DATE: August 12, 1959


TO: F. L. Culler, Jr.

FROM: S. H. Jury and M. E. Whatley

ABSTRACT

A set of equations was written which allowed the calculation of equilibrium concentrations in the solvent phase of nitric acid and uranyl nitrate, given the initial TBP concentration in the solvent and the aqueous phase concentrations of acid and uranium. An ORACLE subroutine was written based on these equations which will calculate a set of equilibrium values in about 35 milliseconds. The subroutine was incorporated into a short program to calculate equilibrium points. A set of calculated points are presented in graphical form for 5, 20, 30, 40, and 100% TBP for nitric acid concentrations up to 7 M and uranyl nitrate concentrations up to 0.6 M in the aqueous phase. Since these calculations were based on limited data, it is the purpose of this memo to invite comment on their accuracy. The equations were reworked from a Russian paper by A. M. Rozen and L. P. Khorkhorina, using empirical polynomial fits for some poorly defined parameters, and were based principally on data from J. W. Codding. This project was undertaken to provide a subroutine to calculate equilibria in a general purpose ORACLE program to calculate the performance of multi-stage compound extraction cascades with more than one significant solute.

NOTICE

This document contains information of a preliminary nature and was prepared primarily for internal use at the Oak Ridge National Laboratory. It is subject to revision or correction and therefore does not represent a final report. The information is not to be abstracted, reprinted or otherwise given public dissemination without the approval of the ORNL patent branch, Legal and Information Control Department.
DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.
This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights, or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.
A number of investigators\(^{(1,2)}\) have studied the aqueous uranyl nitrate-nitric acid system with TBP diluted with a petroleum hydrocarbon. McKays\(^{(3,4,5)}\) and others have also made numerous contributions. There remains however the need for a generalized correlation of these works for column design. This work devotes itself to such an attempt.

Rozen\(^{(2)}\) sets forth the argument that uranyl nitrate is extracted according to the equation:

\[
\mathrm{UO}_2^{2+} + 2\mathrm{NO}_3^- + 2\text{TBP} = \mathrm{UO}_2(\mathrm{NO}_3)_2 \cdot 2\text{TBP}
\]

and thus:

\[
K_u = \frac{[\mathrm{UO}_2(\mathrm{NO}_3)_2 \cdot 2\text{TBP}]}{[\mathrm{UO}_2^{2+}][\mathrm{NO}_3^-]^2[\text{TBP}]^2}
\]

where:

- \(K_u\) = The thermodynamic equilibrium constant.
- \([\cdot]\) = Refer to activities.

The \(\mathrm{UO}_2^{2+}\) and \(\mathrm{NO}_3^-\) activities in the aqueous phase are used because at equilibrium their activities in the two phases are equal.

Nitric acid is apparently extracted according to the equation:

\[
\mathrm{H}^+ + \mathrm{NO}_3^- + \text{TBP} = \mathrm{HNO}_3 \cdot \text{TBP}
\]

For this equation the equilibrium relation may be written as:

\[
K = \frac{[\mathrm{HNO}_3 \cdot \text{TBP}]}{[\mathrm{H}^+][\mathrm{NO}_3^-][\text{TBP}]}
\]

Equation 2 may also be written in terms of concentrations and activity coefficients thus:

\[
K = \frac{\gamma_{\mathrm{H}^+}(\mathrm{HNO}_3 \cdot \text{TBP})}{\gamma_{\mathrm{H}^+}(\mathrm{H}^+)[\mathrm{NO}_3^-][\text{TBP}]}
\]

where:

- \((\cdot)\) = Refer to concentrations. (See Table 1a for nomenclature).
Table 1a  Nomenclature

$W = \text{aqueous phase acid concentration, moles/liter.}$

$Z = \text{organic phase acid concentration, moles/liter.}$

$T_0 = \text{TBP concentration in the organic phase, moles/liter.}$

$X = \text{aqueous phase uranyl nitrate concentration, moles/liter.}$

$Y = \text{organic phase uranyl nitrate concentration, moles/liter.}$

$\gamma = \text{activity coefficient of uranyl nitrate in aqueous acid.}$

$\gamma_T = \text{the activity coefficient of TBP.}$

$\gamma_\theta = \text{the activity coefficient of } UO_2(NO_3)_2 \cdot 2\text{TBP.}$

