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SOLVENT EXTRACTION STUDY OF THE
SYSTEM MONAZITE RARE EARTH
NITRATES - NITRIC ACID - WATER -
TRIBUTYL PHOSPHATE

by

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EARTH NITRATES - NITRIC ACID - WATER - TRIBUTYL PHOSPHATE*

Brooks Martin Sharp and Morton Smutz

ABSTRACT

Using single stage equilibrium data for the systems shown below, plus the assumption of mutual immiscibility of water and tributyl phosphate (TBP), a calculation method was developed to give the stagewise conditions in a cascade of equilibrium stages with all species present in the flow streams.

- I $\text{La}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O
- II $\text{Pr}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O
- III $\text{Nd}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O
- IV $\text{Sm}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O
- V $\text{La}(\text{NO}_3)_3$ - $\text{Pr}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O
- VI $\text{Nd}(\text{NO}_3)_3$ - $\text{Pr}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O
- VII $\text{Sm}(\text{NO}_3)_3$ - $\text{Pr}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O

The calculation method was checked via a series of simulated column experiments. The agreement between predicted and experimental stagewise conditions was considered reasonable, and the calculation is considered useful for engineering work.

As the calculation is tedious and time consuming, digital computer programs were written for the IBM 7074 to calculate the stagewise conditions in cascades of interest. It is hoped these programs will be useful in design and optimization studies.

*This report is based on a Ph. D. thesis submitted by Brooks Martin Sharp November, 1963, to Iowa State University, Ames, Iowa.

NOMENCLATURE

The following three paragraphs are explanatory notes on the nomenclature used in this thesis.

(1) All molalities are expressed in terms of the nitrate group associated with the solute in question. For example, a solution containing one kilogram of water and one molecular weight (324.9 gms.) of $\text{La}(\text{NO}_3)_3$ would be three molal $\text{La}(\text{NO}_3)_3$.

(2) For a doubly subscripted quantity, the first subscript is the solute subscript and the second subscript is a "location" subscript, referring to the phase, stream, or stage with which the quantity is associated.

(3) If used as a subscript S, R, and F denote that the quantity subscripted refers to a stream in an extraction cascade. If used as a variable S, R, and F denote the solvent flow rate in a stream in an extraction cascade. In the text, a reference to stream R_n or S_n denotes a reference to the stream as a whole.

- M - molality, moles of a solute per kilogram of solvent
- K - distribution coefficient, ratio of molality of a solute in an organic phase to molality of the solute in the equilibrium aqueous phase
- β - separation factor, ratio of two distribution coefficients
- X - ratio of molality of a solute in aqueous solution to total molality of the solution

- x - ratio of molality of a rare earth solute in aqueous solution to total rare earth molality of the solution
- Y - ratio of molality of a solute in organic solution to total molality of the solution
- y - ratio of molality of a rare earth solute in organic solution to total rare earth molality of the solution
- S - flow rate of solvent in an organic stream, kgm. TBP/unit time
- R - flow rate of solvent in an aqueous stream, kgm. H₂O/unit time
- F - flow rate of solvent in a feed stream, kgm. H₂O/unit time
- T - total number of solutes
- α - flow rate ratio, S/R

Subscripts

- i, j - arbitrary solute
- t - total solutes present, expressed as equivalents of nitrate
- RE - total rare earth nitrate solutes present
- La - lanthanum nitrate
- Pr - praseodymium nitrate
- Nd - neodymium nitrate
- Sm - samarium nitrate
- HNO₃ - nitric acid
- n - arbitrary stage in extraction cascade
- org. - organic phase
- aq. - aqueous phase

SUMMARY

Using single stage equilibrium data for the systems shown below, plus the assumption of mutual immiscibility of water and tributyl phosphate (TBP), a calculation method was developed to give the stagewise conditions in a cascade of equilibrium stages with all species present in the flow streams.

- I $\text{La}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$
- II $\text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$
- III $\text{Nd}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$
- IV $\text{Sm}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$
- V $\text{La}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$
- VI $\text{Nd}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$
- VII $\text{Sm}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$

The calculation method was checked via a series of simulated column experiments. The agreement between predicted and experimental stagewise conditions was considered reasonable, and the calculation is considered useful for engineering work.

As the calculation is tedious and time consuming, digital computer programs were written for the IBM 7074 to calculate the stagewise conditions in cascades of interest. It is hoped these programs will be useful in design and optimization studies.

INTRODUCTION

The elements of atomic number 57 to 71 are commonly known as the rare earths or lanthanides. They occur in nature as rather complex mixtures, and due to their chemical similarity are quite difficult to separate. The term rare earths is a misnomer, and these elements represent a potentially rich source of metals. The abundance, industrial potential, physical properties, and chemistry of the rare earths have been discussed extensively in the recent literature (1,2,3,4, 5,6,7) and will not be elaborated on here.

Spedding and Powell (8) have developed ion exchange techniques which have been used at the Ames Laboratory of the Atomic Energy Commission and by several chemical companies to prepare the pure lanthanides in industrial quantities. The work discussed in this thesis is a continuation of a long term project sponsored by the Chemical Engineering Division of Ames Laboratory to investigate the application of solvent extraction to the separation of the rare earths. It is thought that either a solvent extraction process or a combination of solvent extraction and ion exchange might possess certain advantages over the present process, such as more continuous operation and larger throughputs per dollar of capital investment.

Specifically, the purpose of this research was to propose and verify a calculation method to give the stagewise conditions

in a multistage cascade operating with the system $\text{La}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{Nd}(\text{NO}_3)_3 - \text{Sm}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$. If considered desirable, as was the case, the method was to be programmed for digital computer calculation.

