=I+1
IM=I-1
PFX1=LAQM(IM)
PFX2=LAQM(I)
PFX3=LORM(IP)
PFX4=LORM(I)
NCOM1=I
IF(LAQM(IM).EQ.1) NCOM1=IM
NCOM2=IP
IF(LAQM(I).EQ.1) NCOM2=I
NCOM3=I
IF(LORM(IP).EQ.1) NCOM3=IP
NCOM4=IM
IF(LORM(I).EQ.1) NCOM4=I
AFLEXI=AFLEX(I)
OFLEXI=OFLEX(I)
AFLOWI=AQPCFL(IM)
OFLOWI=ORPCFL(IP)
AFLOWO=AQPCFL(I)
OFLOWO=ORPCFL(I)
AFLOWD=PFX1*AFLOWI-PFX2*AFLOWO+AFLEXI
OFLOWD=PFX3*OFLOWI-PFX4*OFLOWO+OFLEXI
ASVOLI=ASVOL(I)
OSVOLI=OSVOL(I)

TEMP=-TEMPD
IF(NTEM.EQ.1) GO TO 651
IF(NTOP.EQ.1) TEMPC=TMIX(TEMPO
ATS(NCOM1)=TEMPC
ATS(NCOM2)=TEMPC
OTS(NCOM3)=TEMPC
OTS(NCOM4)=TEMPC

651 DO 66 K=1,NCOM
QQQ=QASJ(K,NCOM1)
QQQ=QQQ+QA(K,NCOM1)*COEFJ
ASX(K)=QQQ
AAA=QOSJ(K,NCOM3)+QO(K,NCOM3)*COEFJ
OSX(K)=AAA
QQQ=QASJ(K,NCOM2)+QA(K,NCOM2)*COEFJ
AAA=QOSJ(K,NCOM4)+QO(K,NCOM4)*COEFJ
SAT(K)=QQQ
SOT(K)=AAA
AQ(K)=(XASJ(K,1)+QA(K,1)*COEFJ)/GMW(K)
OR(K)=(XOSJ(K,1)+QA(K,1)*COEFJ)/GMW(K)
CONTINUE
IREP=0
NCONT=0

660 IF(NQREV.EQ.0) GO TO 661
F=CTBP+3.65145
BBB=1.0-F+2.0*(OR(1)+OR(2)+OR(3))
CCC=-F+2.0*(OR(2)+OR(3))+OR(1)
CCC=BBB**2-4.0*CCC
TBP=(-BBB+SQRT(CCC))/2.0

661 CALL DISCO(TBP,TEMPC,NMIX)
PIX=0.0
IF(NBXN.EQ.0) PIX=PIXF(NCOM,AQ)
PXF=PIX
HRXN=1.7E+02
IF(TAU.EQ.0.0) HRXN=1.74*EXP(3.1E+04/1.987*(1.0/303.16-1.0/(273.16
+TEMPC)))
IREP=IREP+1
NCONT=0
RTAU=TAU*AQ(5)
DO 67 K=1,NCOM
QQQ=0.0
AQK=AQ(K)
ORK=OR(K)
DADK=DAD(K)
RXNAM=SX(K)+RTAU+CX(K)+PFX+HRXN
TRNSFR=AREA(K)+TRNSCO(K)+DADK+AQ(K)-OR(K)
AAA=PFX1-AFLOW1+ASX(K)-PFX2-AFLOW2+SAT(K)+AFLEX1-XAFX(K,I)
IF(NQREV.EQ.1) GO TO 662
AAA=AAA+OFLEX1-XOFX(K,I)
IF(NCOM3.NE.1) AAA=AAA+PFX3+OFLOW3+OSX(K)
IF(NCOM4.NE.1) AAA=AAA-PFX4+OFLOW4+OSX(K)
IF(NCOM3.EQ.1) QQQ=QQQ+PFX3+OFLOW3+AQK+GMWK
IF(NCOM4.EQ.1) QQQ=QQQ-PFX4+OFLOW4+AQK+GMWK
AAA=AAA+QQQ+DADK+RXNAM*ASVOLI
AAA=AAA*TRK/(ASVOLI+DADK*OSVOLI)
GO TO 663
662 QQQ=PFX3+OFLOW3+OSX(K)-PFX4+OFLOW4+SAT(K)+OFLEX1-XOFX(K,I)+TRNSFR
AAA=AAA-TRNSFR
AAA=(AAA/ASVOLI+RXNAM)*TRK
QQQ=TRK*QQQ/OSVOLI
663 QAN(K,I)=AAA
IF(NQREV.EQ.0) QQQ=AAA*DAEK
QON(K,I)=QQQ
AAA=(XASJ(K,I)+AAA+COEFJ)/GMWK
CAQ(K)=AAA
QQQ=(XOSJ(K,I)+QQQ+COEFJ)/GMWK
COR(K)=QQQ
67 CONTINUE
673 K=1,NCOM
PHIA(K,I)=PHIA(K,I)+QAN(K,I)*COEFI
PHIO(K,I)=PHIO(K,I)+QON(K,I)*COEFI
673 CONTINUE
681 CONTINUE
CONTINUE  
CONTINUE  
CONTINUE  
NPRINT=1  
DO 74 I=2,NMS1  
DO 73 K=1,NCON  
AAA=XASJ(K,I)  
QQQ=PHIA(K,I)*REC6  
QQQ=QQQ+AAA  
CALL CHECK(QQQ,NCHECK)  
IF(NCHECK. EQ.1) GO TO 62  
XASJ(K,I)=QQQ  
AQ(K)=QQQ/GMW(K)  
IF(QQQ. GT.0.0) QQQ=ABS((QQQ-AAA)/QQQ)  
IF(QQQ. GT.TLRNCE) NPRINT=0  
IF(NQREV. EQ.0) GO TO 73  
AAA=XOSJ(K,I)  
QQQ=PHIO(K,I)*REC6  
QQQ=QQQ+AAA  
CALL CHECK(QQQ,NCHECK)  
IF(NCHECK. EQ.1) GO TO 62  
XOSJ(K,I)=QQQ  
OR(K)=QQQ/GMW(K)  
IF(QQQ. GT.0.0) QQQ=ABS((QQQ-AAA)/QQQ)  
IF(QQQ. GT.TLRNCE) NPRINT=0  
CONTINUE  
IF(NQREV. EQ.1) GO TO 732  
TEMP=ATSI(I)  
CALL DISCO(TBP,TEMP,NMIX)  
DO 731 K=1,NCON  
QQQ=XASJ(K,I)*DAD(K)  
XOSJ(K,I)=QQQ  
OR(K)=QQQ/GMW(K)  
CONTINUE  
731  CONTINUE  
732  F=CTBP+3.65145  
BBB=1.0-F+2.0*(OR(1)+OR(2)+OR(3))  
CCC=F+2.0*(OR(2)+OR(3))+OR(1)  
CCC=BBB*2-4.0*CCC  
TBP=(-BBB+SQR(CCC))/2.0  
TBPM(I)=TBP  
CONTINUE  
ZET=ZET+TRK  
PZEIT=PZEIT+TRK  
ICNT=ICNT+1  
IF(NPRINT. EQ.0) GO TO 75  
HFI=0.0  
PZEIT=HPRINT  
75  IF(PZEIT. LT. HPRINT) GO TO 76  
PZEIT=0.0  
CALL PRINTS  
76  IF(ZEIT. GT. HFI) GO TO 100  
TRK=H  
GO TO 62  
77  CONTINUE  
STOP
C

SUBROUTINE CITY

SUBROUTINE READY(VOL,VAQR)
COMMON/ALL/ NTOP,NPROUT,NCOM,NMS,NMS1,NMS2,NQSEP,NQOP,ICNT
DIMENSION VOL(102),VAQR(102)
10 READ(1,2000) I,J,QQQ,AAA
2000 FORMAT(2I3,4X,2F10.0)
DO 20 K=I,J
KP=K+1
VOL(KP)=QQQ
VAQR(KP)=AAA
20 CONTINUE
IF(J.NE.NMS) GO TO 10
RETURN
END

SUBROUTINE FEEDST
COMMON/UTO/ I
COMMON/UT1/ CON(6),TEMPD,TEMPF,TEMPC,SPH
COMMON/UT3/ NDXN,NAQ,NOR
COMMON/BLOCKO/ AFLORC(102),OFLOPC(102),AQPCFL(102),ORPCFL(102)
COMMON/BLOCK7/ LAQM(102),LORM(102),NAQM(102),NORM(102)
COMMON/ALL/ NTOP,NPROUT,NCOM,NMS,NMS1,NMS2,NQSEP,NQOP,ICNT
COMMON/FEEDS/ XAFX(6,102),XOFX(6,102),AFLEX(102),OFLEX(102)
COMMON/FEEDT/ TAFX(102),TOFX(102).
COMMON/MOLWG/ GMW(6)
COMMON/TBP/ TLRNCE,STBP,PCNTBP,TBPM(102)
COMMON/TEMP/ ATS(102),OTS(102),TEMPA1,TEMPO1,TEP02
COMMON/TIMES/ H,HHI,HLO,HPRINT,TAU,PRTIME,ZEIT,PRZEIT,PRNTME
WRITE (3,3000)
3000 FORMAT(1//,5X,' FEED & PRODUCT!',1X,'STAGE I NITRIC ACID!',
'.', 'URANIUM | PU(IV) | PU(III) | REDUCTANT '|',
'.', 'NITRATE ION | FLOW RATE | TEMPERATURE')
WRITE (3,3001)
3001 FORMAT(3,5X,'STREAM DATA',1X,'NO. | (MOL/L) | ',
'.', '(G/L) | (G/L) | (G/L) | (MOL/L) | (MOL/L) |',
'.', '(L/MIN) | (CENT.))')
10 READ(1,3004) J,JPHASE,FLOW,(CON(I),I=1,6),TEMPF,INDEX
3004 FORMAT(13,11,8F8.0,11)
JP=J+1
IF(TMPF.NE.TEMPD) NTOP=1
AAA=CON(1)
CON(1)=CON(1)*1.008
C
JPHASE=0 ORG, 1 AQU
IF(JPHASE.EQ.1) GO TO 12
IF(JPHASE.EQ.0) STOP
OFLEX(JP)=FLOW
NOR=1
NORM(JP)=1
IF(TMPF.NE.0.0) TOFX(JP)=TEMPF
DO 11 I=1,6
IF(CON(I).EQ.0.0) GO TO 11
XOFX(I,JP)=CON(I)
11 CONTINUE
IF (I .GT. NCOM) NCOM = I
11 CONTINUE
GO TO 15
12 NAQM(JP) = 1
NAQ = 1
AFLEX(JP) = FLOW
1F (TEMPF .NE. 0.0) TAFX(JP) = TEMPF
1F (CON(5) .EQ. 0.0) GO TO 13
NQOP = 0
NRDXN = 0
13 DO 14 I = 1, 6
1F (CON(I) .EQ. 0.0) GO TO 14
XAFX(I, JP) = CON(I)
1F (I .GT. NCOM) NCOM = I
14 CONTINUE
1F (JPHASE .EQ. 0) WRITE (3, 3002) PCNTBP, J, AAA, (CON(I), I = 2, 6), FLOW,
.TEMPF
1F (JPHASE .EQ. 1) WRITE (3, 3003) J, AAA, (CON(I), I = 2, 6), FLOW, TEMPF
3002 FORMAT (', 7X, F5.1,' % TBP I', 1X, I3, 2X, 'I ',
.7 (1PE10.3,' I'), 0PF4.1)
3003 FORMAT (', 7X, 'AQUEOUS I', 1X, I3, 2X, 'I ',
.7 (1PE10.3, ' I'), 0PF4.1)
1F (INDEX .EQ. 1) GO TO 10
RETURN
END

SUBROUTINE FLOWS
COMMON/BLOCKO/ AFLOPC(102), OFLOPC(102), AQPCFL(102), ORPCFL(102)
COMMON/ALL/ NTOP, NPROUT, NCOM, NMS, NMS1, NMS2, NQSEP, NQOP, ICNT
COMMON/FEEDS/ XAFX(6, 102), XOFX(6, 102), AFLEX(102), OFLEX(102)
COMMON/FEEDT/ TAFX(102), TOFX(102)
COMMON/TEMPS/ ATS(102), OTS(102), TEMPA1, TEMPA2, TEMPO1, TEMPO2
COMMON/VOLS/ ASVOL(102), OSVOL(102), TSVOL(102), VAQOR(102)
DO 16 I = 2, NMS1
1M = I - 1
J = NMS2 - IM
JP = J + 1
AAA = AFLOPC(IM) + AFLEX(I)
QQQ = OFLOPC(JP) + OFLEX(J)
AFLOPC(I) = AAA
OFLOPC(J) = QQQ
16 CONTINUE
CALL HOLDUP
WRITE (3, 7014)
7014 FORMAT (', 8X, 'STAGE I TRANSFER UNIT VOLUMES I',
. ' TRANSFER UNIT FLOW RATE')
WRITE (3, 7015)
7015 FORMAT (', 9X, 'NO. I AQUEOUS I ORGANIC I AQUEOUS I ORGANIC')
WRITE (3, 7016)
7016 FORMAT (', 13X, 4 (' I ', 10X))
1D 17 I = 2, NMS1
1M = I - 1
WRITE (3, 7017) IM, ASVOL(I), OSVOL(I), AFLOPC(I), OFLOPC(I)
7017 FORMAT (', 8X, 13, 2X, 4 (' I ', 1PE10.3))
SUBROUTINE MOLVOL(TCONC,NOR,NAQ)
COMMON/BL0CK2/ AQ(6),OR(6)
COMMON/BL0CK4/ CONVA,CONVO,TEMP
COMMON/ALL/ NTOP,NPROUT,NCOM,NMS,NMS1,NMS2,NQSEP,NQ0P,ICNT
COMMON/TBP/ TLRNCE,CTBP,PCNTBP,TBPM(102)
F=CTBP
ICONC=TCONC
T=3.65145*F
IF(ICONC.EQ.1) GO TO 10
ICONC=T/(2.0+0.092*T)
POS=T/(2.0+0.18*T)
HOS=T*(1.0-0.00609*(3.95-0.0144*TEMP)*(F**1.65))/(1.0+0.043*T)
WO=(3.95-0.0144*TEMP)*(F**1.65)*(1.0-OR(2)/UOS-OR(3)/POS-
0.65*OR(1)/HOS)
GO TO 11
10 WO=(4.2-0.015*TEMP)*(F**1.69)*(T-2.0*OR(2)-2.0*OR(3)-
0.6*OR(1))/T
11 CONVO=1.0
IF(NOR.EQ.0) GO TO 12
CONVO=1.0+TCONC*(0.097*OR(2)+0.139*OR(3)+0.043*OR(1)+0.0174*WO)
CONVO=CONVO**ICONC
12 CONVA=1.0
IF(NAQ.EQ.0) GO TO 13
CONVA=0.0724*AQ(2)+0.13*AQ(3)+0.0309*AQ(1)+0.031*AQ(6)
CONVA=(1.0+TCONC*CONVA)**ICONC
13 RETURN
END