$f_H = \text{factor defined by Equation (6).}$

$\gamma_{UO_2^{2+}}, \gamma_{H^+}, \gamma_{NO_3^-} = \text{ion activity coefficients.}$

$\gamma_{eH} = \text{the activity coefficient of } HNO_3 \cdot \text{TBP.}$

$\mu = \text{ionic strength.}$

$C_i = \text{concentration of } i^{\text{th}} \text{ ion } M/L.$

$Z_i = \text{valence of } i^{\text{th}} \text{ ion.}$

$f_{u_i} = \text{factor defined by Equation (7).}$

Note: In the article by Rozen $N_x$ was used to represent $W$ and $N_y$ to represent $Z$. In the ORACLE code $N_x$ and $N_y$ are used instead of $W$ and $Z.$
If we define $K_1$ as:

$$K_1 = \frac{K \gamma_{H^+} \gamma_{NO_3} \gamma_T}{\gamma_{\Omega H}}$$

and note that

$$(HNO_3 \cdot TBP) = Z$$

$$(H^+) = W$$

$$(NO_3^-) = W + 2X$$

$$(TBP) = T_0 - 2Y - Z$$

then

$$K_1 = \frac{Z}{W(W + 2X)(T_0 - 2Y - Z)}$$

If we now define $f_H$ as:

$$f_H = K_1 W(2X + W)$$

then:

$$Z = f_H(T_0 - 2Y - Z).$$

Rozen used an average value of 0.2 for $K_1$. As will be seen later, $K_1$ is actually a function of ionic strength, $\mu$, and the value of 0.2 is only a fair approximation.

Equation (1) may also be written in terms of activity coefficients and concentrations:

$$K_u = \frac{\gamma_{\Omega}[UO_2(NO_3)_2 \cdot 2TBP]}{\gamma_{UO_2^{2+}}(UO_2^{2+}) \gamma_{NO_3^{-}}(NO_3^-) \gamma_T^2(TBP)^2}.$$

Rozen defined the activity coefficient, $\gamma$, of uranyl nitrate in the aqueous phase as:

$$\gamma^3 = \gamma_{UO_2^{2+}} \gamma_{NO_3^{-}}.$$

He also defined $\bar{K_u}$ as:

$$\bar{K_u} = K_u \frac{\gamma_T^2}{\gamma_{\Omega}}.$$

Since:

$$[UO_2(NO_3)_2 \cdot 2TBP] = Y$$
we may write:

\[ \tilde{K}_u = \frac{Y}{(T_0 - 2Y - Z)^2 X7^2 Y^3 (2X + W)^2} \]  \hspace{1cm} (11)

Rozen wrote this equation in the form:

\[ Y = f_u (T_0 - 2Y - Z)^2 \]  \hspace{1cm} (12)

where \( f_u \) is defined as:

\[ f_u = \tilde{K}_u X7^2 (2X + W)^2. \]  \hspace{1cm} (13)

Rozen's table of \( \tilde{K}_u \) was fit by the empirical expression:

\[ \tilde{K}_u = 86.01 - 25.59 T_0 + 2.718 T_0^2 \]  \hspace{1cm} (14)

Rozen's datum points as well as the fit given by equation (14) are plotted in Fig. 1.

The \( K_1 \) and \( \gamma \) were computed from Coddington's data using the previous resulting equations. They were plotted against ionic strength as shown in Fig. 2. The plots were fit to the empirical expressions:

\[ K_1 = 0.385 - 0.155 (W + 3X) + 0.024 (W + 3X)^2 \]  \hspace{1cm} (15)

and

\[ \gamma = 0.34 + 0.199 (W + 3X) \]  \hspace{1cm} (16)

The empirical curves are also shown in Fig. 2.

The \( W + 3X \) terms in the empirical equations derive from the definition of ionic strength which is:

\[ \mu = 1/2 \sum C_i Z_i^2. \]  \hspace{1cm} (17)

Thus, this equation may be written:

\[ \mu = 1/2[C_{UO_2}^++(2)^2 + C_{H^+}(1)^2 + C_{NO_3}^-(1)^2] = 1/2[4X + W + (2X + W)] = 3X + W \]  \hspace{1cm} (18)

The suggestion that \( \gamma \) and \( K_1 \) should be a function of \( \mu \) comes from the work of McKay.