The basic problem in this project, as in many projects of this type, was to develop a method of calculating the conditions in one equilibrium phase with the contacting equilibrium phase completely specified. Because of the large number of solutes present it is practically impossible to systematically investigate the equilibrium of the system of interest over the range of composition and concentration encountered in a solvent extraction cascade. Therefore the basic approach was to use experimentally determined equilibrium data for contributing systems to predict the equilibrium of the more complex system of interest.

The function of the nitric acid is threefold. The solvent, TBP, has a relatively high viscosity and a specific gravity approximately equal to that of water (about 0.98 at 20°C .). These characteristics have led to slow phase separation and emulsion formation in the past. The inclusion of nitric acid promotes rapid phase separation and inhibits emulsion formation. Also, the separation factors between the rare earth nitrates have been found to increase with increasing nitrate concentration of the system. The inclusion of nitric acid allows high nitrate concentrations without the

phase separation and emulsion problems mentioned above. On the debit side of the discussion, nitric acid is also extracted by TBP and complicates the system as an extra solute which must be considered.

PREVIOUS WORK

The first study of solvent extraction separation of the rare earths was made in 1937 by Fischer et al. (9). Since that time a large number of systems have been investigated, primarily by single stage "shakeups", and often using radioactive rare earth tracers. Typical studies are (10,11,12,13, 14,15). The field has also been reviewed extensively (16,17, 18,19).

In recent years most workers have followed one of two distinct approaches. The more fundamental approach has been based on the thermodynamic equilibrium constants for postulated complexing reactions between the solutes in the aqueous phase and the organic extractant. In contrast, several workers have approached the problem from a pragmatic point of view, obtaining equilibrium data for simple systems and then making approximations to extrapolate the available data to systems of interest. These two approaches are considered in more detail in the following sections.

Thermodynamic Equilibrium Constant Approach

Many thermodynamic studies have been reported in the literature, typical studies being (20,21,22,23,24,25). In general, the conclusions were that the extraction of many

solutes such as nitric acid and rare earth nitrates from aqueous solution by TBP may be considered the result of a reaction of the type

where b is the solvation number, that is, the number of TBP molecules complexed with one molecule of the extracted compound. For the rare earth nitrates b has been established to be three, and for nitric acid b is usually taken as one, although for nitric acid solubility considerations show such a simple picture to be impossible. That is, the solubility of nitric acid in TBP grossly exceeds the theoretical maximum as given by complete formation of $HNO_3 \cdot TBP$ in the organic phase. The present trend (26,27,28) is to consider the nitric acid extraction as an initial formation of $HNO_3 \cdot TBP$ followed by solubility of excess acid in the complex.

Rozen and Khorkhorina (29) have approached the equilibrium of the system $UO_2(NO_3)_2 - HNO_3 - TBP$ plus diluent - H_2O by a consideration of the proposed complexing reactions

and

The equilibrium constant values for these reactions plus

material balances make possible a calculation of the equilibrium organic concentrations if the aqueous concentrations are known. Several questionable assumptions are, however, necessary. No activity data are available for the reactants in the organic phase and so the activity coefficients of all organic constituents (the free TBP and the solvated complexes) are assumed to be unity. Activity measurements of uranyl nitrate in aqueous solution and of nitric acid in aqueous solution are available (30), but no justification is given by the authors for their use of these activity data for mixtures of uranyl nitrate and nitric acid. Also, as pointed out previously, the proposed reaction involving nitric acid is inadequate over the allowable nitric acid concentration range.

Jury and Whatley (31) have written a digital computer subroutine based on the equations of Rozen and Khorkhorina to calculate equilibrium points in the system discussed above. They do not compare their results with distribution data. Referring to their calculated distribution curves the authors conclude "Beyond the insipid observation that these curves seem to follow the behavior of what is known about the system, there is no quantitative criteria available for evaluating their accuracy". Although many of their calculated distributions appear reasonable, it is to be noted that under some conditions such as low values of the TBP concentration and high

values of the uranyl nitrate concentration the equations predict negative values of the solvent phase nitric acid concentration, which is, of course, impossible.

Olander (32) has written a digital computer program for multistage, multicomponent cascade design making use of equations of the form of Equation 1 alternating with material balance calculations. He assumed:

- (1) unit activity coefficients for all species,
- (2) complete dissociation of the solutes in the aqueous phase, and
- (3) no competing side reactions.

The first two assumptions are certainly in error to some undetermined extent, and the third is open to question. His program is for a center fed cascade and involves a multiple trial and error, the extract and raffinate conditions first being assumed and then working toward the center stage by stage from both ends with a match at the feed point the criteria of correct choice of the end streams. He states that it is impossible at present to estimate activity coefficients of mixed electrolytes containing more than two solutes and also to estimate the activity coefficients of the complexes and the unbound TBP in the organic phase. Consequently his calculation must be regarded solely as an order of magnitude approximation to the true number of theoretical stages.

Empirical Approach

Weaver et al. (33) produced better than a kilogram of 95% pure gadolinium oxide starting with a mixture of rare earth oxides containing about 30% gadolinium oxide. They used a 60:40 mixture of TBP in a hydrocarbon diluent and extracted a highly acidified solution of the rare earth nitrates many times in both batch extractions and counter-current extractions in a York Scheibel column. Their approach was primarily trial and error, empirically adjusting the operating conditions from extraction to extraction.

Peppard and Mason (34) report several simulated column extractions of milligram quantities of mixed rare earths. The aqueous phases were either acidified chloride or nitrate solutions and the organic extractant was TBP either undiluted or mixed with a light hydrocarbon diluent. No design procedure was given. In each case they obtained two enriched fractions, the light rare earths preferring the aqueous and the heavies preferentially extracting into the organic.