SUBROUTINE PRINTS
COMMON/BL0CK0/ AFLOPC(102),OFLOPC(102),AQPCFL(102),ORPCFL(102)
COMMON/BL0CK1/ ARY(6),STOICH(6)
COMMON/BL0CK2/ AQ(6),OR(6)
COMMON/BL0CK4/ CONVA,CONVO,TEMP
COMMON/BL0CK6/ XASJ(6,102),X0SJ(6,102)
COMMON/ALL/ NTOP,NPROUT,NCOM,NMS
NMS1,NMS2,NQSEP,NQ0P,ICNT
COMMON/MOLWGT/ GMW(6)
COMMON/PULSE/ ENDIAM,CLDIAM,PLSAMP,PLFREQ,PFLOW
COMMON/TBP/ TLRNCE,CTBP,PCNTBP,TBPM(102)
COMMON/TEMPS/ ATS(102),OTS(102),TEMPA1,TEMPA2,TEMP01,TEMP02
COMMON/TIMES/ H,HHI,HLO,HPRINT,TAU,PRTIME,ZEIT,PRZEIT,PRNTME
COMMON/VOLS/ ASVOL(102),OSVOL(102),TSVOL(102),VAQOR(102)
DIMENSION OOUTH(102),OUTS(102),QON(6,102)
TCONC=1.0
IF(ZEIT.NE.0.0) GO TO 10
PRNTME=HLO
8000 FORMAT(11,8H,1,'INITIAL PROFILE OF THE SETTLERS AT TIME=','
,F7.2,' MINUTES')
GO TO 11
101
10  PRNTME=ZEIT+HLO
WRITE (3,8001) PRNTME,PFLOW
8001  FORMAT('1*///\\/8X,'PROFILE OF THE SETTLERS AT TIME=','   ,F7.2,' MINUTES, CURRENT PULSED FLOW IS ','1PE10.3,' L/MIN')
11  WRITE (3,8002)
8002  FORMAT(' 8X,'AQUEOUS PHASE DATA FOR THE SETTLERS')
WRITE (3,8003)
8003  FORMAT(' 8X,'STAGE I NITRIC ACID | URANIUM | PU(IV) | ',PU(III) | REDUCTANT | NITRATE ION | DENSITY | SETTLER',   ,FLOW | TEMPERATURE')
WRITE (3,8004)
8004  FORMAT(' 9X,'NO. | (MOL/L) | (G/L) | (G/L) | ',(G/L) | (G/L) | (G/L) | (G/L) | (G/L) | (G/L) | (L/MIN) | (CENTIGRADE)')
WRITE (3,8005)
8005  FORMAT(' 13X,9 C I »,10X))
AQUIN=0.0
ORUIN=0.0
APUIN=0.0
OPUIN=0.0
DO 16 J=2,NMS1
TEMP=ATS(J)
DO 13 I=1,6
AQ(I)=XASJ(I,J)/GMW(I)
OR(I)=XOSJ(I,J)/GMW(I)
13  CONTINUE
NOR=1
NAQ=1
TCONC=1.0
CALL MOLVOL(TCONC,NOR,NAQ)
AOUTM=(1.0E3-72.4*AQ(2)-130.0*(AQ(3)+AQ(4))-30.9*AQ(1)-31.0*   .AQ(6))/(1.0E3/.99707)+0.39404*AQ(2)+0.49202*(AQ(3)+AQ(4))+/   .0.06301*AQ(1)+0.2123*AQ(6)
AOUTS(J)=AQ(J)/CONV(J)
BOUTM=1.0E3-17.4*OR(2)-97.0*(OR(3)+OR(4))-43.0*   .OR(1))*1.0E3/(1.0+1.8)/((273.6/266.32+227.5/170.34*1.8)*1.0E3)+   .0.01802*OR(2)+0.39404*OR(2)+0.49202*(OR(3)+OR(4))+0.06301*OR(1)
AOUTS=AFLOPC(J)*CONVA
BOUTS(J)=OFLOPC(J)*CONVO
AQUIN=AQUIN+(AQ(2)+AQ(5))*GMW(2)*ASVOL(J)/CONVA
ORUIN=ORUIN+(OR(2)+OR(5))*GMW(2)*OSVOL(J)/CONVO
APUIN=APUIN+(AQ(3)+AQ(4))*GMW(3)*ASVOL(J)/CONVA
OPUIN=OPUIN+(OR(3)+OR(4))*GMW(3)*OSVOL(J)/CONVO
DO 14 I=2,6
AQ(I)=AQ(I)/GMW(I)/CONVA
14  CONTINUE
QON(I,J)=OR(I)/GMW(I)/CONVO
AQ(I)=AQ(I)/CONVA
JM=J-1
WRITE (3,8006) JM,(AQ(I),I=1,6),AOUTM,AOUTS,TEMP
8006  FORMAT(' 9X,1X,9*("1PE10.3)')
16  CONTINUE
WRITE (3,8007)
8007  FORMAT(' 8X,'ORGANIC PHASE DATA FOR THE SETTLERS')
IF(TAU.EQ.0.0) THEN
WRITE (3,8008)
8008  FORMAT(102)
8008 FORMAT(' ',8X,'STAGE I NITRIC ACID I URANIUM I PU(IV) I ',
       ', U HOLDUP I PU HOLDUP I TBP CONC I DENSITY I SETTLER ',
       ',FLOW I TEMPERATURE')
WRITE (3,8009)
8009 FORMAT(' ',9X,'NO. I (MOL/L) I (G/L) I (G/L) I ',
       'GRAMS I GRAMS I (MOL/L) I (G/ML) I (L/MIN) I ',
       ',(CENTIGRADE)')
ELSE
WRITE (3,8018)
8018 FORMAT(' ',9X,'STAGE I NITRIC ACID I URANIUM I PU(IV) I ',
       ',PU(III) I REDUCTANT I TBP CONC I DENSITY I SETTLER ',
       ',FLOW I TEMPERATURE')
WRITE (3,8019)
8019 FORMAT(' ',9X,'NO. I (MOL/L) I (G/L) I (G/L) I ',
       '(G/L) I (G/L) I (MOL/L) I (G/ML) I (L/MIN) I ',
       ',(CENTIGRADE)')
END IF
8010 FORMAT(' ',13X,9 C I ',10X))
WRITE (3,8010)
DO 17 J=2,NMS1
JM=J-1
UHOLD=Q0N(2,J)*OSVOL(J)
PHOLD=QON(3,J)*OSVOL(J)
TEMP=OTS(J)
IF(TAU.EQ.0.0) THEN
WRITE (3,8011) JM,(QON(I,J),I=1,3),UHOLD,PHOLD,TBPM(J),OOUTM(J),
       .OOUTS(J),TEMP
ELSE
WRITE (3,8011) JM,(QON(I,J),I=1,5),TBPM(J),OOUTM(J),
       .OOUTS(J),TEMP
END IF
8011 FORMAT(' ',9X,I3,1X,9 C I ',1PE10.3))
17 CONTINUE
TPUIN=APUIN+OPUIN
TUIN=AQUIN+ORUIN
8012 FORMAT('0',1SX,' INVENTORIES: ',3X, 'AQUEOUS', 6X, 'ORGANIC', 6X,
       'TOTAL')
WRITE (3,8012)
8013 FORMAT(' ',15X,'PLUTONIUM',5X,3 (1PE10.3,3X))
WRITE (3,8013) APUIN,OPUIN,TPUIN
8014 FORMAT(' ',15X,'URANIUM',7X,3 (1PE10.3,3X))
WRITE (3,8014) AQUIN,ORUIN,TUIN
RETURN
END

FUNCTION TMIX(TEMPC)
COMMON/UTO/ I
COMMON/BLOCKO/ AFOLOPC(102),OFLOPC(102),AQPCFL(102),ORPCFL(102)
COMMON/BLOCK6/ XASJ(6,102),X0SJ(6,102)
COMMON/ALL/ NTOP,NPROUT,NCOM,NMS,NMS1,NMS2,NQSEP,NQOP,ICNT
COMMON/COEFS/ PFX1,PFX2,PFX3,PFX4
COMMON/FEEDS/ XAFX(6,102),XOFX(6,102),AFLEX(102),OFLEX(102)
COMMON/FEEDT/ TAFX(102),TOFX(102)
COMMON/TEMPC/ NCOM1,NCOM2,NCOM3,NCOM4,NTEM
COMMON/TEMPS/ ATS(102),OTS(102),TEMPA1,TEMPA2,TEMP01,TEMP02
COMMON/TIMES/ H, HHI, HLO, HPRINT, TAU, PRTIME, ZEIT, PZEIT, PRZEIT, PRNTME
COMMON/VOLS/ ASVOL(102), OSVOL(102), TSVOL(102), VAQOR(102)
IM=I+1
IP=I+1
ATMIX=AQPCFL(IM)*PFX1*ATS(NCOM1)-AQPCFL(I)*PFX2*ATS(NCOM2)
 +AFLEX(I)*TAFX(I)
OTMIX=OPRCFL(IP)*PFX3*OTS(NCOM3)-OPRCFL(I)*PFX4*OTS(NCOM4)
 +OFLEX(I)*TOFX(I)
TMIX=ATMIX*SPH*OTMIX
ATMIX=AQPCFL(IM)*PFX1-AQPCFL(I)*PFX2+AFLEX(I)
OTMIX=OPRCFL(IP)*PFX3-OPRCFL(I)*PFX4+OFLEX(I)
TMIX=TMIX/(ATMIX+SPH*OTMIX)
NTMN=1
RETURN
END

SUBROUTINE DISCO(TBP, TEMPC, NMIX)
COMMON/BLOCK2/ AQ(6), OR(6)
COMMON/BLOCK3/ CX(6), SX(6), DAD(6), CMA(6), CMO(6), SAT(6), SOT(6)
COMMON/ALL/ NTOP, NPROUT, NCOM, NMS, NMS1, NMS2, NQSEP, NQOP, ICNT
COMMON/TBP/ TLRCNO, CTBP, PCNTBP, TBPM(102)
COMMON/TIMES/ H, HHI, HLO, HPRINT, TAU, PRTIME, ZEIT, PZEIT, PRZEIT, PRNTME
F=CTBP
HAM=AQ(1)
UAM=AQ(2)
PAM=AQ(3)
P3M=AQ(4)
RAM=AQ(5)
SAM=AQ(6)
XAM=UAM+PAM
IF(XAM.LT.1.0E-10) XAM=3.14159
XAM=PAM/XAM
TNM=HAM+2.0*UAM+(4.0-2.0*XAM)*PAM+SAM+3.0*P3M+RAM
IF(TNM.LT.1.0E-10) TNM=1.0E-9
IF(TNM.GT.2.0E+01) TNM=2.0E+01
TEMPRK=1.0E3/(TEMPC+273.16)
DRT=TEMPRK-3.3539
UK=3.7*TNM**1.57+1.4*TNM**3.9+0.011*TNM**7.3
U4K=UK*(5.41E-02+6.58E-04*TNM**2)
TBPDEP=4.0*F**(0.17)-3.0
TEMDEP=EXP(-0.2*DRT)
UK=UK*TBPDEP
PK=UK*(0.20+0.55*F+1.25+0.0074*TNM**2)
HK1=0.135*TNM**0.62+0.0052*TNM**3.44
IF(F.LT.1.0) HK1=HK1*(1.0-0.54*EXP(-15.0*F))
UK=UK*EXP(2.5*DRT)
PK=PK*TEMDEP
HK1=HK1*EXP(0.34*DRT)
U4K=U4K*TEMDEP*TBPDEP
P3K=PK*1.138E-02
IF(TAU.EQ.0.0) U4K=0.0
HK2=HK1
IF(NMIX.EQ.0) GO TO 11
TF=TBP
GO TO 12
A = 2.0 * (UK * UAM + PK * PAM + HK2 * HAM + U4K * RAM) + 3.0 * P3K * P3M

B = HK1 * HAM + 1.0

C = -3.65145 * CTBP

TF = (-B + SQRT(B**2 - 4.0 * A * C)) / (2.0 * A)