The scatter of the triangular and circle datum points in Fig. 2 suggested difficulty in Coddington's measurement of acid and uranyl in the presence of each
Fig. 1. A Plot of Data from Table I of Article by Rozen.
Fig 2 Calculated Data and the Empirical Expressions for Them

\[ \gamma = 0.34 + 0.199(W + 3x) \]

\[ K_i = 0.385 - 0.155(W + 3x) + 0.024(W + 3x)^2 \]
other. In the case of $K_1$, it was decided therefore to fit $K_1$ to the pure acid runs, i.e., the square points, of Codding's data. These points show a much better consistency within themselves.

The equations for $K_1$, $\gamma$, $\bar{K}_u$, etc., when rearranged and ordered, comprise a set from which equilibrium can be explicitly calculated. These equations are given in Table 1b.

**DISCUSSION OF EQUATION DEVELOPMENT**

It is a recognized fact that TBP and water have limited solubilities in each other and that these vary with uranyl and acid. Also the nitric acid associates to some extent in water as does uranyl nitrate. In this calculation these effects and others were taken into account indirectly through their effects on $\gamma$, $K_1$, and $\bar{K}_u$. In other words, $\gamma$ and $K_1$ were selected as functions of ionic strength so that Codding's experimental data at 30% TBP would be fit. Rozen had already determined $K_u$ as such a function of $T_0$ as to make the calculations fit at other values of $T_0$. More complete experimental information is badly needed to test the validity of the set of equations and resulting code presented. Although many investigators have worked with the subject system, Codding is one of the few who measured $Y$ and $Z$ for corresponding measured values of $X$, $W$, and $T_0$ at equilibrium.

**SUBROUTINE CHARACTERISTICS**

A digital computer subroutine which employs the equations in Table 1 is given in Appendix I. Since an iterative calculation of the performance of a 20 stage solvent extraction column might use this routine up to 200,000 times, it was essential that the routine be as fast as possible. An attempt to code it in the usual 8-32 pseudo code showed that a minimum time of about 300 milliseconds would be required per set of equilibrium values. This rate would result in over 16 hours of calculating time for equilibrium calculations alone. By coding in fixed point, and using many time savers, the calculating time was cut to about 55 milliseconds, which would require about two hours of equilibrium calculating time for the same problem.

Among the time saving devices employed was the avoidance of general purpose subroutines from the ORACLE compiler. This subroutine does its own conversion from an 8-32 input to fixed point and has its own loop for extracting a square root. It does use the compiler subroutine O0065 to convert the calculated numbers from fixed point to floating point.

The necessity for repeated recalculating $\bar{K}_u$, which is a function of TBP concentration alone, was eliminated by storing the previous value of $\bar{K}_u$ and using it if an examination of the TBP concentration revealed it to be unchanged.

There are eight constants which are specified in the set of equations. If consideration of more equilibrium data indicates it necessary, the values of these numbers in the code can be easily changed. The locations of these numbers are given in the Appendix.
Table 1b: Equations for Calculating Uranyl Nitrate and Nitric Acid Equilibrium Solvent Phase Concentrations from Initial TBP Concentration and Aqueous Phase Concentrations

\[ K_1 = 0.385 - 0.155(W + 3X) + 0.024(W + 3X)^2 \]  \hspace{1cm} (19)

\[ f_H = K_1W(2X + W) \]  \hspace{1cm} (20)

\[ Ku = 86.01 - 25.59T_0 + 2.718T_0^2 \]  \hspace{1cm} (21)

\[ \gamma = 0.34 + 0.199(W + 3X) \]  \hspace{1cm} (22)

\[ f_u = Ku\gamma^3(2X + W)^2 \]  \hspace{1cm} (23)

\[ F = \frac{f_u}{(1 + f_H)^2} \]  \hspace{1cm} (24)

\[ Y = 1/2[T_0 - (1/4F\sqrt{1 + 8FT_0} - 1)] \]  \hspace{1cm} (25)

\[ Z = \frac{f_H}{1 + f_H}(T_0 - 2Y) \]  \hspace{1cm} (26)
There are limits to the range of variables over which this routine will produce valid results. At low values of TBP concentration and high uranium concentrations it calculates negative values for the nitric acid concentration in the solvent phase. Some typical deviations are given in Table 2.