A series of reports by Michigan Chemical Corporation (35, 36, 37, 38, 39, 40, 41, 42, 43) describe the bench and pilot plant scale separation of yttrium from the rare earths and the division of the rare earths into a light enriched and a heavy enriched fraction. Some work was also done in attempting to strip lanthanum from a rare earth and yttrium mixture. The

solvent used in the latter study was monododecyl phosphoric acid plus hydrocarbon diluent and the aqueous phase acidified chloride or acetate solutions of the rare earths. In some cases a chelating agent was added to the aqueous strip. Yttrium of 98% purity was obtained.

At Ames Laboratory of the Atomic Energy Commission Bochinski (44) demonstrated the partial separation of the rare earths. He distributed the acid free nitrates between undiluted, water equilibrated TBP and water. He developed a design procedure based on two assumptions concerning the equilibrium distribution of the system. They are:

- (1) an average equilibrium curve may be used for all mixtures of the rare earths and
- (2) the separation factors between the rare earths are independent of the composition of the rare earth solutes and a function only of the total concentration of solutes present in an equilibrium stage.

Bochinski then "pinched" the total solute concentration, thus by assumption 2 holding the separation factors constant. He based his calculations on an oxides per liter basis.

Using Bochinski's method Schoenherr (45) set up a pilot plant separation run. Because of the aforementioned phase separation and emulsion formation problems he acidified the system with nitric acid. The stages were preloaded with a fixed nitric acid concentration, the feed and strip were also

at this acid concentration, and the organic was pre-equilibrated with an aqueous of the specified acidity. Under these conditions it was hoped that the acid concentration in the system would remain constant and Bochinski's method could be used to predict the stagewise rare earth compositions and concentrations. This condition was not realized and it was found that the acid, if included, must be considered as a solute. Schoenherr (46), Sharp (47), and Dinnin (48) then collected distribution data for various acidified systems, the object being to predict the equilibrium of the complex acidified systems of interest.

The project described in this report is essentially a continuation of this work carried out at the Ames Laboratory. After a consideration of the state of development of the field of thermodynamic chemistry applied to concentrated, multicomponent ionic solutions, it was the opinion of the author that an empirical approach of this type was more likely to yield a realistic design procedure than the thermodynamic equilibrium constant approach.

METHOD OF CALCULATION

In this section the proposed calculation method will be discussed in detail. The data used in the calculation method are single stage "shake-up" distributions for the systems

- I $\text{La}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$,
- II $\text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$,
- III $\text{Nd}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$,
- IV $\text{Sm}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$,
- V $\text{La}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$,
- VI $\text{Nd}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$,
- VII $\text{Sm}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$.

The data for systems I, II, V, VI, and VII were collected by the author by the method described in detail by Sharp (47). The bulk of the data for systems III and IV were taken from the work of Schoenherr (46), supplemented to a small degree by work of the author. A complete compilation of the equilibrium data used is given in Appendix B.

Equilibrium Phase Calculation

The method to be discussed in this section is the calculation of all concentrations of one equilibrium phase with all concentrations of the contacting phase specified. The general procedure was:

- (1) to obtain values of K_t and K_{HNO_3} by interpolation using data obtained from the contributing two solute systems and then use the defining equations

$$K_t = (M_t)_{\text{org.}} / (M_t)_{\text{aq.}}, \quad (4)$$

$$K_{\text{HNO}_3} = (M_{\text{HNO}_3})_{\text{org.}} / (M_{\text{HNO}_3})_{\text{aq.}}, \quad (5)$$

$$M_{\text{RE}} = M_t - M_{\text{HNO}_3}, \quad (6)$$

to calculate the total molality, HNO_3 molality, and the rare earth molality of the unspecified phase, followed by

- (2) the use of separation factors between the rare earths obtained from data for the contributing three solute systems in one of the equations

$$(M_i)_{\text{org.}} = \frac{(M_{\text{RE}})_{\text{org.}} \times \beta_{i-\text{Pr}} \times (M_i)_{\text{aq.}}}{\sum_{i=1}^T (\beta_{i-\text{Pr}} \times (M_i)_{\text{aq.}})}, \quad (7)$$

$$(M_i)_{\text{aq.}} = \frac{(M_{\text{RE}})_{\text{aq.}} \times (M_i)_{\text{org.}}}{\beta_{i-\text{Pr}} \times \sum_{i=1}^T ((M_i)_{\text{org.}} / \beta_{i-\text{Pr}})}, \quad (8)$$

to calculate the rare earth molalities of the unspecified phase. Equations 7 and 8 follow directly from the definition of separation factor and are applicable, of course, only to the rare earths present.

Considering this calculation in more detail, the data from systems I, II, III, and IV were processed to give a series of plots of K_t and K_{HNO_3} versus the composition of an equilibrium phase with the total molality of the same phase as parameter. Typical plots are shown in Figures 1 through 8. A complete compilation of the values from these plots is given in Appendix D.

The separation factors from systems V, VI, and VII were plotted versus the total molality of the organic phase as shown in Figure 9. In each case the rare earth separation factors are seen to be, to a good approximation, a function of the total nitrate molality of the equilibrium organic phase and relatively independent of the phase composition. This observation parallels Bochinski's (44) observation of the acid free system. The curves of Figure 9 were fitted to straight lines by the least squares method to give

$$\beta_{\text{La-Pr}} = 0.8187 - 0.1106(M_t)_{\text{org.}} \quad , \quad (9)$$

$$\beta_{\text{Nd-Pr}} = 1.0448 + 0.09874(M_t)_{\text{org.}} \quad , \quad (10)$$

$$\beta_{\text{Sm-Pr}} = -0.3795 + 0.9214(M_t)_{\text{org.}} \quad . \quad (11)$$

These correlations were assumed to hold with $(M_t)_{\text{org.}}$ greater than 1.75.