DAD(4) = P3K * TF**3

DAD(5) = 0.0

IF (TAU .GT. 0.0) DAD(5) = U4K * TF**2

DAD(6) = 0.0

DAD(1) = HK1 * (TF + 1.0) * TF

DAD(2) = UK * TF**2

DAD(3) = PK * TF**2

TBP = TF

RETURN

END

SUBROUTINE CHECK(AAA, NCHECK)

COMMON/UT2/ TBASE, TRK, PCNT

IF (AAA .LT. 0.0) GO TO 10

GO TO 12

10 IF (ABS(AAA) .GT. TBASE) GO TO 11

AAA = 0.0

GO TO 12

11 TRK = TRK / 2.0

WRITE (3, 7000) TRK

7000 FORMAT (' ', 15X, 'TIME IN THE RUNGE-KUTTA INTEGRATION PROCEDURE ',
           'CHANGED TO ', E10.3, ' MINUTES')

NCHECK = 1

12 RETURN

END

FUNCTION PIXF(J, AQ)

COMMON/ALL/ NTOP, NPROUT, NCOM, NMS, NMS1, NMS2, NQSEP, NQOP, ICNT

COMMON/RATE/ NPX(6), NAX(6)

COMMON/TIMES/ H, HHI, HLO, HPRINT, TAU, PRTIME, ZEIT, PZEIT, PRZEIT, PRNTME

DIMENSION AQ(6)

IF (AQ(1) .GT. 1.0E-10) GO TO 10

PIXF = 1.0E-3

DPI = 0.0

GO TO 15

10 NRX = NPX(1)

PIXF = AQ(1)**NRX

IF (TAU .GT. 0.0) GO TO 13

IF (AQ(4) .GT. 1.0E-10) GO TO 11

PIXF = 1.0E-3

DPI = 0.0

GO TO 15

11 TNM = AQ(1) + 2.0 * AQ(2) + 4.0 * AQ(3) + AQ(6) * 0.33

NRX = NPX(6)

PIXF = PIXF * TNM**NRX

DO 12 K = 3, 5

QQQ = AQ(K)

NRX = NPX(K)

IF (NRX .EQ. 0) GO TO 12

12 CONTINUE

DAD(4) = P3K * TF**3

DAD(5) = 0.0

IF (TAU .GT. 0.0) DAD(5) = U4K * TF**2

DAD(6) = 0.0

DAD(1) = HK1 * (TF + 1.0) * TF

DAD(2) = UK * TF**2

DAD(3) = PK * TF**2

TBP = TF

RETURN

END
IF(QQQ.LT.0.0) PIXF=0.0
PIXF=PIXF*QQQ**NRX
CONTINUE
GO TO 15
DO 14 K=2,5
QQQ=AQ(K)
NRX=NFX(K)
IF(NRX.EQ.0) GO TO 14
IF(QQQ.LT.0.0) PIXF=0.0
PIXF=PIXF*QQQ**NRX
CONTINUE
14 RETURN
15 RETURN
END

SUBROUTINE GAUSIN(ISEED,STDDV1,STDDV2,XNORM1,XNORM2)
PI=3.141593
UNIF1=RANDU(ISEED)
UNIF2=RANDU(ISEED)
UNIF1=-2.0*ALOG(UNIF1)
UNIF2=2.0*UNIF2*PI
XNORM1=SQRT(UNIF1)*COS(UNIF2)
XNORM2=SQRT(UNIF1)*SIN(UNIF2)
XNORM1=XNORM1*STDDV1+1.0
XNORM2=XNORM2*STDDV2+1.0
RETURN
END

REAL FUNCTION RANDU(IY)
INTEGER IY
INTEGER IA, IC, ITWO, M2, M, MIC
DOUBLE PRECISION HALFM
REAL S
DOUBLE PRECISION DATAN, DSQRT
DATA M2/0.0/ ITWO/2.0 /
IF(M2.NE.0) GO TO 20
M=1
10 M2=M
ITWO=ITWO+M2
IF(M.GT.M2) GO TO 10
HALFM=M2
IA=8*IDINT(HALFM*DATAN(1.0D0)/8.0D0)+5
IC=2*IDINT(HALFM*(0.5DO-DSQRT(3.DO)/6.DO))+1
MIC=(M2-IC)+M2
S=0.5/HALFM
IY=IY*IA
IF(IY.GT.MIC) IY=(IY-M2)-M2
IY=IY+IC
IY=IY+ITWO
IF(IY.LT.0) IY=(IY+M2)+M2
RANDU=FLOAT(IY)*S
RETURN
END

SUBROUTINE HOLDUP
COMMON/BLOCK0/ AFLOPC(102),OFLOPC(102),AQPCFL(102),ORPCFL(102)
COMMON/ALL/ NTOP,NPROUT,NCOM,NMS,NMS1,NMS2,NQSEP,NQOP,ICNT
COMMON/PULSE/ ENDIAM,CLDIAM,PLSAMP,PLFREQ,PFLOW
COMMON/VOLS/ ASVOL(102),OSVOL(102),TSVOL(102),VAQOR(102)
ENDSEC=7.854E-01*ENDIAM**2*6.0E+01
CNTSEC=7.854E-01*CLDIAM**2*6.0E+01
AAA=2.0*PLSAMP*PLFREQ
DUDC=(AFLOPC(2)-OFLOPC(2))/ENDSEC
ASVOL(2)=VAQOR(2)*TSVOL(2)
OSVOL(2)=(1.0-VAQOR(2))*TSVOL(2)
DUDC=(AFLOPC(NMS1)-OFLOPC(NMS1))/ENDSEC
ASVOL(NMS1)=VAQOR(NMS1)*TSVOL(NMS1)
OSVOL(NMS1)=(1.0-VAQOR(NMS1))*TSVOL(NMS1)
DO J=3,NMS
DUDC=(AFLOPC(J)-OFLOPC(J))/CNTSEC
ASVOL(J)=VAQOR(J)*TSVOL(J)
OSVOL(J)=(1.0-VAQOR(J))*TSVOL(J)
CONTINUE
RETURN
END
B. Organization and Subroutine Structure of CUSEP

The organization in CUSEP is diagramed in Scheme I below. The computational sequence cycles through the Runge-Kutta and output sections of program MAIN. The MAIN program and the various subroutines are discussed below in the order that they appear in the printout of CUSEP. The details of how data is input into CUSEP is given in Appendix D, section C.

**SCHEME I**

**MAIN:** There are two computational schemes available in CUSEP, one an equilibrium calculation, the other allowing deviations from mass transfer equilibrium. The user controls the method that is to be used by the parameter NQSEP. If NQSEP is 0, an equilibrium calculation results; if NQSEP is 1, deviations from mass transfer equilibrium are assumed, mass transfer areas and coefficients must then be input. Program MAIN controls the reading of all input data, then sets up the flow rates of the two phases through the contactor, calculates the concentrations as a function of time, and directs the printout of the profiles. Throughout CUSEP, the six components of interest are assigned the following locations in all pertinent vectors and matrices in both aqueous and organic phases;
First element: $H^+$
Second element: $UO_2^{2+}$
Third element: $Pu^{4+}$
Fourth element: $Pu^{3+}$
Fifth element: $U^{4+}$ or HAN
Sixth element: $NO_3^-$

All concentrations are read into CUSEP in units of grams per liter, except for the $H^+$ concentration, which is in units of molarity. The nitrate ion concentration, as read in by CUSEP, represents the total for all the inextractable salts. If there are no inextractable salts, the nitrate ion concentration should be input as zero.

READVL: This subroutine reads in the height of a typical mass transfer unit (MTU) and the volume fraction for the aqueous phase. At the present, this must be estimated from holdup data. The input is in the form $(I, J, H, F_a)$ where MTU's $I$ through $J$ have a height $H$ (units of cm) and the aqueous volume fraction is $F_a$. For example, the input $(1,10,5.0,0.1)$ means that MTU's 1 through 10 have a height of 5.0 cm and the aqueous volume fraction is 0.1 or 10% of the total volume in these MTU's. READVL will continue reading data until the value of $J$ above equals the total number of MTU's (input by the variable NMS) in the column. The format for the input is $(2I3, 4X, 2F10.0)$.

FEEDST: This subroutine reads in all feed stream information. Only one feed stream of each phase can enter any one MTU in the column. The form of the input is $(J, JPHASE, FLOW, CON1, \ldots, CON6, TEMPF, INDEX)$, where $J$ is the MTU where the feed stream enters, JPHASE defines the stream phase as organic ($JPHASE = 0$) or
aqueous (JPHASE=1), FLOW is the flow rate in L/min, CON1 through CON6 are the concentrations of the six components in the feed in g/L, TEMPF is the feed temperature in degrees Fahrenheit and INDEX is a control parameter: if INDEX=1, more feed stream data is to be read in; if INDEX=0, the subroutine is terminated. The format for the input is (I3,I1,8F8.0,I1).

FLOWS: This subroutine generates the flow patterns for the aqueous and organic phases through the column. It then prints out in tabular form the volumes and flow rates of the aqueous and organic phases in each MTU.

MOLVOL: This subroutine interconverts molal and molar units for flows and concentrations.

PRINTS: This subroutine prints a table of the profile of the column, showing concentrations, flows, densities, temperatures, and inventories. The frequency of this printing is controlled by the user with the control parameter HPRINT. The table also shows the total elapsed time.

TMIX: This function accounts for the instantaneous heat transfer between phases as they mix in each MTU.

DISCO: This subroutine calculates, for a given set of concentrations in the two phases of a MTU, the free TBP concentration when needed and the equilibrium distribution coefficients as functions of these concentrations.

CHECK: This subroutine insures that negative concentrations are not generated by the Runge-Kutta integration procedure. Depending on the magnitude of a negative concentration, CHECK either clips the value at zero or halves the integration time increment, printing a statement of its new value.

PIXF: This function calculates the rate of reduction of Pu$^{4+}$ by either U$^{4+}$ or HAN.

GAUSIN: As an option to the user, this subroutine randomly fluctuates the feed stream concentrations about their input concentrations as a mean value. The fluctuated values are constrained to form a normal error distribution about the mean value with a standard deviation that is set by the user.
RANDU: This subroutine generates the random numbers that are needed by subroutine GAUSIN.

HOLDUP: This subroutine calculates the volume of the typical MTU and distributes it according to the input holdup percentages.

BUILT-IN FUNCTIONS: CUSEP uses the following built-in functions:

ABS, ALOG, COS, DATAN, DSQRT, EXP, FTIME, SIN, IDINT, SQRT.

C. The Arrangement and Format of Input to CUSEP

On the next pages are listed the different types of data records, their contents and their format, that are needed as input for CUSEP. CUSEP reads in the information using the Fortran file FT001F001 (IBM computers) or FOR001 (DEC VAX COMPUTERS). If a record is optional, then the option parameter and its value needed to call the record are shown parenthetically after the record number. The subroutine which reads the record is shown under the card number. The variables and the column numbers from which they are read are shown with the allowed range of values in parenthesis. The equivalence sign indicates that the variable to its left is assigned to those variables to its right. Any special instructions for a card are given after the last variable listed. Appendix D, section D contains a glossary of major variables and input parameters in CUSEP listed in alphabetical order.
<table>
<thead>
<tr>
<th>CARD NO.</th>
<th>COLUMNS</th>
<th>FORMAT, VARIABLE, ASSIGNMENT (RANGE)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>MAIN</td>
<td>Format(6E10.3)</td>
</tr>
<tr>
<td></td>
<td>1-10</td>
<td>H</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>HHI</td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>HPRINT</td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>TBASE</td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>TAU</td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>TEMPD</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(TAU≥0.0)</td>
</tr>
<tr>
<td>2</td>
<td>MAIN</td>
<td>Format(3I4)</td>
</tr>
<tr>
<td></td>
<td>1-4</td>
<td>NMS</td>
</tr>
<tr>
<td></td>
<td>5-8</td>
<td>NTITLE</td>
</tr>
<tr>
<td></td>
<td>9-12</td>
<td>NQSEP</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1≤NMS≤100)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1≤NTITLE≤10)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(0 or 1)</td>
</tr>
<tr>
<td>3</td>
<td>MAIN</td>
<td>Format(10A8)</td>
</tr>
<tr>
<td></td>
<td>1-80</td>
<td>TITLE(NTITLE,10)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(as many cards as the value of NTITLE, no more than 10)</td>
</tr>
<tr>
<td>4 (NQSEP=1)</td>
<td>MAIN</td>
<td>Format(2I3, 4X, F8.0)</td>
</tr>
<tr>
<td></td>
<td>1-3</td>
<td>I</td>
</tr>
<tr>
<td></td>
<td>4-6</td>
<td>J</td>
</tr>
<tr>
<td></td>
<td>11-18</td>
<td>QQQ = AREA(I) to AREA(J)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1≤I, J≤NMS)</td>
</tr>
<tr>
<td>CARD NO.</td>
<td>COLUMNS</td>
<td>FORMAT, VARIABLE, ASSIGNMENT (RANGE)</td>
</tr>
<tr>
<td>---------</td>
<td>---------</td>
<td>-------------------------------------</td>
</tr>
<tr>
<td>5 (NQSEP=1)</td>
<td>Format(2I3, 4X, 6E10.3)</td>
<td></td>
</tr>
<tr>
<td>MAIN</td>
<td>1-3</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>4-6</td>
<td>J ( (1 \leq i, j \leq \text{NMS}) )</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>( \text{CON}(1) = \text{TRANSCO}(1,i) ) to ( \text{TRANSCO}(1,j) )</td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>. .</td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>. .</td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>. .</td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>. .</td>
</tr>
<tr>
<td></td>
<td>61-70</td>
<td>( \text{CON}(6) = \text{TRANSCO}(6,i) ) to ( \text{TRANSCO}(6,j) )</td>
</tr>
<tr>
<td>(repeat until ( j = \text{NMS} ))</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| 6 | Format(4F10.0) |
| MAIN | 1-10 | PCNTBP \( (0 \leq \text{PCNTBP} \leq 100) \) |
| | 11-20 | TLRNCE \( (0 \leq \text{TLRNCE} \leq 100) \) |
| | 21-30 | STDDV1 \( (0 \leq \text{STDDV1} \leq 100) \) |
| | 31-40 | STDDV2 \( (0 \leq \text{STDDV2} \leq 100) \) |