Table 2 Calculated Values Showing Limits of Subroutine

<table>
<thead>
<tr>
<th>TBP % by vol</th>
<th>Aqueous Phase</th>
<th>Solvent Phase</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HNO₃ M</td>
<td>Uranyl Nitrate M</td>
</tr>
<tr>
<td>40</td>
<td>1.0</td>
<td>0.8</td>
</tr>
<tr>
<td>30</td>
<td>2.0</td>
<td>0.6</td>
</tr>
<tr>
<td>20</td>
<td>3.5</td>
<td>0.8</td>
</tr>
<tr>
<td>5</td>
<td>3.0</td>
<td>0.5</td>
</tr>
<tr>
<td>5</td>
<td>2.0</td>
<td>0.5</td>
</tr>
<tr>
<td>5</td>
<td>2.0</td>
<td>0.8</td>
</tr>
<tr>
<td>5</td>
<td>1.0</td>
<td>0.8</td>
</tr>
</tbody>
</table>

The low negative values are inherent in the equations, and since they vary smoothly, an iteration procedure could use them. It is not, in fact, certain that the acid in the organic solvent remains positive in the real system. In any case, the effect was not noticed for aqueous uranium concentrations less than 0.5 M (120 gms U/liter) at TBP concentrations over 20%, and was noticed at only slightly lower uranium concentrations for the lower TBP concentrations.

The very large negative numbers for nitric acid concentration and the corresponding ridiculous solvent uranium concentrations found at 0.8 M uranium with 5% TBP represents a limitation of the code stemming from its fixed point nature. This is an unmonitored failure which, if allowed to occur, would ruin a calculation. Another manifestation of the fixed point limitation is the overflow from using aqueous phase uranium concentrations over 0.7 M (170 gms U/liter) with high (100%) TBP concentrations. The subroutine, however, will catch this error, type "Ouch" on the keyboard typewriter and stop the calculation.
RESULTS OF CALCULATION

To test the subroutine a short program was written and used. The TBP concentrations used were 5, 20, 30, 40, and 100% by volume (0.19, 0.72, 1.06, 1.43, and 3.46 moles per liter respectively), and the aqueous phase nitric acid concentrations were 0.05, 0.5, 1.0, 2.0, 3.0, 3.5, 4.0, and, in some cases, 6.0 and 7.0 moles per liter. Ten values of aqueous phase uranium concentration were used ranging from 0.001 to 0.8 moles per liter. The results are shown graphically in Figs. 3 through 7. The plot of calculated curves for 30% TBP also includes Codding's data for purpose of comparison.

Beyond the insipid observation that these curves seem to follow the behavior of what is known about the system, there is no quantitative criteria for evaluating their accuracy. One of the purposes of this report is to invite those with equilibrium points from the many years of study of this system to comment on the validity of these curves.

THE ORACLE PROGRAM

The ORACLE program used to calculate the curves is available for calculating additional points. It is comprised of an administrative item, the subroutine to be tested, and a short edited output. The administrative item is given in Appendix II.

The input for the program is of the following form:

(a) Ten values for aqueous phase uranium concentration in moles per liter in "packed decimal" numbers.

(b) Any number of sets of TBP and nitric acid concentrations, in that order, in mole per liter in "packed decimal" numbers.

The code will read in the values of X and use them for every subsequent set of TBP and nitric acid concentrations which it will read as it calculates. The calculated answers will be punched out on paper tape, printing a separate table for each set of TBP and nitric acid concentrations, listing the values of X, Z, and Y (Appendix III).

REFERENCES


Fig 3 Calculated Distribution for 5% TBP
Fig 4 Calculated Distribution for 20% TBP

- $W$, Aqueous Phase Nitric Acid Concentration, mole/liter
- $Y$, Organic Phase Uranium Concentration, mole/liter
- $Z$, Organic Phase Nitric Acid Concentration, mole/liter
Fig. 5a. Calculated Distribution for 30% TBP.
Fig 6a. Calculated Distribution for 40% TBP.
Fig 7a Calculated Distribution for 100% TBP
Fig. 5b, 30% TBP

Fig. 6b, 40% TBP

Fig. 7b, 100% TBP
APPENDIX I

**Subroutine 00200**

This subroutine calculates the equilibrium concentrations of uranyl nitrate and nitric acid in the organic solvent phase when the corresponding concentrations in the aqueous phase and the initial TBP concentration are given.