At this point a gross assumption was made. It was assumed that Equations 9, 10, and 11 would hold also in the five

Figure 1. Nitric acid distribution coefficient for $RE(NO_3)_3 - HNO_3 - TBP - H_2O$ systems as a function of the composition of the organic phase at $(M_t)_{org.}$ equal to 3.0

Figure 2. Nitric acid distribution coefficient for $\text{RE}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O systems as a function of the composition of the organic phase at $(M_t)_{\text{org}}$ equal to 3.5

Figure 3. Total distribution coefficient for $RE(NO_3)_3$ - HNO_3 - TBP - H_2O systems as a function of the composition of the organic phase at $(M_t)_{org.}$ equal to 3.0

Figure 4. Total distribution coefficient for $RE(NO_3)_3$ - HNO_3 - TBP - H_2O systems as a function of the composition of the organic phase at $(M_t)_{org.}$ equal to 3.5

Figure 5. Nitric acid distribution coefficient for $RE(NO_3)_3 - HNO_3 - TBP - H_2O$ systems as a function of the composition of the aqueous phase at $(M_t)_{aq.}$ equal to 5.0

Figure 6. Nitric acid distribution coefficient for $RE(NO_3)_3$ - HNO_3 - TBP - H_2O systems as a function of the composition of the aqueous phase at $(M_t)_{aq.}$ equal to 7.0

Figure 7. Total distribution coefficient for $RE(NO_3)_3 - HNO_3 - TBP - H_2O$ systems as a function of the composition of the aqueous phase at $(M_t)_{aq.}$ equal to 5.0

Figure 8. Total distribution coefficient for $RE(NO_3)_3 - HNO_3 - TBP - H_2O$ systems as a function of the composition of the aqueous phase at $(M_t)_{aq.}$ equal to 7.0

Figure 9. Separation factor between $RE(NO_3)_3$ and $Pr(NO_3)_3$ for $RE(NO_3)_3 - Pr(NO_3)_3 - HNO_3 - TBP - H_2O$ systems as a function of concentration of the organic phase

solute system $\text{La}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{Nd}(\text{NO}_3)_3 - \text{Sm}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$. The limitations of such a sweeping assumption may only be ascertained empirically, therefore the usefulness of the approximation must be judged by the comparison with experimental results in the Verification of Model section.

Sample calculation

A sample calculation is now given to illustrate this method. It was assumed that an equilibrium organic phase has the following concentrations:

$$(M_t)_{\text{org.}} = 3.0261 \quad ,$$

$$(M_{\text{HNO}_3})_{\text{org.}} = 2.3590 \quad ,$$

$$(M_{\text{La}})_{\text{org.}} = 0.0397 \quad ,$$

$$(M_{\text{Pr}})_{\text{org.}} = 0.0460 \quad ,$$

$$(M_{\text{Nd}})_{\text{org.}} = 0.0706 \quad ,$$

$$(M_{\text{Sm}})_{\text{org.}} = 0.5108 \quad ,$$

$$(M_{\text{RE}})_{\text{org.}} = 0.6671 \quad .$$

From these data were calculated

$$Y_{\text{HNO}_3} = (M_{\text{HNO}_3})_{\text{org.}} / (M_t)_{\text{org.}} = 2.3590 / 3.0261 = 0.7796 \quad ,$$

$$Y_{\text{RE}} = (M_{\text{RE}})_{\text{org.}} / (M_t)_{\text{org.}} = 0.6671 / 3.0261 = 0.2204 \quad ,$$

$$y_{\text{La}} = (M_{\text{La}})_{\text{org.}} / (M_{\text{RE}})_{\text{org.}} = 0.0397 / 0.6671 = 0.0595 \quad ,$$

$$y_{\text{Pr}} = (M_{\text{Pr}})_{\text{org.}} / (M_{\text{RE}})_{\text{org.}} = 0.0460 / 0.6671 = 0.0690 \quad ,$$

$$y_{\text{Nd}} = (M_{\text{Nd}})_{\text{org.}} / (M_{\text{RE}})_{\text{org.}} = 0.0706 / 0.6671 = 0.1058 \quad ,$$

$$y_{\text{Sm}} = (M_{\text{Sm}})_{\text{org.}} / (M_{\text{RE}})_{\text{org.}} = 0.5108 / 0.6671 = 0.7657 \quad .$$

To obtain the value of K_t it was first assumed that all the rare earth nitrates present were $\text{La}(\text{NO}_3)_3$. That is, $Y_{\text{RE}} = Y_{\text{La}} = 0.2204$. Then, by straight line interpolation between the total molality parameters of Figures 3 and 4, a value of K_t was obtained that would hold for the case of $(M_t)_{\text{org.}} = 3.0261$ and $Y_{\text{RE}} = Y_{\text{La}} = 0.2204$. This was $K_t = 0.4031$. Exactly the same procedure was then followed to get values for K_t assuming, in succession, that all the rare earths present were $\text{Pr}(\text{NO}_3)_3$, $\text{Nd}(\text{NO}_3)_3$, and $\text{Sm}(\text{NO}_3)_3$. To then get the K_t used in the calculation each K_t derived from the assumption of only one rare earth solute was multiplied by the fraction of the rare earths present as that particular solute. In other words, the contribution from the $\text{La}(\text{NO}_3)_3$ system to the final value of K_t was assumed to be equal to the value of K_t for the $\text{La}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ system multiplied by y_{La} . Or arithmetically, the contribution was $(0.4031) \times (0.0595) = 0.0240$. The sum of the four contributions was then the value of K_t used.

Exactly the same procedure, using Figures 1 and 2 was then used to get a value of K_{HNO_3} for the case in question.