| 7 | Format(4F10.0) |
| MAIN | 1-10 | PLSAMP |
| | 11-20 | PLFREQ |
| | 21-30 | CLDIAM |
| | 31-40 | ENDIAM |

113
<table>
<thead>
<tr>
<th>CARD NO.</th>
<th>COLUMNS</th>
<th>FORMAT, VARIABLE, ASSIGNMENT (RANGE)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1-3</td>
<td>Format(2I3, 4X, 2F10.0)</td>
</tr>
<tr>
<td></td>
<td>4-6</td>
<td>I</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>J</td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>QQQ = HGT(I) to HGT(J)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>AAA = VAQOR(I) to VAQOR(J)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(repeat until J=NMS)</td>
</tr>
</tbody>
</table>

| 9       | 1-3     | Format(I3, I1, 8F8.0, I1)            |
|         | 4       | J                                    |
|         | 5-12    | JPHASE                               |
|         | 13-20   | FLOW = OFLEX(J) or AFLEX(J)          |
|         | 21-28   | CON(1) = XOFX(1,J) or XAFX(1,J)      |
|         | 29-36   | .                                    |
|         | 37-44   | .                                    |
|         | 45-52   | .                                    |
|         | 53-60   | CON(6) = XOFX(6,J) or XAFX(6,J)      |
|         | 61-68   | TEMPF = TOFX(J) or TAFX(J)           |
|         | 69      | INDEX                                |
|         |         | (repeat if INDEX=1)                  |

114
D. Glossary of Major Variables and Input Parameters

This glossary lists alphabetically the major variables and input parameters that are used in CUSEP. If a variable for an organic quantity differs in name from that for an aqueous one only by the replacement of the letter A by O, it is not included in the list as a separate entry, but is shown in square brackets after the aqueous variable description. The dimensions of vectors and matrices are listed after the variable name. Where necessary, the specific units that must be assigned to a variable are also shown.

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFLEX(102)</td>
<td>The aqueous feed stream flow rates in L/min. [OFLEX(102)]</td>
</tr>
<tr>
<td>AFLOPC(102)</td>
<td>The unpulsed aqueous flow in the column. [OFLOPC(102)]</td>
</tr>
<tr>
<td>AQ(6)</td>
<td>The aqueous concentrations of the six components, usually in a specific MTU. [OR(6)]</td>
</tr>
<tr>
<td>AQPCFL(102)</td>
<td>The aqueous flow in the column including the contribution of the pulse to the flow. [ORPCFL(102)]</td>
</tr>
<tr>
<td>AREA(102)</td>
<td>The mass transfer area in a MTU in square decimeters.</td>
</tr>
<tr>
<td>ASVOL(102)</td>
<td>The volume of the aqueous phase in a MTU. [OSVOL(102)]</td>
</tr>
<tr>
<td>ATS(102)</td>
<td>The temperature of the aqueous phase in a MTU. [OTS(102)]</td>
</tr>
<tr>
<td>CLDIAM</td>
<td>The internal diameter of the working section of the column in cm.</td>
</tr>
<tr>
<td>CX(6)</td>
<td>The stoichiometric changes in the concentrations of the components due to the reduction of Pu(IV) by either U(IV) or HAN.</td>
</tr>
<tr>
<td>DAD(6)</td>
<td>The vector of the distribution coefficients of the components in the system.</td>
</tr>
<tr>
<td>ENDIAM</td>
<td>The diameter of the end sections of the column in cm. Both the top and bottom of the column are assumed to have the same diameter.</td>
</tr>
<tr>
<td>GMW(6)</td>
<td>The gram molecular weights of the components in the system.</td>
</tr>
<tr>
<td>H</td>
<td>The time increment in minutes to be used in the Runge-Kutta integration. The value of H may be changed during one step of a calculation, but</td>
</tr>
</tbody>
</table>
reverts back to the input value at the end of that step. The new value is printed each time that a change occurs. H usually is in the range 0.001 to 0.01 minutes.

HGT(102)  The height of a MTU or an end section in cm.

HHI     The time in minutes at which the calculation is to stop. If the pulse frequency is low, a steady-state solution to the equations may result and the calculation automatically stops at that point, regardless of the value of HHI.

HPRINT  The time in minutes between printings of the concentration profiles and other system information.

JPHASE  The phase of a feed stream. JPHASE must be input as zero for an organic feed stream, or as one for an aqueous one.

NAX(6)  The vector for the exponents of the concentrations of each species in the rate law for the auto-oxidation of U(IV) to U(VI) in a partitioning contactor.

NCOM    The highest numbered component with a non-zero concentration.

NMS     The number of MTU in the column. NMS may range from 1 to 100.

NPX(6)  The vector for the exponents of the concentrations of each species in the rate law for the reduction of Pu(IV) to Pu(III) by either U(IV) or HAN.

NQSEP   The computational option being used in a calculation. If NQSEP=0, mass transfer equilibrium is assumed throughout the column; if NQSEP=1, deviations from mass transfer equilibrium are assumed, and mass transfer areas and coefficients must be included in the input.

NTITLE  The number of title cards to be read and subsequently printed as the introduction to the output. The number must not exceed 10.

PCNTBP  The TBP concentration in volume percent.

PFLOW   The instantaneous value of the flow due to the effect of the pulse.

PHIA(6,102)  The matrix of changes in the aqueous concentrations as calculated by
fourth order Runge-Kutta integration.  

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLFREQ</td>
<td>The linear pulse frequency in cycles per minute (cpm).</td>
</tr>
<tr>
<td>PLSAMP</td>
<td>The linear pulse amplitude in cm.</td>
</tr>
<tr>
<td>QA(6,102)</td>
<td>The matrix of the successive corrections to the aqueous phase concentrations during Runge-Kutta integration.</td>
</tr>
<tr>
<td>SPH</td>
<td>The specific heat of the organic phase.</td>
</tr>
<tr>
<td>STDDV1</td>
<td>The standard deviation of the normal error distribution of the fluctuated aqueous phase feed stream concentrations about the input value as a mean. The deviation is input as a percentage.</td>
</tr>
<tr>
<td>STDDV2</td>
<td>The standard deviation of the normal error distribution of the fluctuated organic phase feed stream concentrations about the input value as a mean. The deviation is input as a percentage.</td>
</tr>
<tr>
<td>SX(6)</td>
<td>The stoichiometric changes in the concentrations of the species due to auto-oxidation of U(IV) to U(VI).</td>
</tr>
<tr>
<td>TAU</td>
<td>The value of the rate constant in reciprocal minutes for the auto-oxidation of U(IV) to U(VI). The rate is assumed to be first order in the concentration of U(IV). If HAN is the reductant in a partitioning column, TAU must be set equal to zero, otherwise CUSEP will assume that U(IV) is the reductant.</td>
</tr>
<tr>
<td>TBASE</td>
<td>This sets the permissible level of clipping in the Runge-Kutta integration. Negative concentrations smaller than TBASE are set equal to zero, and the calculation is allowed to continue without changing the value of H.</td>
</tr>
<tr>
<td>TEMPD</td>
<td>The default temperature of the system in degrees Fahrenheit. If a feed stream temperature differs from TEMPD, function TMIX will take account of temperature gradients in the column.</td>
</tr>
<tr>
<td>TLRNCE</td>
<td>This parameter sets the tolerance for the test of convergence to steady state after each Runge-Kutta integration step. It is input as a percentage,</td>
</tr>
</tbody>
</table>
typically 0.1%.

**TRNSCO(6,102)** The matrix of mass transfer coefficients for the components in the column MTU's in units of decimeters/min. The product of this variable with the AREA variable gives the interphase mass transfer rate in L/min.

**TSVOL(102)** The total volume of a MTU.

**VAQOR(102)** The fraction of the total volume of a MTU that is aqueous.

**XAFX(6,102)** The concentrations of components in the aqueous feed streams. Element 1 must be in molarity units, the others in units of g/L.  

**XASJ(6,102)** The concentrations of the components in the aqueous phase of the column.
APPENDIX E

Databases for Model Development

Tables E1 to E3 contain databases for the development of the steady state inventory models. Tables E4 to E6 contain flow sheet conditions used to generate databases for the nonsteady state inventory model. The steady state inventories corresponding to the flow sheet conditions and the standard deviations calculated from least squares deviations of the model predictions from the database are also given in Tables E4 to E6. The standard deviations are calculated as a fraction of the steady state inventory.
<table>
<thead>
<tr>
<th>U (g/L)</th>
<th>PU (g/L)</th>
<th>ACID (H)</th>
<th>T (C)</th>
<th>NO. STAGE</th>
<th>SCRUB STAGES</th>
<th>T/RATIO TO ORG FLOW RATE</th>
<th>FEED TO ORG FLOW RATE RATIO</th>
<th>A/D PHASE RATIO</th>
<th>T/RATIO</th>
<th>U INV</th>
<th>U FRACT</th>
<th>PU INV</th>
<th>PU FRACT</th>
<th>DEVI</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.294</td>
<td>0.300</td>
<td>0.000</td>
<td>0.000</td>
<td>5.4200E+04</td>
<td>-9.0228</td>
<td>5.3900E+02</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6800E+04</td>
<td>-0.0234</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>1.0300E+05</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6100E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
<tr>
<td>0.00</td>
<td>285.00</td>
<td>2.66</td>
<td>2.94</td>
<td>25.0</td>
<td>0</td>
<td>100.0</td>
<td>0.300</td>
<td>0.196</td>
<td>0.300</td>
<td>0.190</td>
<td>0.000</td>
<td>0.000</td>
<td>9.6000E+04</td>
<td>-0.0231</td>
</tr>
</tbody>
</table>

**Table E1**

Flowsheet Data on a Type Aqueous to Organic Extraction Contactors Used to Generate a Data Base with PUBG. The resultant PUBG Inventories and Fractional Deviations of Model Calculations from PUBG Inventories are also given.
| U (g/L) | PU (g/L) | ACID (H) | T (C) | NO. STAGE | SCRUB STAGES | SCRUB | TO ORG VOL | SCRUB TO ORG FLOW RATE | A/O FLOW RATE | A/O | TBP | U INV | U FRACT | PU INV | PU FRACT |
|--------|---------|----------|------|-----------|--------------|-------|-------------|------------------------|----------------|-----|-----|-------|--------|--------|--------|----------|
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.200 | 0.1300     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.290 | 0.2194     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.320 | 0.2594     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.390 | 0.3454     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.500 | 0.4000     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.619 | 0.4700     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.619 | 0.4700     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.619 | 0.4700     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.619 | 0.4700     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.619 | 0.4700     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.619 | 0.4700     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.619 | 0.4700     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.619 | 0.4700     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |
| 285.00 | 2.46    | 1.06     | 25.0 | 8         | 150.0        | 0.619 | 0.4700     | 0.190                   | 0.35           | 1.10E+05 | -0.0462 | 1.41E+05 | -0.0913 |

**RESULTS OF LEAST SQUARES**

**ORDER OF CALC = 2**

<table>
<thead>
<tr>
<th>U CONS</th>
<th>PU CONS</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.0971</td>
<td>-0.0730</td>
</tr>
</tbody>
</table>