The subroutine entry in ORNL Compiler pseudo code is:

```
ff 000 00 200
    -- ggg -- hhh
    -- jjj -- ----
    -- kkk -- mmm
```

where ggg and hhh are the addresses of the memory cells containing the aqueous phase concentrations of nitric acid and uranyl nitrate in mols per liter respectively.

jjj is the address of the initial concentration of TBP in the organic solvent in mols per liter.

kkk and mmm are the addresses which are to receive respectively the organic solvent phase concentrations of nitric acid and uranyl nitrate in mols per liter.

All numbers are in 8-32 floating point.

There are eight constants necessary to the calculation which appear in the equations:

\[ K_u = a_1 T_0^2 - a_2 T_0 + a_3 \]

\[ K_1 = a_4 (W + 3X)^2 - a_5 (W + 3X) + a_6 \]

\[ \gamma = a_7 (W + 3X) + a_8 \]

These constants are multiplied by scale factors and stored in the routine.
Table 3 Location of Constants for Calculation

<table>
<thead>
<tr>
<th>Constant</th>
<th>Scale Factor</th>
<th>Relative Address</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$2^{-2}$</td>
<td>06a</td>
</tr>
<tr>
<td>2</td>
<td>$2^{-3}$</td>
<td>06b</td>
</tr>
<tr>
<td>3</td>
<td>$2^{-7}$</td>
<td>06c</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>06d</td>
</tr>
<tr>
<td>5</td>
<td>$2^{-7}$</td>
<td>06e</td>
</tr>
<tr>
<td>6</td>
<td>$2^{-7}$</td>
<td>06f</td>
</tr>
<tr>
<td>7</td>
<td>1</td>
<td>070</td>
</tr>
<tr>
<td>8</td>
<td>$2^{-7}$</td>
<td>071</td>
</tr>
</tbody>
</table>

All constants are used as binary fractions.

A copy of the subroutine is included (see following pages).
<table>
<thead>
<tr>
<th>Item Number: 00200</th>
<th>Page 1</th>
</tr>
</thead>
</table>

**Key Words:**
00200, 69, 0, 9, 0, 0, 0, 0, 0

**Code:**

<table>
<thead>
<tr>
<th>Code</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>000</td>
<td>20</td>
</tr>
<tr>
<td>001</td>
<td>20</td>
</tr>
<tr>
<td>002</td>
<td>20</td>
</tr>
<tr>
<td>003</td>
<td>20</td>
</tr>
<tr>
<td>004</td>
<td>60</td>
</tr>
<tr>
<td>005</td>
<td>24</td>
</tr>
<tr>
<td>006</td>
<td>24</td>
</tr>
<tr>
<td>007</td>
<td>54</td>
</tr>
<tr>
<td>008</td>
<td>5f</td>
</tr>
<tr>
<td>009</td>
<td>24</td>
</tr>
<tr>
<td>00a</td>
<td>24</td>
</tr>
<tr>
<td>00b</td>
<td>51</td>
</tr>
<tr>
<td>00c</td>
<td>22</td>
</tr>
<tr>
<td>00d</td>
<td>27</td>
</tr>
<tr>
<td>00e</td>
<td>24</td>
</tr>
<tr>
<td>00f</td>
<td>1c</td>
</tr>
<tr>
<td>010</td>
<td>4a</td>
</tr>
<tr>
<td>011</td>
<td>25</td>
</tr>
<tr>
<td>012</td>
<td>24</td>
</tr>
<tr>
<td>013</td>
<td>7f</td>
</tr>
<tr>
<td>014</td>
<td>22</td>
</tr>
<tr>
<td>015</td>
<td>60</td>
</tr>
<tr>
<td>016</td>
<td>1b</td>
</tr>
<tr>
<td>017</td>
<td>5f</td>
</tr>
<tr>
<td>018</td>
<td>00</td>
</tr>
<tr>
<td>019</td>
<td>00</td>
</tr>
</tbody>
</table>
Item Number: 00200  Page 2