The values so obtained were

$$K_t = 0.5200 \quad ,$$

$$K_{\text{HNO}_3} = 0.6114 \quad .$$

The values of $(M_t)_{\text{aq.}}$, $(M_{\text{HNO}_3})_{\text{aq.}}$, and $(M_{\text{RE}})_{\text{aq.}}$ were then calculated from Equations 4, 5 and 6 to be

$$(M_t)_{\text{aq.}} = (M_t)_{\text{org.}}/K_t = 3.0261/0.5200 = 5.8194 \quad ,$$

$$(M_{\text{HNO}_3})_{\text{aq.}} = (M_{\text{HNO}_3})_{\text{org.}}/K_{\text{HNO}_3} = 2.3590/0.6114 = 3.8584 \quad ,$$

$$(M_{\text{RE}})_{\text{aq.}} = (M_t)_{\text{aq.}} - (M_{\text{HNO}_3})_{\text{aq.}} = 5.8194 - 3.8584 = 1.9610 \quad .$$

Using $(M_t)_{\text{org.}} = 3.0261$ the separation factors were calculated as

$$\beta_{\text{La-Pr}} = 0.4840 \quad ,$$

$$\beta_{\text{Nd-Pr}} = 1.3436 \quad ,$$

$$\beta_{\text{Sm-Pr}} = 2.4087 \quad .$$

Note that, by definition, $\beta_{\text{Pr-Pr}}$ is equal to 1.0.

The rare earth molalities of the aqueous phase were then calculated by Equation 8 as follows:

$$\begin{aligned} \sum_{i=1}^T ((M_i)_{\text{org.}}/\beta_{i-\text{Pr}}) &= (M_{\text{La}})_{\text{org.}}/\beta_{\text{La-Pr}} + (M_{\text{Pr}})_{\text{org.}}/\beta_{\text{Pr-Pr}} + \\ &\quad (M_{\text{Nd}})_{\text{org.}}/\beta_{\text{Nd-Pr}} + (M_{\text{Sm}})_{\text{org.}}/\beta_{\text{Sm-Pr}} \quad , \\ \sum_{i=1}^T ((M_i)_{\text{org.}}/\beta_{i-\text{Pr}}) &= 0.0397/0.4840 + 0.0460/1.0000 + \\ &\quad 0.0706/1.3436 + 0.5108/2.4087 \quad , \end{aligned}$$

$$\sum_{i=1}^T ((M_i)_{\text{org.}} / \beta_{i-\text{Pr}}) = 0.3926$$

$$(M_{\text{La}})_{\text{aq.}} = \frac{(M_{\text{RE}})_{\text{aq.}} \times (M_{\text{La}})_{\text{org.}}}{\beta_{\text{La-Pr}} \times \sum_{i=1}^T ((M_i)_{\text{org.}} / \beta_{i-\text{Pr}})}$$

$$= \frac{(1.9610)(0.0397)}{(0.4840)(0.3926)} = 0.4097$$

and in exactly the same manner

$$(M_{\text{Pr}})_{\text{aq.}} = 0.2298 \quad ,$$

$$(M_{\text{Nd}})_{\text{aq.}} = 0.2625 \quad ,$$

$$(M_{\text{Sm}})_{\text{aq.}} = 1.0592 \quad .$$

If the reverse calculation had been desired, the same procedure would have been followed, first using plots of the type portrayed in Figures 5, 6, 7, and 8 to get K_t and K_{HNO_3} , calculating then $(M_t)_{\text{org.}}$, $(M_{\text{HNO}_3})_{\text{org.}}$, and $(M_{\text{RE}})_{\text{org.}}$, and then, after calculating the separation factors, using Equation 7 to calculate the rare earth molalities.

Application to Multistage Calculations

It was desired to apply the model to the calculation of the stagewise conditions in an ideal multistage cascade. Referring to Figures 10 and 11 it is seen that if any point on

Figure 10. Cascade I

Figure 11. Cascade II

the operating line is known, that is, if two streams passing each other are completely defined, the conditions for any number of stages may be calculated "backwards" through the column if the operating line equation is known. The direction such a calculation would follow is shown by the dashed arrows in Figures 10 and 11. Obviously, but to ensure clarity, the calculation would be composed of alternating applications of the equilibrium model and the operating line.

In the present work, the assumption of mutual immiscibility of water and TBP was made. Writing a general operating line for the cascade pictured in Figure 10 gives

$$\left[(M_1)_{S_0} \times S_0 \right] + \left[(M_1)_{R_n} \times R_n \right] = \left[(M_1)_{S_{n-1}} \times S_{n-1} \right] + \left[(M_1)_{R_1} \times R_1 \right] \quad (12)$$

By the assumption of mutual immiscibility $S_0 = S_{n-1}$ and $R_n = R_1$ and so the subscripts may be deleted, and after rearrangement

$$(M_1)_{R_n} = \alpha(M_1)_{S_{n-1}} - \alpha(M_1)_{S_0} + (M_1)_{R_1} \quad (13)$$

The assumption of mutual immiscibility of water and TBP was felt to be justified. The solubility of TBP in water is very low, on the order of tenths of a gram per liter, and the solubility of water in TBP does not exceed approximately six percent by weight. Because the solvent is normally equi-

librated with water before use, the assumption of constant water content does not introduce a large error.

Using the proposed equilibrium model and operating lines of the form of Equation 13 several calculations of the stage-wise conditions in various cascades were carried out. The procedure was to arbitrarily choose the end conditions, either R_1 and S_0 for the cascade in Figure 10, or R_0 and S_1 for the cascade in Figure 11, and then to proceed as explained previously. The purposes of these calculations were to obtain a "feel" for the possible separations that could be made with the system and to select several predictions for experimental verification.

At this point an unexpected problem arose. In several of the calculations the total molality was "pinched" at a high value. This was done to impress high separation factors on the system, since, with the equilibrium model proposed the separation factors increase with increased total concentration. In each case in which this was done the individual concentrations also quickly "pinched". When the end conditions and flow ratio were chosen so that the total concentration changed from stage to stage no such "pinch" of the individual solutes was calculated.