**REL. STD. DEV. FOR U = 0.0418**

**REL. STD. DEV. FOR PU = 0.0412**
### Table E2

<table>
<thead>
<tr>
<th>Stage Type</th>
<th>Flow Rate (G/L)</th>
<th>U (G/L)</th>
<th>PU</th>
<th>H (+)</th>
<th>U farmer (G/L)</th>
<th>AVG Temp</th>
<th>A/O</th>
<th>U Conc. (C)</th>
<th>PHASE</th>
<th>INV. FRACT.</th>
<th>INV. FRACT.</th>
<th>INV. FRACT.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>8.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>76.082</td>
<td>35.000</td>
<td>0.530</td>
<td>1.2675E+05</td>
<td>0.0104</td>
<td>2.5275E+05</td>
<td>0.0416</td>
</tr>
<tr>
<td>2</td>
<td>8.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>76.082</td>
<td>35.000</td>
<td>0.660</td>
<td>1.2227E+05</td>
<td>0.0557</td>
<td>5.9089E+05</td>
<td>0.0241</td>
</tr>
<tr>
<td>3</td>
<td>8.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>76.082</td>
<td>35.000</td>
<td>0.990</td>
<td>1.2068E+05</td>
<td>0.1013</td>
<td>4.8522E+05</td>
<td>0.0179</td>
</tr>
<tr>
<td>4</td>
<td>8.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>37.059</td>
<td>35.000</td>
<td>0.530</td>
<td>6.0638E+04</td>
<td>0.1243</td>
<td>2.4816E+05</td>
<td>0.0239</td>
</tr>
<tr>
<td>5</td>
<td>8.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>37.059</td>
<td>35.000</td>
<td>0.660</td>
<td>5.6705E+04</td>
<td>0.1291</td>
<td>5.0829E+05</td>
<td>0.0175</td>
</tr>
<tr>
<td>6</td>
<td>8.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>37.059</td>
<td>35.000</td>
<td>0.990</td>
<td>5.4073E+04</td>
<td>0.1327</td>
<td>4.6196E+05</td>
<td>0.0155</td>
</tr>
<tr>
<td>7</td>
<td>8.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>66.050</td>
<td>35.000</td>
<td>0.330</td>
<td>1.0004E+05</td>
<td>-0.0260</td>
<td>2.5174E+05</td>
<td>0.0370</td>
</tr>
<tr>
<td>8</td>
<td>8.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>66.050</td>
<td>35.000</td>
<td>0.660</td>
<td>9.6150E+04</td>
<td>-0.0058</td>
<td>3.2960E+05</td>
<td>0.0233</td>
</tr>
<tr>
<td>STAGE</td>
<td>TYPE</td>
<td>FLOW RATE (g/L)</td>
<td>U (g/L)</td>
<td>PU</td>
<td>HI (L)</td>
<td>UI (g/L)</td>
<td>PHASE</td>
<td>INV.</td>
<td>U CONC. (C)</td>
<td>A/O RATIO</td>
<td>U FRACT.</td>
<td>INV.</td>
</tr>
<tr>
<td>-------</td>
<td>------</td>
<td>----------------</td>
<td>--------</td>
<td>----</td>
<td>-------</td>
<td>--------</td>
<td>-------</td>
<td>-----</td>
<td>-------------</td>
<td>-----------</td>
<td>----------</td>
<td>-----</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1.480</td>
<td>34.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>10</td>
<td>60.200</td>
<td>76.600</td>
<td>0.710</td>
<td>0.077</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>1</td>
<td>1.480</td>
<td>34.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>1</td>
<td>1.480</td>
<td>34.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>1</td>
<td>0.400</td>
<td>34.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>60.200</td>
<td>76.600</td>
<td>0.710</td>
<td>0.077</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>19.400</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**TABLE E2.** (CONTINUED FROM PREVIOUS PAGE)
<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>FLOW RATE (g/L)</th>
<th>U (g/L)</th>
<th>H+ (L/L)</th>
<th>U IV (L/L)</th>
<th>AVD TEMP (°C)</th>
<th>A/D PHASE RATIO</th>
<th>AVD U INV (GRAMS)</th>
<th>AVD U FRACT. INV (GRAMS)</th>
<th>AVD PU INV (GRAMS)</th>
<th>AVD PU FRACT. INV (GRAMS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>0.610 0.000 0.000 0.200 0.000</td>
<td>62.850 35.000 0.660 8.33582E+04 -0.0648 4.5468E+03 0.0254</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>1</td>
<td>0.610 0.000 0.000 0.200 0.000</td>
<td>62.850 35.000 0.990 7.8921E+04 -0.0647 5.7776E+03 0.0205</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>10</td>
<td>0.610 0.000 0.000 0.200 0.000</td>
<td>62.850 35.000 0.530 9.0263E+04 -0.0186 4.7606E+03 0.0368</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>10</td>
<td>0.610 0.000 0.000 0.200 0.000</td>
<td>62.850 35.000 0.660 8.35587E+04 -0.0276 7.6407E+03 0.0384</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>1</td>
<td>0.610 0.000 0.000 0.200 0.000</td>
<td>62.850 35.000 0.990 7.90873E+04 -0.0344 9.2368E+03 0.0390</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>10</td>
<td>0.610 0.000 0.000 0.200 0.000</td>
<td>62.850 35.000 0.530 9.3615E+04 0.0004 7.2049E+03 0.0129</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>10</td>
<td>0.610 0.000 0.000 0.200 0.000</td>
<td>62.850 35.000 0.660 8.64058E+04 0.0042 1.1321E+04 0.0255</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>10</td>
<td>0.610 0.000 0.000 0.200 0.000</td>
<td>62.850 35.000 0.990 8.15682E+04 0.0046 1.3942E+04 0.0298</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>STAGE</td>
<td>TYPE</td>
<td>FLOW (G/L)</td>
<td>U (G/L)</td>
<td>PU INV. (%)</td>
<td>UM (G/L)</td>
<td>A/D PHASE</td>
<td>U CONC. (G/L)</td>
<td>TEMP (°C)</td>
<td>A/D PHASE</td>
<td>U CONC. (GRAMS)</td>
<td>FRACT. INV. (GRAMS)</td>
</tr>
<tr>
<td>-------</td>
<td>------</td>
<td>------------</td>
<td>---------</td>
<td>-------------</td>
<td>---------</td>
<td>-----------</td>
<td>----------</td>
<td>-----------</td>
<td>-----------</td>
<td>----------------</td>
<td>------------------</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>20.100</td>
<td>0.000</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>10.000</td>
<td>5.000</td>
<td>0.000</td>
<td>10.000</td>
<td>5.000</td>
<td>10.000</td>
<td>5.000</td>
<td>0.000</td>
<td>10.000</td>
<td>5.000</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>20.100</td>
<td>0.000</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>10.000</td>
<td>5.000</td>
<td>0.000</td>
<td>10.000</td>
<td>5.000</td>
<td>10.000</td>
<td>5.000</td>
<td>0.000</td>
<td>10.000</td>
<td>5.000</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>20.100</td>
<td>0.000</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>10.000</td>
<td>5.000</td>
<td>0.000</td>
<td>10.000</td>
<td>5.000</td>
<td>10.000</td>
<td>5.000</td>
<td>0.000</td>
<td>10.000</td>
<td>5.000</td>
</tr>
<tr>
<td>7</td>
<td>7</td>
<td>20.100</td>
<td>0.000</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
</tr>
<tr>
<td>8</td>
<td>8</td>
<td>10.000</td>
<td>5.000</td>
<td>0.000</td>
<td>10.000</td>
<td>5.000</td>
<td>10.000</td>
<td>5.000</td>
<td>0.000</td>
<td>10.000</td>
<td>5.000</td>
</tr>
<tr>
<td>9</td>
<td>9</td>
<td>20.100</td>
<td>0.000</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
<td>0.000</td>
<td>20.100</td>
<td>0.000</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>10.000</td>
<td>5.000</td>
<td>0.000</td>
<td>10.000</td>
<td>5.000</td>
<td>10.000</td>
<td>5.000</td>
<td>0.000</td>
<td>10.000</td>
<td>5.000</td>
</tr>
</tbody>
</table>

**TABLE E2. (CONTINUED FROM PREVIOUS PAGE)**
### TABLE E2. (CONTINUED FROM PREVIOUS PAGE)

#### FEED STREAM DATA

<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>FLOW RATE</th>
<th>U CONC. (g/L)</th>
<th>PU</th>
<th>H+</th>
<th>U IV</th>
<th>AVG TEMP</th>
<th>A/O</th>
<th>U PHASE INV</th>
<th>FRACT. INV</th>
<th>FRACT. DEVI</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(g/L)</td>
<td>(g/L)</td>
<td>(g/L)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>76.00E- 2</td>
<td>35.000</td>
<td>0.990</td>
<td>1.195054+05</td>
<td>0.085E+03</td>
</tr>
<tr>
<td>10</td>
<td>1</td>
<td>1.680</td>
<td>34.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>71.772</td>
<td>35.000</td>
<td>0.330</td>
<td>1.24055E+05</td>
<td>0.051E+03</td>
</tr>
<tr>
<td>20</td>
<td>1</td>
<td>1.680</td>
<td>34.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>71.772</td>
<td>35.000</td>
<td>0.660</td>
<td>1.21635E+05</td>
<td>0.090E+03</td>
</tr>
<tr>
<td>18</td>
<td>1</td>
<td>1.680</td>
<td>34.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>71.772</td>
<td>35.000</td>
<td>0.990</td>
<td>1.19813E+05</td>
<td>0.130E+03</td>
</tr>
<tr>
<td>35</td>
<td>1</td>
<td>1.680</td>
<td>34.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>68.793</td>
<td>35.000</td>
<td>0.330</td>
<td>8.22554E+04</td>
<td>-0.080E+03</td>
</tr>
<tr>
<td>36</td>
<td>1</td>
<td>1.680</td>
<td>34.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>58.793</td>
<td>35.000</td>
<td>0.660</td>
<td>7.57646E+04</td>
<td>-0.090E+03</td>
</tr>
<tr>
<td>37</td>
<td>1</td>
<td>1.680</td>
<td>34.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>58.793</td>
<td>35.000</td>
<td>0.990</td>
<td>7.14266E+04</td>
<td>-0.111E+03</td>
</tr>
<tr>
<td>38</td>
<td>1</td>
<td>1.680</td>
<td>34.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>62.444</td>
<td>35.000</td>
<td>0.330</td>
<td>9.96738E+04</td>
<td>-0.042E+03</td>
</tr>
</tbody>
</table>

#### OTHER DATA, INVENTORIES, AND DEVI. FROM MODEL CALC.

<table>
<thead>
<tr>
<th></th>
<th>AVG</th>
<th>U CONC.</th>
<th>PHI</th>
<th>PHASE</th>
<th>INV.</th>
<th>FRACT.</th>
<th>INV.</th>
<th>FRACT.</th>
<th>DEVI.</th>
<th>(GRAMS)</th>
<th>(GRAMS)</th>
<th>(DEVI.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>STAGE</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>1</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>1</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

Note: The table continues with more data points, showing various stages, flow rates, and concentrations, along with other model calculations and inventories.
<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>FLOW RATE</th>
<th>U (g/L)</th>
<th>PU (g/L)</th>
<th>HI (g/L)</th>
<th>UIV (g/L)</th>
<th>AVG U CONC.</th>
<th>TEMPERATURE</th>
<th>A/O</th>
<th>PHASE</th>
<th>INV.</th>
<th>FRACT.</th>
<th>INV.</th>
<th>FRACT.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(C)</td>
<td>(GRAMS)</td>
<td></td>
<td>(GRAMS)</td>
<td></td>
<td></td>
<td>(GRAMS)</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>62.444</td>
<td>35.000</td>
<td>0.660</td>
<td>0.0080</td>
<td>2.91716E+03</td>
<td>0.0258</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>60.200</td>
<td>76.600</td>
<td>0.710</td>
<td>0.077</td>
<td>0.000</td>
<td>62.444</td>
<td>35.000</td>
<td>0.990</td>
<td>0.0216</td>
<td>3.61419E+03</td>
<td>0.0108</td>
<td></td>
<td></td>
</tr>
<tr>
<td>41</td>
<td>1</td>
<td>0.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>63.001</td>
<td>35.000</td>
<td>0.330</td>
<td>0.0665</td>
<td>2.52147E+03</td>
<td>0.0369</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>60.200</td>
<td>76.600</td>
<td>0.710</td>
<td>0.077</td>
<td>0.000</td>
<td>63.001</td>
<td>35.000</td>
<td>0.660</td>
<td>0.0677</td>
<td>3.90495E+03</td>
<td>0.0231</td>
<td></td>
<td></td>
</tr>
<tr>
<td>42</td>
<td>1</td>
<td>0.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>63.001</td>
<td>35.000</td>
<td>0.990</td>
<td>0.0686</td>
<td>4.83395E+03</td>
<td>0.0183</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>60.200</td>
<td>76.600</td>
<td>0.710</td>
<td>0.077</td>
<td>0.000</td>
<td>63.001</td>
<td>35.000</td>
<td>0.330</td>
<td>0.0586</td>
<td>2.51648E+03</td>
<td>0.0374</td>
<td></td>
<td></td>
</tr>
<tr>
<td>43</td>
<td>1</td>
<td>0.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>66.207</td>
<td>35.000</td>
<td>0.660</td>
<td>0.0256</td>
<td>3.90557E+03</td>
<td>0.0232</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>60.200</td>
<td>76.600</td>
<td>0.710</td>
<td>0.077</td>
<td>0.000</td>
<td>66.207</td>
<td>35.000</td>
<td>0.990</td>
<td>0.0126</td>
<td>4.85595E+03</td>
<td>0.0183</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### TABLE 2. (CONTINUED FROM PREVIOUS PAGE)