01a:  00 000 00 000
01b:  24 f01 1c 020
01c:  22 ea7 4a 04d
01d:  5f f00 25 f00
01e:  51 01f 24 e80
01f:  40 000 1c 000
020:  7f f01 24 f02
021:  1c 020 22 ea7
022:  4a 04d 5f f00
023:  25 f00 51 024
024:  24 e80 1c 000
025:  7f f02 24 f02
026:  20 f02 20 f02
027:  20 f01 5f f03
028:  60 f03 38 06d
029:  22 06e 5f f00
02a:  60 f00 38 f03
02b:  40 000 1b 007
02c:  4f 04d 20 06f
02d:  4f 04d 5f f00
02e:  24 f02 20 f02
02f:  20 f01 5f f04
030:  60 f04 38 f01
031:  40 000 1b 007
032:  4f 04d 5f f05
033:  60 f05 38 f00
034:  40 000 1b 007
035:  4f 04d 5f f00
036: 60 f03 38 070
037: 20 071 4f 04d
038: 5f f03 60 f03
039: 38 f04 40 000
03a: 1b 007 4f 04d
03b: 5f f05 60 f05
03c: 38 f02 40 000
03d: 1b 007 4f 04d
03e: 5f f06 60 f06
03f: 38 f03 40 000
040: 1b 007 4f 04d
041: 5f f06 60 f06
042: 38 f03 40 000
043: 1b 007 4f 04d
044: 5f f05 60 f05
045: 38 f04 5f f03
046: 24 f00 20 e01
047: 4f 04d 5f f04
048: 22 f03 4b 04d
049: 24 f03 3a f04
04a: 38 019 3b f04
04b: 7f f02 40 000
04c: 38 01a 43 04f
04d: 8a 04e 43 04e
04e: 00 210 c1 238
04f: 1b 007 20 069
050: 4f 04d 5f f03
051: 60 ec5 12 001
<table>
<thead>
<tr>
<th>Item Number</th>
<th>00200</th>
</tr>
</thead>
<tbody>
<tr>
<td>052</td>
<td>4f 054 1c 001</td>
</tr>
<tr>
<td>053</td>
<td>12 002 4c 051</td>
</tr>
<tr>
<td>054</td>
<td>7f f05 25 f03</td>
</tr>
<tr>
<td>055</td>
<td>10 001 3a f05</td>
</tr>
<tr>
<td>056</td>
<td>7f f06 24 f05</td>
</tr>
<tr>
<td>057</td>
<td>10 001 20 f06</td>
</tr>
<tr>
<td>058</td>
<td>5f f06 60 f06</td>
</tr>
<tr>
<td>059</td>
<td>22 f05 5f f06</td>
</tr>
<tr>
<td>05a</td>
<td>25 f06 22 eb0</td>
</tr>
<tr>
<td>05b</td>
<td>7f f05 48 054</td>
</tr>
<tr>
<td>05c</td>
<td>24 f05 18 002</td>
</tr>
<tr>
<td>05d</td>
<td>22 e01 18 009</td>
</tr>
<tr>
<td>05e</td>
<td>3b f02 7f f02</td>
</tr>
<tr>
<td>05f</td>
<td>38 f00 3b f04</td>
</tr>
<tr>
<td>060</td>
<td>7f f05 24 01a</td>
</tr>
<tr>
<td>061</td>
<td>22 f02 5f f06</td>
</tr>
<tr>
<td>062</td>
<td>ff 000 00 065</td>
</tr>
<tr>
<td>063</td>
<td>40 f05 50 f05</td>
</tr>
<tr>
<td>064</td>
<td>80 f06 40 f06</td>
</tr>
<tr>
<td>065</td>
<td>24 f05 20 e07</td>
</tr>
<tr>
<td>066</td>
<td>5f 000 24 f06</td>
</tr>
<tr>
<td>067</td>
<td>20 e06 5f 000</td>
</tr>
<tr>
<td>068</td>
<td>43 000 00 000</td>
</tr>
<tr>
<td>069</td>
<td>00 200 00 000</td>
</tr>
<tr>
<td>06a</td>
<td>56 f9c 10 000</td>
</tr>
<tr>
<td>06b</td>
<td>06 65d c2 000</td>
</tr>
<tr>
<td>06c</td>
<td>56 028 10 000</td>
</tr>
<tr>
<td>06d</td>
<td>03 014 60 000</td>
</tr>
<tr>
<td>Item</td>
<td>Code</td>
</tr>
<tr>
<td>------</td>
<td>------</td>
</tr>
<tr>
<td>06e</td>
<td>00</td>
</tr>
<tr>
<td>06f</td>
<td>00</td>
</tr>
<tr>
<td>070</td>
<td>19</td>
</tr>
<tr>
<td>071</td>
<td>00</td>
</tr>
</tbody>
</table>
APPENDIX II