The study of this "pinch" based on the limit of a sequence that can be written describing the molality of a general component in successive streams of a cascade is an inter-

esting problem the author has not been able to solve completely. A discussion of this approach is given in Appendix C.

As the stagewise calculation is quite tedious and time consuming, four digital computer programs were written for various cascades of interest. These programs were compiled and debugged on the IBM 7074. Although some calculations were made with each program they are intended primarily for future use in design and optimization studies, and as guides for further programming. A complete discussion of these programs is given in Appendix D.

VERIFICATION OF MODEL

A specification of the source and method of preparation of the materials used in the experimental phase of this project follows:

Tributyl phosphate Commercial grade TBP, obtained from Commercial Solvents Corporation, was pre-equilibrated with distilled water before use as the solvent. The TBP was stored in contact with a water phase to ensure equilibrium.

Nitric acid Reagent grade nitric acid was used in all laboratory work.

Rare earth nitrate solutions The oxides of La, Pr, Nd, and Sm, 99.9 percent pure, were obtained from the ion exchange group of the Ames Laboratory of the Atomic Energy Commission. Stock nitrate solutions of each rare earth were prepared by dissolving the oxides in boiling, concentrated nitric acid. After complete reaction, the excess nitric acid was boiled off and distilled water added. All feed solutions for the simulated column experiments were prepared by mixing these stock solutions, reagent grade concentrated nitric acid and distilled water.

As mentioned previously, the simulated column technique was used to obtain experimental stagewise conditions for comparison with the predicted values. Briefly, a simulated column experiment is a batchwise approximation to a continuous counter-

current cascade. The error in the approximation may be made arbitrarily small by increasing the number of cycles the experiment is run. The mechanics and mathematical demonstrations involved will not be gone into here as this technique has been discussed extensively by Scheibel (49,50,51,52).

Four of the prediction calculations discussed in the Method of Calculation section were chosen for simulation. The experiments were carried out in laboratory glassware at room temperature, using 1/100 horsepower laboratory stirrers for the mixing steps. A minimum of two minutes mixing and three minutes settling time was maintained for each contact.

Along with the phases from the final cycle, the leaving aqueous phase from each cycle was retained and analyzed as a check on the approach to steady state. In all cases the number of cycles was felt to be sufficient.

All organic and aqueous phases from the final cycle were analyzed for total oxides, nitric acid content, and rare earth composition. The analytical methods used are discussed in Appendix A.

A complete compilation of the experimental conditions and the final experimental-predicted comparisons from these four simulations is given on pages 32 to 52. In each case, the first figure gives all pertinent experimental conditions, including the simulation pattern and the continuous cascade being simu-

lated, and is followed by both tabular and graphic experimental-predicted concentration and composition comparisons.

TOTAL NUMBER OF CYCLES - 11

, FLOW RATE RATIO = $\alpha = 0.5$

VOLUME R_{11} /INJECTION = 74.6 ml.

, CONCENTRATION R_{11} : $M_{HNO_3} = 1.86$, $M_{RE} = 6.89$

VOLUME S_0 /INJECTION = 30.7 ml.

, CONCENTRATION S_0 : $M_{HNO_3} = 0.00$, $M_{RE} = 0.00$

Figure 12. General information pertaining to Simulated Column Experiment I

Table 1. Comparison of experimental and predicted compositions and concentrations for Simulated Column Experiment I

	Weight % La ₂ O ₃ in total oxides <u>exp. pred.</u>		Weight % Pr ₆ O ₁₁ in total oxides <u>exp. pred.</u>		Weight % Nd ₂ O ₃ in total oxides <u>exp. pred.</u>		Weight % Sm ₂ O ₃ in total oxides <u>exp. pred.</u>		Grams total oxides per gram of so- lution <u>exp. pred.</u>		Grams HNO ₃ per gram of solution <u>exp. pred.</u>	
R ₁	32.3	32.3	25.2	25.3	25.6	25.0	17.0	17.3	0.191	0.195	0.039	0.037
R ₂	30.0	29.5	26.8	24.8	25.0	25.6	18.2	20.1	0.208	0.211	0.055	0.053
R ₃	28.0	29.2	25.4	24.5	25.9	25.4	20.7	21.0	0.206	0.208	0.060	0.060
R ₄	28.8	29.3	24.7	24.4	25.7	25.3	20.8	21.1	0.204	0.207	0.062	0.062
R ₅	28.4	29.3	26.4	24.4	25.4	25.2	19.8	21.0	0.204	0.207	0.062	0.062
R ₆	29.9	29.3	25.2	24.4	25.0	25.2	19.9	21.0	0.203	0.207	0.062	0.063
R ₇	29.7	29.3	24.8	24.4	25.4	25.2	20.2	21.0	0.202	0.207	0.062	0.063
R ₈	29.1	29.3	24.4	24.4	28.8	25.2	17.8	21.0	0.202	0.207	0.062	0.063
R ₉	29.2	29.3	24.8	24.4	26.5	25.2	19.5	21.0	0.202	0.207	0.062	0.063
R ₁₀	30.1	29.3	24.9	24.4	26.0	25.2	18.9	21.0	0.205	0.207	0.062	0.063
R ₁₁	29.0	29.3	24.9	24.4	26.5	25.2	19.6	21.0	0.204	0.207	0.062	0.063
S ₁	12.1	13.1	22.4	21.6	28.4	28.8	37.1	36.6	0.088	0.088	0.054	0.054

Table 1 (Continued)