<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>FLOW RATE</th>
<th>U (g/L)</th>
<th>PU (g/L)</th>
<th>H+ (g/L)</th>
<th>U+IV (g/L)</th>
<th>AVG CONC. (g/L)</th>
<th>TEMP (°C)</th>
<th>A/V</th>
<th>PHASE RATIO</th>
<th>INV. (GRAMS)</th>
<th>U FRACT. INV. (GRAMS)</th>
<th>PU FRACT. INV. (GRAMS)</th>
<th>FRACT. DEV.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.400</td>
<td>0.000</td>
<td>0.610</td>
<td>35.000</td>
<td>0.330</td>
<td>9.6147E+04</td>
<td>0.000</td>
<td>2.5321E+03</td>
<td>0.000</td>
<td>0.0546</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>1.400</td>
<td>94.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>1.400</td>
<td>35.000</td>
<td>0.660</td>
<td>9.0091E+04</td>
<td>0.000</td>
<td>3.9288E+03</td>
<td>0.000</td>
<td>0.0233</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>1.400</td>
<td>94.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>1.400</td>
<td>35.000</td>
<td>0.990</td>
<td>8.6043E+04</td>
<td>0.000</td>
<td>4.0623E+03</td>
<td>0.000</td>
<td>0.0194</td>
</tr>
<tr>
<td>20</td>
<td>2</td>
<td>19.400</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>19.400</td>
<td>35.000</td>
<td>0.330</td>
<td>1.0001E+05</td>
<td>0.000</td>
<td>2.4944E+03</td>
<td>0.000</td>
<td>0.0332</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>1.400</td>
<td>94.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>1.400</td>
<td>35.000</td>
<td>0.660</td>
<td>9.5510E+04</td>
<td>0.000</td>
<td>3.8013E+03</td>
<td>0.000</td>
<td>0.0199</td>
</tr>
<tr>
<td>20</td>
<td>2</td>
<td>19.400</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>19.400</td>
<td>35.000</td>
<td>0.990</td>
<td>8.6043E+04</td>
<td>0.000</td>
<td>4.0623E+03</td>
<td>0.000</td>
<td>0.0194</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>1.400</td>
<td>94.230</td>
<td>0.000</td>
<td>0.930</td>
<td>208.500</td>
<td>1.400</td>
<td>35.000</td>
<td>0.330</td>
<td>9.5438E+04</td>
<td>0.000</td>
<td>3.9483E+03</td>
<td>0.000</td>
<td>0.0289</td>
</tr>
<tr>
<td>STAGE</td>
<td>TYPE</td>
<td>FLOW RATE</td>
<td>U</td>
<td>PU</td>
<td>H(+1)</td>
<td>UTIL</td>
<td>AVG U CONC.</td>
<td>TEMP</td>
<td>A/O</td>
<td>PHASE</td>
<td>INV</td>
<td>FRACT.</td>
<td>INV</td>
<td>FRACT.</td>
</tr>
<tr>
<td>-------</td>
<td>------</td>
<td>------------</td>
<td>---</td>
<td>----</td>
<td>-------</td>
<td>------</td>
<td>-------------</td>
<td>------</td>
<td>-----</td>
<td>--------</td>
<td>-----</td>
<td>--------</td>
<td>-----</td>
<td>--------</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0.610</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>65.287</td>
<td>35.000</td>
<td>0.990</td>
<td>8.8519E+04</td>
<td>-0.0767</td>
<td>4.8793E+03</td>
<td>0.0294</td>
<td></td>
</tr>
<tr>
<td>57</td>
<td>10</td>
<td>1.400</td>
<td>34.230</td>
<td>0.000</td>
<td>1.930</td>
<td>209.600</td>
<td>65.287</td>
<td>35.000</td>
<td>0.150</td>
<td>9.3162E+04</td>
<td>-0.0113</td>
<td>2.565E+03</td>
<td>0.0295</td>
<td></td>
</tr>
<tr>
<td>58</td>
<td>10</td>
<td>1.400</td>
<td>34.230</td>
<td>0.000</td>
<td>1.930</td>
<td>209.600</td>
<td>65.287</td>
<td>35.000</td>
<td>0.660</td>
<td>8.5096E+04</td>
<td>-0.0259</td>
<td>3.9760E+03</td>
<td>0.0259</td>
<td></td>
</tr>
<tr>
<td>59</td>
<td>10</td>
<td>1.400</td>
<td>34.230</td>
<td>0.000</td>
<td>1.930</td>
<td>209.600</td>
<td>65.287</td>
<td>35.000</td>
<td>0.990</td>
<td>8.1039E+04</td>
<td>-0.0372</td>
<td>4.9201E+03</td>
<td>0.0220</td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>10</td>
<td>1.400</td>
<td>34.230</td>
<td>0.000</td>
<td>1.930</td>
<td>209.600</td>
<td>65.287</td>
<td>35.000</td>
<td>0.150</td>
<td>9.3162E+04</td>
<td>-0.0113</td>
<td>2.565E+03</td>
<td>0.0295</td>
<td></td>
</tr>
<tr>
<td>61</td>
<td>10</td>
<td>1.400</td>
<td>34.230</td>
<td>0.000</td>
<td>1.930</td>
<td>209.600</td>
<td>65.287</td>
<td>35.000</td>
<td>0.350</td>
<td>9.9691E+04</td>
<td>0.0784</td>
<td>2.5089E+03</td>
<td>-0.0011</td>
<td></td>
</tr>
</tbody>
</table>
TABLE E2. (CONTINUED FROM PREVIOUS PAGE)

<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>FEED STREAM DATA</th>
<th>OTHER DATA, INVENTORIES, AND DEVI FROM MODEL CALC.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>AG (1)</td>
<td>FLOW U (G/L)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ORG (2)</td>
<td>RATE (G/L)</td>
</tr>
<tr>
<td>62</td>
<td>1</td>
<td>1</td>
<td>0.610</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1.480</td>
</tr>
<tr>
<td>63</td>
<td>10</td>
<td>2</td>
<td>80.200</td>
</tr>
<tr>
<td>20</td>
<td>2</td>
<td>19.400</td>
<td>0.000</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1.687</td>
<td>75.970</td>
</tr>
<tr>
<td>64</td>
<td>7</td>
<td>11</td>
<td>1.687</td>
</tr>
<tr>
<td>STAGE</td>
<td>TYPE</td>
<td>AG. (1)</td>
<td>ORG. (2)</td>
</tr>
<tr>
<td>-------</td>
<td>------</td>
<td>---------</td>
<td>---------</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.067</td>
<td>0.000</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
</tr>
<tr>
<td>67</td>
<td>7</td>
<td>2</td>
<td>4.167</td>
</tr>
<tr>
<td>11</td>
<td>2</td>
<td>1.250</td>
<td>0.000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>AG. (1)</th>
<th>ORG. (2)</th>
<th>FLOW RATE (Q/L)</th>
<th>U (G/L)</th>
<th>PU (G/L)</th>
<th>HI (M)</th>
<th>UINV (G/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.067</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>68</td>
<td>7</td>
<td>2</td>
<td>4.167</td>
<td>78.570</td>
<td>0.022</td>
<td>0.280</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>11</td>
<td>2</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>AG. (1)</th>
<th>ORG. (2)</th>
<th>FLOW RATE (Q/L)</th>
<th>U (G/L)</th>
<th>PU (G/L)</th>
<th>HI (M)</th>
<th>UINV (G/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.067</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>69</td>
<td>7</td>
<td>2</td>
<td>4.167</td>
<td>78.570</td>
<td>0.022</td>
<td>0.280</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>11</td>
<td>2</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>AG. (1)</th>
<th>ORG. (2)</th>
<th>FLOW RATE (Q/L)</th>
<th>U (G/L)</th>
<th>PU (G/L)</th>
<th>HI (M)</th>
<th>UINV (G/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.067</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>70</td>
<td>7</td>
<td>2</td>
<td>4.167</td>
<td>78.570</td>
<td>0.022</td>
<td>0.280</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>11</td>
<td>2</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>AG. (1)</th>
<th>ORG. (2)</th>
<th>FLOW RATE (Q/L)</th>
<th>U (G/L)</th>
<th>PU (G/L)</th>
<th>HI (M)</th>
<th>UINV (G/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.067</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>71</td>
<td>7</td>
<td>2</td>
<td>4.167</td>
<td>78.570</td>
<td>0.022</td>
<td>0.280</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>11</td>
<td>2</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>AG. (1)</th>
<th>ORG. (2)</th>
<th>FLOW RATE (Q/L)</th>
<th>U (G/L)</th>
<th>PU (G/L)</th>
<th>HI (M)</th>
<th>UINV (G/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.067</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>0.063</td>
<td>0.000</td>
<td>0.000</td>
<td>1.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>71</td>
<td>7</td>
<td>2</td>
<td>4.167</td>
<td>78.570</td>
<td>0.022</td>
<td>0.280</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>11</td>
<td>2</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>
### TABLE E2. (CONTINUED FROM PREVIOUS PAGE)

<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>FLOW</th>
<th>U</th>
<th>PU</th>
<th>H(1)</th>
<th>U(IV)</th>
<th>AVG</th>
<th>TEMP</th>
<th>A/D</th>
<th>U</th>
<th>U</th>
<th>PU</th>
<th>PU</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(G/L)</td>
<td>(G/L)</td>
<td>(G/L)</td>
<td>(G/L)</td>
<td>(G/L)</td>
<td>(G/L)</td>
<td>(G/L)</td>
<td>(G/L)</td>
<td>(G/L)</td>
<td>(G/L)</td>
<td>(G/L)</td>
<td>(G/L)</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1.883</td>
<td>0.000</td>
<td>0.000</td>
<td>0.600</td>
<td>0.000</td>
<td>0.000</td>
<td>0.600</td>
<td>0.000</td>
<td>0.000</td>
<td>0.600</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.067</td>
<td>100.000</td>
<td>0.000</td>
<td>1.200</td>
<td>100.000</td>
<td>0.000</td>
<td>1.200</td>
<td>100.000</td>
<td>0.000</td>
<td>1.200</td>
<td>100.000</td>
<td>0.000</td>
</tr>
<tr>
<td>72</td>
<td>7</td>
<td>6.167</td>
<td>75.870</td>
<td>0.822</td>
<td>0.390</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>72</td>
<td>11</td>
<td>1.850</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1.883</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.067</td>
<td>100.000</td>
<td>0.000</td>
<td>1.500</td>
<td>100.000</td>
<td>0.000</td>
<td>1.500</td>
<td>100.000</td>
<td>0.000</td>
<td>1.500</td>
<td>100.000</td>
<td>0.000</td>
</tr>
<tr>
<td>73</td>
<td>7</td>
<td>6.167</td>
<td>75.870</td>
<td>0.822</td>
<td>0.480</td>
<td>0.000</td>
<td>0.000</td>
<td>0.480</td>
<td>0.000</td>
<td>0.000</td>
<td>0.480</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>74</td>
<td>11</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1.883</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.067</td>
<td>100.000</td>
<td>0.000</td>
<td>1.500</td>
<td>100.000</td>
<td>0.000</td>
<td>1.500</td>
<td>100.000</td>
<td>0.000</td>
<td>1.500</td>
<td>100.000</td>
<td>0.000</td>
</tr>
<tr>
<td>75</td>
<td>7</td>
<td>6.167</td>
<td>75.870</td>
<td>0.822</td>
<td>0.480</td>
<td>0.000</td>
<td>0.000</td>
<td>0.480</td>
<td>0.000</td>
<td>0.000</td>
<td>0.480</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>76</td>
<td>11</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

**OTHER DATA, INVENTORIES, AND DEV. FROM MODEL CALC.**

- **STAGE 1**
  - **Type 1**
  - **Flow** 1.883 (G/L)
  - **U** 0.000 (G/L)
  - **PU** 0.600 (G/L)
  - **INV. FRACT.** -0.0837

- **STAGE 72**
  - **Type 7**
  - **Flow** 6.167 (G/L)
  - **U** 75.870 (G/L)
  - **PU** 0.822 (G/L)
  - **INV. FRACT.** 0.0973

- **STAGE 75**
  - **Type 7**
  - **Flow** 6.167 (G/L)
  - **U** 75.870 (G/L)
  - **PU** 0.822 (G/L)
  - **INV. FRACT.** 0.0973

- **STAGE 76**
  - **Type 7**
  - **Flow** 6.167 (G/L)
  - **U** 75.870 (G/L)
  - **PU** 0.822 (G/L)
  - **INV. FRACT.** 0.0973
### Table E2. (Continued from previous page)

<table>
<thead>
<tr>
<th>Stage</th>
<th>Type</th>
<th>Flow Rate</th>
<th>U (g/L)</th>
<th>U (g/L)</th>
<th>H(+) (g/L)</th>
<th>U INV</th>
<th>Other Data, Inventories, and Dev. From Model Calc.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>AVG TEMP U CONC. A/O U U PU PU CONC. ICI PHASE INV. FRACT. INV. FRACT.</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>50.204 30.000 0.660 5.83500E+04 0.036 7.05729E+02 -0.0627</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>50.204 30.000 0.990 5.61113E+04 0.033 8.02461E+02 -0.0556</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>33.575 30.000 0.330 3.76783E+04 0.064 4.47421E+02 -0.0689</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>33.575 30.000 0.640 3.48309E+04 0.072 7.12729E+02 -0.0522</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>1.250</td>
<td>0.000</td>
<td>0.000</td>
<td>0.200</td>
<td>0.000</td>
<td>33.575 30.000 0.990 3.29279E+04 0.079 8.90045E+02 -0.0466</td>
</tr>
</tbody>
</table>
### TABLE E2. (CONTINUED FROM PREVIOUS PAGE)

| STAGE | TYPE | FLOW (G/L) | U (G/L) | H+ (G/L) | U+ (G/L) | AVG TEMP (°C) | A/G RATIO | U CONC. (GRAMS) | P/U CONC. (GRAMS) | PHASE INV. FRACT. | U INV. FRACT. | PU INV. FRACT. | OTHER DATA, INVENTORIES, AND DEV. FROM MODEL CALC. |
|-------|------|------------|---------|----------|----------|---------------|-----------|----------------|-----------------|-----------------|---------------|---------------|---------------|--------------------------------------------------|
| 1     | 1    | 1.003      | 0.000   | 0.000    | 0.200    | 0.000         | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 2     | 1    | 0.067      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 3     | 1    | 0.043      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 4     | 1    | 0.047      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 5     | 1    | 0.067      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 6     | 1    | 0.043      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 7     | 1    | 0.067      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 8    | 7    | 6.167      | 75.870  | 0.822    | 0.280    | 0.000         | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 9    | 11   | 1.250      | 0.000   | 0.000    | 0.000    | 0.000         | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 10   | 1    | 1.003      | 0.000   | 0.000    | 0.200    | 0.000         | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 11   | 1    | 0.067      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 12   | 1    | 0.043      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 13   | 1    | 0.047      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 14   | 1    | 0.067      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 15   | 1    | 0.043      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 16   | 1    | 0.047      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 17   | 1    | 0.067      | 100.000 | 0.000    | 1.500    | 100.000       | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 18   | 7    | 6.167      | 75.870  | 0.822    | 0.280    | 0.000         | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |
| 19   | 11   | 1.250      | 0.000   | 0.000    | 0.000    | 0.000         | 0.000     | 0.000          | 0.000           | 0.000           | 0.000         | 0.000         | 0.000                     |