ORACLE Program to Calculate Test Points

This program was written for the express purpose of testing subroutine 00200. It reads in ten values of X and uses them for calculating equilibrium values for any number of sets of values of TB and nitric acid concentration. All input numbers must be in moles per liter in packed decimal form. The code is available in paper tape form from the author on request. The operating instructions are as follows:

1. Load code to 000.

2. Place input tape under reader.

3. 43 000. The ten values of X will be read in, the first set of T0 and W will be read in, and the answers will be punched out as the calculation proceeds. It will continue to read pairs of T0 and W as long as they appear.

4. If the limits of the fix point scaling are exceeded the word "Ouch" will be typed on the console typewriter and the calculation will stop. To read in the next case, 43 020.

A copy of the administrative item is included (see following pages).
<table>
<thead>
<tr>
<th>Key Words</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>00001, 22, 3, 0, 0, 0, 0, 0, 0</td>
<td>000: ff 000 00 035</td>
</tr>
<tr>
<td></td>
<td>001: 40 800 40 809</td>
</tr>
<tr>
<td></td>
<td>002: ff 000 00 035</td>
</tr>
<tr>
<td></td>
<td>003: 40 80a 40 80b</td>
</tr>
<tr>
<td></td>
<td>004: 24 008 51 013</td>
</tr>
<tr>
<td></td>
<td>005: 24 008 51 00f</td>
</tr>
<tr>
<td></td>
<td>006: 88 fff 43 008</td>
</tr>
<tr>
<td></td>
<td>00 000 a0 001</td>
</tr>
<tr>
<td></td>
<td>007: 04 014 88 80a</td>
</tr>
<tr>
<td></td>
<td>008: 60 007 40 800</td>
</tr>
<tr>
<td></td>
<td>009: ff 000 00 098</td>
</tr>
<tr>
<td></td>
<td>00a: 88 fff 43 00c</td>
</tr>
<tr>
<td></td>
<td>00 000 a0 002</td>
</tr>
<tr>
<td></td>
<td>00b: 04 014 88 80b</td>
</tr>
<tr>
<td></td>
<td>00c: 60 00b 40 000</td>
</tr>
<tr>
<td></td>
<td>00d: ff 000 00 098</td>
</tr>
<tr>
<td></td>
<td>00e: 88 fff 43 010</td>
</tr>
<tr>
<td></td>
<td>00 000 a0 003</td>
</tr>
<tr>
<td></td>
<td>00f: 04 014 88 800</td>
</tr>
<tr>
<td></td>
<td>010: 60 00f 40 000</td>
</tr>
<tr>
<td></td>
<td>011: ff 000 00 098</td>
</tr>
<tr>
<td></td>
<td>012: ff 000 00 200</td>
</tr>
<tr>
<td></td>
<td>013: 40 80b 40 800</td>
</tr>
<tr>
<td></td>
<td>014: 40 80a 40 000</td>
</tr>
<tr>
<td></td>
<td>015: 40 80c 40 80d</td>
</tr>
<tr>
<td></td>
<td>016: 60 017 43 018</td>
</tr>
<tr>
<td>Item Number: 00001</td>
<td>Page 2</td>
</tr>
<tr>
<td>-------------------</td>
<td>--------</td>
</tr>
<tr>
<td>017: 04 014 80 80c</td>
<td></td>
</tr>
<tr>
<td>018: ff 000 00 098</td>
<td></td>
</tr>
<tr>
<td>019: 60 01a 43 01b</td>
<td></td>
</tr>
<tr>
<td>01a: 04 014 80 80d</td>
<td></td>
</tr>
<tr>
<td>01b: ff 000 00 098</td>
<td></td>
</tr>
<tr>
<td>01c: 8c e35 24 013</td>
<td></td>
</tr>
<tr>
<td>01d: 20 eb1 51 013</td>
<td></td>
</tr>
<tr>
<td>01e: 51 00f 20 ea3</td>
<td></td>
</tr>
<tr>
<td>01f: 22 015 4b 010</td>
<td></td>
</tr>
<tr>
<td>020: 8c e35 8c e35</td>
<td></td>
</tr>
<tr>
<td>021: 8c e2f 43 002</td>
<td></td>
</tr>
</tbody>
</table>
APPENDIX III