	Weight % La ₂ O ₃ in		Weight % Pr ₆ O ₁₁ in		Weight % Nd ₂ O ₃ in		Weight % Sm ₂ O ₃ in		Grams total oxides per gram of so- lution		Grams HNO ₃ per gram of solution	
	<u>total</u> <u>oxides</u>		<u>total</u> <u>oxides</u>		<u>total</u> <u>oxides</u>		<u>total</u> <u>oxides</u>		<u>exp.</u> <u>pred.</u>		<u>exp.</u> <u>pred.</u>	
	exp. pred.		exp. pred.		exp. pred.		exp. pred.		exp. pred.		exp. pred.	
S ₂	8.0	10.0	19.9	19.1	28.8	27.4	43.3	43.5	0.085	0.083	0.071	0.074
S ₃	9.4	9.6	18.8	18.6	28.1	26.7	43.8	45.2	0.082	0.080	0.076	0.080
S ₄	9.3	9.5	19.1	18.5	27.5	26.6	44.1	45.4	0.081	0.078	0.078	0.082
S ₅	9.4	9.6	19.0	18.5	27.1	26.6	44.5	45.4	0.080	0.078	0.078	0.083
S ₆	10.0	9.6	18.7	18.5	27.0	26.6	44.4	45.3	0.081	0.078	0.078	0.083
S ₇	10.1	9.6	19.0	18.5	27.2	26.6	43.6	45.3	0.080	0.078	0.078	0.083
S ₈	7.5	9.6	20.5	18.5	28.3	26.6	43.7	45.3	0.081	0.078	0.078	0.083
S ₉	10.2	9.6	19.0	18.5	26.0	26.6	44.8	45.3	0.081	0.078	0.077	0.083
S ₁₀	8.2	9.6	19.8	18.5	27.5	26.6	44.5	45.3	0.081	0.078	0.077	0.083

Figure 13. Stagewise aqueous rare earth oxide composition for Simulated Column Experiment I

Figure 14. Stagewise organic rare earth oxide composition for Simulated Column Experiment I

Figure 15. Stagewise organic rare earth oxide and nitric acid concentrations for Simulated Column Experiment I

Figure 16. Stagewise aqueous rare earth oxide and nitric acid concentrations for Simulated Column Experiment I

TOTAL NUMBER OF CYCLES - 10

, FLOW RATE RATIO = $\alpha = 8.0$

VOLUME R_0 /INJECTION = 30.0 ml.

, CONCENTRATION $R_0:M_{HNO_3} = 0.00$, $M_{RE} = 0.00$

VOLUME S_{11} /INJECTION = 245.2 ml.

, CONCENTRATION $S_{11}:M_{HNO_3} = 0.00$, $M_{RE} = 0.00$

VOLUME F /INJECTION = 215.6 ml.

, CONCENTRATION $F:M_{HNO_3} = 6.66$, $M_{RE} = 11.69$

CONTINUOUS

CASCADE

BEING

SIMULATED

Figure 17. General information pertaining to Simulated Column Experiment II

Table 2. Comparison of experimental and predicted compositions and concentrations for Simulated Column Experiment II

	Weight % La_2O_3 in total oxides		Weight % Pr_6O_{11} in total oxides		Weight % Nd_2O_3 in total oxides		Weight % Sm_2O_3 in total oxides		Grams total oxides per gram of so- lution		Grams HNO_3 per gram of solution	
	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.
R ₁	7.3	11.2	10.4	9.5	11.4	12.1	70.9	67.3	0.052	0.058	0.139	0.136
R ₂	14.6	19.9	12.9	11.7	11.9	13.2	60.6	55.2	0.072	0.076	0.168	0.167
R ₃	26.4	31.0	15.0	12.3	10.5	12.6	48.2	44.1	0.087	0.092	0.172	0.171
R ₄	37.4	43.4	14.7	11.5	8.6	10.9	39.3	34.2	0.103	0.108	0.165	0.164
R ₅	50.6	55.4	12.0	9.8	7.0	8.7	30.4	26.0	0.122	0.126	0.152	0.151
R ₆	62.8	65.8	9.8	7.9	4.2	6.7	23.2	19.6	0.140	0.145	0.136	0.136
R ₇	72.9	74.0	7.5	6.1	2.6	5.1	17.0	14.9	0.163	0.166	0.117	0.119
R ₈	82.3	80.0	3.4	4.6	1.2	3.9	13.2	11.4	0.184	0.186	0.102	0.104
R ₉	81.3	84.4	6.1	3.6	2.5	3.1	10.1	8.9	0.204	0.207	0.088	0.090
R ₁₀	86.4	87.8	5.8	2.8	1.9	2.4	5.8	7.0	0.220	0.228	0.076	0.077
F	83.0	81.2	2.9	3.0	0.8	3.0	13.2	12.8	0.235	0.238	0.153	0.156
S ₁	0.0	3.8	5.7	5.9	10.8	9.7	83.5	80.6	0.023	0.024	0.108	0.107

Table 2 (Continued)

	Weight % La ₂ O ₃ in total oxides		Weight % Pr ₆ O ₁₁ in total oxides		Weight % Nd ₂ O ₃ in total oxides		Weight % Sm ₂ O ₃ in total oxides		Grams total oxides per gram of so- lution		Grams HNO ₃ per gram of solution	
	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.
S ₂	3.4	5.6	7.1	6.8	11.9	10.3	77.6	77.3	0.029	0.031	0.124	0.122
S ₃	6.5	9.0	8.2	7.8	12.5	10.9	72.8	72.3	0.032	0.035	0.127	0.126
S ₄	10.5	14.1	8.9	8.4	12.4	10.8	68.3	66.7	0.034	0.037	0.129	0.127
S ₅	18.6	20.7	9.2	8.3	11.2	10.2	61.0	60.7	0.037	0.040	0.128	0.126
S ₆	25.5	28.3	9.3	7.8	10.5	9.3	54.6	54.6	0.040	0.044	0.126	0.125
S ₇	36.3	36.1	7.4	6.9	9.9	8.2	46.5	48.8	0.044	0.047	0.124	0.122
S ₈	45.4	43.4	5.7	6.0	8.4	7.1	40.5	43.5	0.047	0.052	0.121	0.119
S ₉	51.2	49.8	5.4	5.1	7.5	6.2	35.9	38.8	0.052	0.056	0.117	0.116
S ₁₀	50.7	55.5	5.0	4.4	5.7	5.5	38.6	34.6	0.057	0.062	0.115	0.114