**RESULTS OF LEAST SQUARES**

ORDER OF CALC = 3

<table>
<thead>
<tr>
<th>U CONSTS</th>
<th>PU CONSTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5930</td>
<td>0.3109</td>
</tr>
<tr>
<td>0.5124</td>
<td>0.4886</td>
</tr>
<tr>
<td>0.0000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

REL. STD. DEV. FOR U = 0.0789
REL. STD. DEV. FOR PU = 0.0468
<table>
<thead>
<tr>
<th>U</th>
<th>TBP</th>
<th>VOL</th>
<th>FLD</th>
<th>RATIO</th>
<th>TEMP</th>
<th>STAGES</th>
<th>H+1</th>
<th>H+2</th>
<th>(aq)</th>
<th>(gmb)</th>
<th>(gmb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.12</td>
<td>1.25</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
</tr>
<tr>
<td>0.24</td>
<td>2.50</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
</tr>
<tr>
<td>0.36</td>
<td>3.75</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
<td>0.18</td>
</tr>
<tr>
<td>0.48</td>
<td>5.00</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
</tr>
<tr>
<td>0.60</td>
<td>6.25</td>
<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
<td>0.30</td>
</tr>
<tr>
<td>0.72</td>
<td>7.50</td>
<td>0.36</td>
<td>0.36</td>
<td>0.36</td>
<td>0.36</td>
<td>0.36</td>
<td>0.36</td>
<td>0.36</td>
<td>0.36</td>
<td>0.36</td>
<td>0.36</td>
</tr>
<tr>
<td>0.84</td>
<td>8.75</td>
<td>0.42</td>
<td>0.42</td>
<td>0.42</td>
<td>0.42</td>
<td>0.42</td>
<td>0.42</td>
<td>0.42</td>
<td>0.42</td>
<td>0.42</td>
<td>0.42</td>
</tr>
<tr>
<td>0.96</td>
<td>10.00</td>
<td>0.48</td>
<td>0.48</td>
<td>0.48</td>
<td>0.48</td>
<td>0.48</td>
<td>0.48</td>
<td>0.48</td>
<td>0.48</td>
<td>0.48</td>
<td>0.48</td>
</tr>
</tbody>
</table>

135
<table>
<thead>
<tr>
<th>U (Org)</th>
<th>PU (Org)</th>
<th>H⁺ (Org)</th>
<th>H⁺ (Ar)</th>
<th>STAGES</th>
<th>TEMP (K)</th>
<th>FLOW RATE</th>
<th>VOL RATIO</th>
<th>TBP</th>
<th>U INV</th>
<th>U FRACT</th>
<th>PU INV</th>
<th>PU FRACT</th>
</tr>
</thead>
<tbody>
<tr>
<td>01</td>
<td>88.620</td>
<td>0.560</td>
<td>0.091</td>
<td>0.040</td>
<td>12</td>
<td>25.00</td>
<td>1.2000</td>
<td>1.3000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.3024</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>02</td>
<td>88.620</td>
<td>0.560</td>
<td>0.091</td>
<td>0.040</td>
<td>12</td>
<td>25.00</td>
<td>1.2000</td>
<td>1.3000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.3024</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>03</td>
<td>88.620</td>
<td>0.560</td>
<td>0.091</td>
<td>0.040</td>
<td>12</td>
<td>25.00</td>
<td>1.2000</td>
<td>1.3000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.3024</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>04</td>
<td>88.620</td>
<td>0.560</td>
<td>0.091</td>
<td>0.040</td>
<td>12</td>
<td>25.00</td>
<td>1.2000</td>
<td>1.3000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.3024</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>05</td>
<td>88.620</td>
<td>0.560</td>
<td>0.091</td>
<td>0.040</td>
<td>12</td>
<td>25.00</td>
<td>1.2000</td>
<td>1.3000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.3024</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>06</td>
<td>88.620</td>
<td>0.560</td>
<td>0.091</td>
<td>0.040</td>
<td>12</td>
<td>25.00</td>
<td>1.2000</td>
<td>1.3000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.3024</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>07</td>
<td>88.620</td>
<td>0.560</td>
<td>0.091</td>
<td>0.040</td>
<td>12</td>
<td>25.00</td>
<td>1.2000</td>
<td>1.3000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.3024</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>08</td>
<td>88.620</td>
<td>0.560</td>
<td>0.091</td>
<td>0.040</td>
<td>12</td>
<td>25.00</td>
<td>1.2000</td>
<td>1.3000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.3024</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>09</td>
<td>91.340</td>
<td>0.853</td>
<td>0.181</td>
<td>0.010</td>
<td>12</td>
<td>25.00</td>
<td>1.3000</td>
<td>1.4000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.4034</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>10</td>
<td>91.340</td>
<td>0.853</td>
<td>0.181</td>
<td>0.010</td>
<td>12</td>
<td>25.00</td>
<td>1.3000</td>
<td>1.4000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.4034</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>11</td>
<td>91.340</td>
<td>0.853</td>
<td>0.181</td>
<td>0.010</td>
<td>12</td>
<td>25.00</td>
<td>1.3000</td>
<td>1.4000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.4034</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>12</td>
<td>91.340</td>
<td>0.853</td>
<td>0.181</td>
<td>0.010</td>
<td>12</td>
<td>25.00</td>
<td>1.3000</td>
<td>1.4000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.4034</td>
<td>6.1599E+01</td>
</tr>
<tr>
<td>13</td>
<td>91.340</td>
<td>0.853</td>
<td>0.181</td>
<td>0.010</td>
<td>12</td>
<td>25.00</td>
<td>1.3000</td>
<td>1.4000</td>
<td>0.3000</td>
<td>5.0006E+04</td>
<td>0.4034</td>
<td>6.1599E+01</td>
</tr>
</tbody>
</table>

REL. STD. DEV. FOR U = 0.0824
REL. STD. DEV. FOR PU = 0.0548
<table>
<thead>
<tr>
<th></th>
<th>U (g/l)</th>
<th>PU (g/l)</th>
<th>ACID FEED</th>
<th>ACID SCRUB</th>
<th>T (C)</th>
<th>NO. STAGE</th>
<th>STAGE SCRUB Vol</th>
<th>SCRUB FEED TO ORG RATIO</th>
<th>SCRUB FEED A/O PHASE RATIO</th>
<th>TPB U</th>
<th>INV</th>
<th>U FRACT DEV</th>
<th>PU FRACT INV</th>
<th>PU FRACT DEV</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>180.00</td>
<td>0.92</td>
<td>2.83</td>
<td>2.01</td>
<td>25.0</td>
<td>3</td>
<td>150.0</td>
<td>0.227</td>
<td>0.511</td>
<td>1.00</td>
<td>30.0</td>
<td>0.0299E+006</td>
<td>0.0096</td>
<td>0.2217E+003</td>
</tr>
<tr>
<td>2</td>
<td>180.00</td>
<td>0.92</td>
<td>2.83</td>
<td>2.01</td>
<td>25.0</td>
<td>4</td>
<td>150.0</td>
<td>0.227</td>
<td>0.512</td>
<td>1.00</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.2217E+003</td>
</tr>
<tr>
<td>3</td>
<td>180.00</td>
<td>0.92</td>
<td>2.83</td>
<td>2.01</td>
<td>25.0</td>
<td>5</td>
<td>150.0</td>
<td>0.227</td>
<td>0.512</td>
<td>1.00</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.2217E+003</td>
</tr>
<tr>
<td>4</td>
<td>180.00</td>
<td>0.92</td>
<td>2.83</td>
<td>2.01</td>
<td>25.0</td>
<td>6</td>
<td>150.0</td>
<td>0.227</td>
<td>0.512</td>
<td>1.00</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.2217E+003</td>
</tr>
<tr>
<td>5</td>
<td>180.00</td>
<td>0.92</td>
<td>2.83</td>
<td>2.01</td>
<td>25.0</td>
<td>7</td>
<td>150.0</td>
<td>0.227</td>
<td>0.512</td>
<td>1.00</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.2217E+003</td>
</tr>
<tr>
<td>6</td>
<td>180.00</td>
<td>0.92</td>
<td>2.83</td>
<td>2.01</td>
<td>25.0</td>
<td>8</td>
<td>150.0</td>
<td>0.227</td>
<td>0.512</td>
<td>1.00</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.2217E+003</td>
</tr>
<tr>
<td>7</td>
<td>285.00</td>
<td>2.44</td>
<td>2.83</td>
<td>2.01</td>
<td>25.0</td>
<td>9</td>
<td>150.0</td>
<td>0.227</td>
<td>0.512</td>
<td>1.00</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.2217E+003</td>
</tr>
<tr>
<td>8</td>
<td>285.00</td>
<td>2.44</td>
<td>2.83</td>
<td>2.01</td>
<td>25.0</td>
<td>10</td>
<td>150.0</td>
<td>0.227</td>
<td>0.512</td>
<td>1.00</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.2217E+003</td>
</tr>
<tr>
<td>9</td>
<td>285.00</td>
<td>2.44</td>
<td>2.83</td>
<td>2.01</td>
<td>25.0</td>
<td>11</td>
<td>150.0</td>
<td>0.227</td>
<td>0.512</td>
<td>1.00</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.2217E+003</td>
</tr>
<tr>
<td>10</td>
<td>285.00</td>
<td>2.44</td>
<td>2.83</td>
<td>2.01</td>
<td>25.0</td>
<td>12</td>
<td>150.0</td>
<td>0.227</td>
<td>0.512</td>
<td>1.00</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.2217E+003</td>
</tr>
<tr>
<td>11</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>3</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>12</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>4</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>13</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>5</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>14</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>6</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>15</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>7</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>16</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>8</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>17</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>9</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>18</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>10</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>19</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>11</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>20</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>12</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>21</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>13</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
<tr>
<td>22</td>
<td>180.00</td>
<td>1.28</td>
<td>4.00</td>
<td>3.00</td>
<td>30.0</td>
<td>14</td>
<td>86.0</td>
<td>0.228</td>
<td>0.491</td>
<td>1.50</td>
<td>30.0</td>
<td>0.0096</td>
<td>0.0096</td>
<td>0.4772E+003</td>
</tr>
</tbody>
</table>

Overall fractional std. dev. for uranium = 0.0016
Overall fractional std. dev. for plutonium = 0.0016
TABLE E6

FLOW SHEET DATA; STEADY STATE INVENTORIES, AND STANDARD DEVIATIONS GIVEN AS A FRACTION OF THE STEADY STATE INVENTORIES FOR COMPARISONS OF TIME DEPENDENT MODEL CALCULATIONS WITH PUBG GENERATED DATABASES FOR STARTUP OF THE PARTITIONING CONTACTOR.