Format for Output of ORACLE Equilibrium Calculation of Uranyl Nitrate Nitric Acid Solvent Concentrations from Aqueous Concentrations.

\[ \text{TBP} = 1.429 \]
\[ \text{HNO}_3 = 6.000 \]

\[
\begin{array}{cccc}
  x   & \text{Ny} & y \\
0.1000E-2 & 1.158 & 0.8204E-1 \\
0.1000E-1 & 0.7265 & 0.3186 \\
0.9999E-1 & 0.3189 & 0.5429 \\
0.1500 & 0.2753 & 0.5672 \\
0.1999 & 0.2496 & 0.5817 \\
0.3000 & 0.2207 & 0.5981 \\
0.3999 & 0.2052 & 0.6071 \\
0.5000 & 0.1961 & 0.6126 \\
0.6000 & 0.1903 & 0.6161 \\
0.7999 & 0.1846 & 0.6199 \\
\end{array}
\]

\[ \text{Ny} = Z \quad x = X \quad y = Y \]

All concentrations are in moles per liter. E-2 means times $10^{-2}$, etc.
### DISTRIBUTION

1. E. L. Anderson (AEC Washington)  
2. F. P. Baranowski (AEC Washington)  
3. R. E. Blanco  
4. J. O. Blomeke  
5. J. C. Breese  
6. K. B. Brown (Y-12)  
7. F. R. Bruce  
8. L. P. Bupp (HAPO)  
9. G. I. Cathers  
10. J. T. Christy (HOO)  
11. W. E. Clark  
12. J. W. Codding (KAPL)  
13. V. R. Cooper (HAPO)  
14. F. L. Culler, Jr.  
15. W. Davis, Jr.  
16. O. C. Dean  
17. W. K. Elster  
18. D. E. Ferguson  
19. L. M. Ferris  
20. J. R. Flanary  
21. M. J. Fortenbery (Y-12)  
22. H. E. Goeller  
23. J. H. Goode  
24. M. J. Googin (Y-12)  
25. A. T. Gresky  
26. P. A. Haas  
27. W. C. Haas, Jr (KAPL)  
28. M. K. Harmon (HAPO)  
29. F. K. Heumann (KAPL)  
30. O. F. Holl (HAPO)  
31. J. M. Holmes  
32. R. W. Horton  
33. A. R. Irvine  
34. H. F. Johnson  
35-40. S. H. Jury  
41. F. Kerze (AEC Washington)  
42. E. Lamb  
43. D. M. Lang (ORGIP)  
44. S. Lawroski (ANL)  
45. R. W. Leuze  
46. J. A. Lieberman (AEC Washington)  
47. R. B. Lindauer  
48. A. P. Litman  
49. J. T. Long  
50. B. Manowitz (BNL)  
51. J. P. McBride  
52. R. A. McNees  
53. R. P. Milford  
54. J. G. Moore  
55. J. W. Morris (SRP)  
56. R. E. Nahler (AEC Washington)  
57. D. M. Paige (ICFP)  
58. F. S. Patton, Jr. (Y-12)  
59. R. H. Rainey  
60. J. T. Roberts  
61. C. A. Rohrman (HAPO)  
62. O. T. Roth (AEC Washington)  
63. A. D. Ryon  
64. J. E. Savolainen  
65. W. F. Schaffer  
66. C. H. Secoy  
67. E. M. Shank  
68. M. J. Skinner  
69. C. M. Slansky (ICFP)  
70. S. H. Smiley (ORCID)  
71. J. A. Sonia (Goodyear Atomic Corp.)  
72. C. E. Stevenson (ICFP)  
73. E. G. Struxness  
74. J. A. Swartout  
75. V. R. Thayer (duPont, Wilmington, Del.)  
76. W. E. Unger  
77. J. Vanderryn (AEC ORO)  
78. F. M. Warzel (ICFP)  
79. C. D. Watson  
80-81. M. E. Whatley  
82. G. C. Williams  
83. C. E. Winters  
84-85. Central Research Library  
86-89. Laboratory Records  
90. Laboratory Records (RC)  
91. Document Reference Section  
92-106. TISE