<table>
<thead>
<tr>
<th>STAGE TYPE</th>
<th>FLOW U</th>
<th>PU</th>
<th>H(+)</th>
<th>U(DIV)</th>
<th>TEMP (C)</th>
<th>VOL. PHASE</th>
<th>VOL. PHASE</th>
<th>U INV</th>
<th>FRACT INV</th>
<th>FRACT GRAMS</th>
<th>U GRAMS</th>
<th>FRACT DEV</th>
<th>U GRAMS</th>
<th>FRACT DEV</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.61</td>
<td>0.0</td>
<td>0.0</td>
<td>0.20</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>0</td>
<td>0.61</td>
<td>34.23</td>
<td>0.0</td>
<td>0.45</td>
<td>208.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>0</td>
<td>0.61</td>
<td>34.23</td>
<td>0.0</td>
<td>0.45</td>
<td>208.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0.61</td>
<td>0.0</td>
<td>0.0</td>
<td>0.20</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>1</td>
<td>0.61</td>
<td>34.23</td>
<td>0.0</td>
<td>0.45</td>
<td>208.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>2</td>
<td>0.61</td>
<td>34.23</td>
<td>0.0</td>
<td>0.45</td>
<td>208.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1</td>
<td>0.61</td>
<td>0.0</td>
<td>0.0</td>
<td>0.20</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>1</td>
<td>0.61</td>
<td>34.23</td>
<td>0.0</td>
<td>0.45</td>
<td>208.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>1</td>
<td>0.61</td>
<td>34.23</td>
<td>0.0</td>
<td>0.45</td>
<td>208.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>1</td>
<td>0.61</td>
<td>0.0</td>
<td>0.0</td>
<td>0.20</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>1</td>
<td>0.61</td>
<td>34.23</td>
<td>0.0</td>
<td>0.45</td>
<td>208.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>1</td>
<td>0.61</td>
<td>34.23</td>
<td>0.0</td>
<td>0.45</td>
<td>208.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>1</td>
<td>0.61</td>
<td>0.0</td>
<td>0.0</td>
<td>0.20</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>1</td>
<td>0.61</td>
<td>34.23</td>
<td>0.0</td>
<td>0.45</td>
<td>208.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>1</td>
<td>0.61</td>
<td>34.23</td>
<td>0.0</td>
<td>0.45</td>
<td>208.46</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>STAGE</td>
<td>TYPE</td>
<td>FLOW RATE (g/L)</td>
<td>U (g/L)</td>
<td>H(+)</td>
<td>ULIV) (g/L)</td>
<td>TEMP (°C)</td>
<td>SCRUB BAKEN PHASE VOL.</td>
<td>EXT. BAKEN PHASE VOL.</td>
<td>INV GRAMS</td>
<td>U FRACT</td>
<td>INV GRAMS</td>
<td>PU FRACT</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td>------</td>
<td>----------------</td>
<td>---------</td>
<td>------</td>
<td>------------</td>
<td>-----------</td>
<td>----------------------</td>
<td>----------------------</td>
<td>-----------</td>
<td>---------</td>
<td>-----------</td>
<td>----------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1.80</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>30.00</td>
<td>1124.21</td>
<td>1.23</td>
<td>752.76</td>
<td>1.21</td>
<td>0.8652E+05</td>
<td>0.077</td>
<td>0.1212E+03</td>
<td>0.048</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.07</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>30.00</td>
<td>1124.50</td>
<td>0.80</td>
<td>326.66</td>
<td>1.16</td>
<td>0.7444E+05</td>
<td>0.029</td>
<td>0.3126E+03</td>
<td>0.056</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>30.00</td>
<td>770.00</td>
<td>1.00</td>
<td>550.00</td>
<td>1.00</td>
<td>0.5404E+05</td>
<td>0.055</td>
<td>0.4560E+03</td>
<td>0.041</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>30.00</td>
<td>770.00</td>
<td>0.43</td>
<td>550.00</td>
<td>0.43</td>
<td>0.5704E+05</td>
<td>0.052</td>
<td>0.2949E+03</td>
<td>0.052</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>30.00</td>
<td>770.00</td>
<td>0.43</td>
<td>550.00</td>
<td>0.43</td>
<td>0.5648E+05</td>
<td>0.024</td>
<td>0.4579E+03</td>
<td>0.046</td>
</tr>
<tr>
<td>6</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>30.00</td>
<td>770.00</td>
<td>0.43</td>
<td>550.00</td>
<td>0.43</td>
<td>0.5648E+05</td>
<td>0.024</td>
<td>0.4579E+03</td>
<td>0.046</td>
</tr>
<tr>
<td>7</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>30.00</td>
<td>770.00</td>
<td>0.43</td>
<td>550.00</td>
<td>0.43</td>
<td>0.5648E+05</td>
<td>0.024</td>
<td>0.4579E+03</td>
<td>0.046</td>
</tr>
<tr>
<td>8</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>30.00</td>
<td>770.00</td>
<td>0.43</td>
<td>550.00</td>
<td>0.43</td>
<td>0.5648E+05</td>
<td>0.024</td>
<td>0.4579E+03</td>
<td>0.046</td>
</tr>
<tr>
<td>9</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>30.00</td>
<td>770.00</td>
<td>0.43</td>
<td>550.00</td>
<td>0.43</td>
<td>0.5648E+05</td>
<td>0.024</td>
<td>0.4579E+03</td>
<td>0.046</td>
</tr>
<tr>
<td>10</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>30.00</td>
<td>770.00</td>
<td>0.43</td>
<td>550.00</td>
<td>0.43</td>
<td>0.5648E+05</td>
<td>0.024</td>
<td>0.4579E+03</td>
<td>0.046</td>
</tr>
<tr>
<td>11</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>30.00</td>
<td>770.00</td>
<td>0.43</td>
<td>550.00</td>
<td>0.43</td>
<td>0.5648E+05</td>
<td>0.024</td>
<td>0.4579E+03</td>
<td>0.046</td>
</tr>
<tr>
<td>STAGE</td>
<td>TYPE</td>
<td>FLOW</td>
<td>U</td>
<td>PU</td>
<td>H(+)</td>
<td>U(IV)</td>
<td>TEMP</td>
<td>(SCRUB BANK)</td>
<td>(EXT. BANK)</td>
<td>U</td>
<td>FRACT</td>
<td>PU</td>
<td>FRACT</td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td>------</td>
<td>-------</td>
<td>---</td>
<td>----</td>
<td>------</td>
<td>-------</td>
<td>------</td>
<td>---------------</td>
<td>-------------</td>
<td>---</td>
<td>--------</td>
<td>----</td>
<td>--------</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.60</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>100.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0.02</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>100.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>0.01</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>100.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>1</td>
<td>0.04</td>
<td>100.00</td>
<td>0.0</td>
<td>1.50</td>
<td>100.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0</td>
<td>7.50</td>
<td>67.85</td>
<td>0.43</td>
<td>0.65</td>
<td>0.0</td>
<td>30.00</td>
<td>770.00</td>
<td>1.00</td>
<td>550.00</td>
<td>1.00</td>
<td>0.3977E+05</td>
<td>0.026</td>
<td>0.6368E+03</td>
</tr>
<tr>
<td>11</td>
<td>0</td>
<td>1.25</td>
<td>0.0</td>
<td>0.0</td>
<td>0.65</td>
<td>0.0</td>
<td>30.00</td>
<td>770.00</td>
<td>1.00</td>
<td>550.00</td>
<td>1.00</td>
<td>0.1274E+05</td>
<td>0.004</td>
<td>0.4705E+03</td>
</tr>
<tr>
<td>12</td>
<td>0</td>
<td>7.50</td>
<td>20.55</td>
<td>0.43</td>
<td>0.65</td>
<td>0.0</td>
<td>30.00</td>
<td>770.00</td>
<td>1.00</td>
<td>550.00</td>
<td>1.00</td>
<td>0.1274E+05</td>
<td>0.004</td>
<td>0.4705E+03</td>
</tr>
<tr>
<td>13</td>
<td>0</td>
<td>1.25</td>
<td>0.0</td>
<td>0.0</td>
<td>0.65</td>
<td>0.0</td>
<td>30.00</td>
<td>770.00</td>
<td>1.00</td>
<td>550.00</td>
<td>1.00</td>
<td>0.1274E+05</td>
<td>0.004</td>
<td>0.4705E+03</td>
</tr>
<tr>
<td>15</td>
<td>0</td>
<td>1.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.60</td>
<td>0.0</td>
<td>30.00</td>
<td>124.40</td>
<td>0.11</td>
<td>47.50</td>
<td>0.48</td>
<td>0.5356E+04</td>
<td>0.017</td>
<td>0.3946E+03</td>
</tr>
<tr>
<td>15</td>
<td>0</td>
<td>0.65</td>
<td>0.0</td>
<td>0.0</td>
<td>0.60</td>
<td>0.0</td>
<td>30.00</td>
<td>124.40</td>
<td>0.11</td>
<td>47.50</td>
<td>0.48</td>
<td>0.3607E+04</td>
<td>0.029</td>
<td>0.3632E+03</td>
</tr>
<tr>
<td>15</td>
<td>0</td>
<td>0.65</td>
<td>0.0</td>
<td>0.0</td>
<td>0.60</td>
<td>0.0</td>
<td>30.00</td>
<td>124.40</td>
<td>0.11</td>
<td>47.50</td>
<td>0.48</td>
<td>0.3607E+04</td>
<td>0.029</td>
<td>0.3632E+03</td>
</tr>
<tr>
<td>15</td>
<td>0</td>
<td>1.67</td>
<td>0.0</td>
<td>0.0</td>
<td>0.60</td>
<td>0.0</td>
<td>30.00</td>
<td>124.40</td>
<td>0.11</td>
<td>47.50</td>
<td>0.48</td>
<td>0.3607E+04</td>
<td>0.029</td>
<td>0.3632E+03</td>
</tr>
<tr>
<td>15</td>
<td>0</td>
<td>0.65</td>
<td>0.0</td>
<td>0.0</td>
<td>0.60</td>
<td>0.0</td>
<td>30.00</td>
<td>124.40</td>
<td>0.11</td>
<td>47.50</td>
<td>0.48</td>
<td>0.3607E+04</td>
<td>0.029</td>
<td>0.3632E+03</td>
</tr>
<tr>
<td>15</td>
<td>0</td>
<td>1.67</td>
<td>0.0</td>
<td>0.0</td>
<td>0.60</td>
<td>0.0</td>
<td>30.00</td>
<td>124.40</td>
<td>0.11</td>
<td>47.50</td>
<td>0.48</td>
<td>0.3607E+04</td>
<td>0.029</td>
<td>0.3632E+03</td>
</tr>
<tr>
<td>15</td>
<td>0</td>
<td>0.65</td>
<td>0.0</td>
<td>0.0</td>
<td>0.60</td>
<td>0.0</td>
<td>30.00</td>
<td>124.40</td>
<td>0.11</td>
<td>47.50</td>
<td>0.48</td>
<td>0.3607E+04</td>
<td>0.029</td>
<td>0.3632E+03</td>
</tr>
</tbody>
</table>

TABLE ES (CONTINUED FROM PREVIOUS PAGE)
<table>
<thead>
<tr>
<th>STAGE</th>
<th>TYPE</th>
<th>FLOW</th>
<th>U</th>
<th>PU</th>
<th>H+</th>
<th>U(V)</th>
<th>TEMP</th>
<th>SCRUB BANK</th>
<th>EXT. BANK</th>
<th>U</th>
<th>FRACT</th>
<th>U</th>
<th>FRACT</th>
<th>PU</th>
<th>FRACT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1.67</td>
<td>0.0</td>
<td>0.0</td>
<td>0.20</td>
<td>0.0</td>
<td>30.00</td>
<td>120.00</td>
<td>1.00</td>
<td>96.00</td>
<td>1.00</td>
<td>0.520E+04</td>
<td>0.047</td>
<td>0.955E+03</td>
<td>0.041</td>
</tr>
<tr>
<td>15</td>
<td>1</td>
<td>1.67</td>
<td>0.0</td>
<td>0.0</td>
<td>0.20</td>
<td>0.0</td>
<td>30.00</td>
<td>128.00</td>
<td>0.17</td>
<td>96.00</td>
<td>0.17</td>
<td>0.565E+04</td>
<td>0.037</td>
<td>0.674E+03</td>
<td>0.186</td>
</tr>
<tr>
<td>16</td>
<td>0</td>
<td>1.12</td>
<td>11.12</td>
<td>0.22</td>
<td>0.0</td>
<td>30.00</td>
<td>128.00</td>
<td>0.17</td>
<td>96.00</td>
<td>0.17</td>
<td>0.547E+04</td>
<td>0.036</td>
<td>0.282E+03</td>
<td>0.135</td>
<td></td>
</tr>
</tbody>
</table>

OVERALL FRACTIONAL STD. DEV. FOR URANIUM = 0.0556
OVERALL FRACTIONAL STD. DEV. FOR PLUTONIUM = 0.0711
<table>
<thead>
<tr>
<th>U (g/L)</th>
<th>Pu (g/L)</th>
<th>Acid Feed Stream (M)</th>
<th>Acid Scrub Stream (M)</th>
<th>T Stage Vol (M)</th>
<th>No. Stages</th>
<th>Scrub to Org Flow (M)</th>
<th>Scrub to Org Ratio</th>
<th>A/O Feed (M)</th>
<th>TBP (M)</th>
<th>U Inv</th>
<th>U Frac</th>
<th>Pu Inv</th>
<th>Pu Frac</th>
<th>Dev</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>69.99</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>104.2</td>
<td>1.254</td>
<td>1.00</td>
<td>1.109</td>
<td>30.00</td>
<td>0.1120E+05</td>
<td>0.0631</td>
<td>0.2277E+02</td>
</tr>
<tr>
<td>2</td>
<td>69.99</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>104.2</td>
<td>1.254</td>
<td>1.00</td>
<td>1.109</td>
<td>30.00</td>
<td>0.1120E+05</td>
<td>0.0631</td>
<td>0.2277E+02</td>
</tr>
<tr>
<td>3</td>
<td>89.99</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>104.2</td>
<td>1.254</td>
<td>1.00</td>
<td>1.109</td>
<td>30.00</td>
<td>0.1120E+05</td>
<td>0.0631</td>
<td>0.2277E+02</td>
</tr>
<tr>
<td>4</td>
<td>89.99</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>104.2</td>
<td>1.254</td>
<td>1.00</td>
<td>1.109</td>
<td>30.00</td>
<td>0.1120E+05</td>
<td>0.0631</td>
<td>0.2277E+02</td>
</tr>
<tr>
<td>5</td>
<td>79.99</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>104.2</td>
<td>1.254</td>
<td>1.00</td>
<td>1.109</td>
<td>30.00</td>
<td>0.1120E+05</td>
<td>0.0631</td>
<td>0.2277E+02</td>
</tr>
<tr>
<td>6</td>
<td>89.99</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>104.2</td>
<td>1.254</td>
<td>1.00</td>
<td>1.109</td>
<td>30.00</td>
<td>0.1120E+05</td>
<td>0.0631</td>
<td>0.2277E+02</td>
</tr>
<tr>
<td>7</td>
<td>0.01</td>
<td>1.88</td>
<td>0.02</td>
<td>0.02</td>
<td>25.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>8</td>
<td>88.33</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>9</td>
<td>91.36</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>10</td>
<td>91.36</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>11</td>
<td>91.36</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>12</td>
<td>91.36</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>13</td>
<td>91.36</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>14</td>
<td>91.36</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>60.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>15</td>
<td>48.36</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>25.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>16</td>
<td>48.36</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>25.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>17</td>
<td>0.01</td>
<td>5.50</td>
<td>0.02</td>
<td>0.02</td>
<td>25.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>18</td>
<td>0.01</td>
<td>5.50</td>
<td>0.02</td>
<td>0.02</td>
<td>25.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>19</td>
<td>91.36</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>25.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
<tr>
<td>20</td>
<td>91.36</td>
<td>0.01</td>
<td>0.02</td>
<td>0.02</td>
<td>25.0</td>
<td>12</td>
<td>145.0</td>
<td>1.200</td>
<td>1.00</td>
<td>1.090</td>
<td>30.00</td>
<td>0.6015E+00</td>
<td>0.0518</td>
<td>0.7825E+02</td>
</tr>
</tbody>
</table>

**Overall Fractional Standard Deviation for U = 0.0676**

**Overall Fractional Standard Deviation for Pu = 0.0658**