Figure 18. Stagewise aqueous rare earth oxide composition for Simulated Column Experiment II

Figure 19. Stagewise organic rare earth oxide composition for Simulated Column Experiment II

Figure 20. Stagewise organic rare earth oxide and nitric acid concentrations for Simulated Column Experiment II

Figure 21. Stagewise aqueous rare earth oxide and nitric acid concentrations for Simulated Column Experiment II

Figure 22. General information pertaining to Simulated Column Experiment III

Table 3. Comparison of experimental and predicted compositions and concentrations for Simulated Column Experiment III

	Weight % La ₂ O ₃ in total oxides		Weight % Pr ₆ O ₁₁ in total oxides		Weight % Nd ₂ O ₃ in total oxides		Weight % Sm ₂ O ₃ in total oxides		Grams total oxides per gram of so- lution		Grams HNO ₃ per gram of solution	
	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.
S ₁	65.8	66.8	10.5	11.4	11.5	12.1	12.3	9.7	0.049	0.060	0.044	0.031
S ₂	43.7	47.4	12.8	12.8	16.7	16.7	26.8	23.1	0.050	0.061	0.098	0.083
S ₃	29.1	28.5	10.7	11.1	17.0	17.4	43.3	43.1	0.039	0.046	0.137	0.128
S ₄	26.9	19.6	7.1	8.2	13.5	14.1	52.5	58.1	0.032	0.035	0.156	0.154
S ₅	17.0	17.8	6.7	6.7	10.2	11.3	66.0	64.3	0.030	0.030	0.163	0.166
R ₁	79.6	79.3	8.2	8.3	7.4	7.2	4.9	5.3	0.118	0.127	0.025	0.016
R ₂	77.8	73.7	9.3	9.7	5.2	9.4	7.7	7.3	0.163	0.183	0.081	0.055
R ₃	64.5	64.3	10.2	10.4	11.3	11.6	13.9	13.6	0.158	0.174	0.148	0.122
R ₄	61.8	58.7	8.7	9.4	9.9	11.3	19.5	20.6	0.139	0.151	0.199	0.182
R ₅	62.4	58.8	7.8	8.3	8.6	9.5	21.2	23.4	0.130	0.136	0.223	0.216
R ₆	63.9	60.4	7.1	7.8	7.5	8.4	21.4	23.4	0.126	0.128	0.232	0.232

Figure 23. Stagewise aqueous rare earth oxide composition for Simulated Column Experiment III

Figure 24. Stagewise organic rare earth oxide composition for Simulated Column Experiment III

Figure 25. Stagewise organic rare earth oxide and nitric acid concentrations for Simulated Column Experiment III

Figure 26. Stagewise aqueous rare earth oxide and nitric acid concentrations for Simulated Column Experiment III

Figure 27. General information pertaining to Simulated Column Experiment IV

Table 4. Comparison of experimental and predicted compositions and concentrations for Simulated Column Experiment IV

	Weight % La_2O_3 in total oxides		Weight % Pr_6O_{11} in total oxides		Weight % Nd_2O_3 in total oxides		Weight % Sm_2O_3 in total oxides		Grams total oxides per gram of so- lution		Grams HNO_3 per gram of solution	
	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.	exp.	pred.
S_1	7.0	9.1	17.9	19.0	21.8	21.8	53.4	50.0	0.052	0.050	0.136	0.142
S_2	6.9	9.1	17.9	19.0	22.3	21.9	52.9	50.1	0.053	0.050	0.135	0.142
S_3	7.1	9.1	18.2	19.2	22.7	22.2	51.9	49.5	0.054	0.052	0.132	0.138
S_4	7.7	10.1	19.7	20.7	25.1	23.6	47.5	45.7	0.059	0.058	0.122	0.127
S_5	14.3	16.0	24.5	24.7	27.6	25.2	33.6	34.1	0.067	0.067	0.088	0.090
R_0		34.0		25.8		20.4		19.8		0.191		0.149
R_1	33.4	34.0	23.9	25.8	20.7	20.4	22.0	19.9	0.193	0.191	0.147	0.149
R_2	33.2	33.9	24.2	25.8	21.7	20.5	21.0	19.9	0.194	0.192	0.145	0.147
R_3	33.5	33.6	25.9	25.9	21.9	20.7	18.8	19.7	0.197	0.196	0.138	0.140
R_4	34.8	34.3	25.8	26.6	22.0	21.1	17.4	18.0	0.204	0.204	0.118	0.117
R_5	36.4	38.9	24.6	27.1	21.8	20.1	17.2	13.9	0.185	0.188	0.072	0.071

Figure 28. Stages aqueous rare earth oxide and nitric acid concentrations for Simulated Column Experiment IV

Figure 29. Stages aqueous rare earth oxide composition for Simulated Column Experiment IV

Figure 30. Stage-wise organic rare earth oxide and nitric acid concentrations for Simulated Column Experiment IV

Figure 31. Stage-wise organic rare earth oxide composition for Simulated Column Experiment IV

CONCLUSIONS

1. The calculation method developed for the multistage multisolute system gave good agreement with experimental data from four simulated column experiments. The conditions for each of the four simulated column experiments were quite different, and the agreement between predicted values and experimental data was believed to be a valid test of the method.

2. The assumption made that the separation factor between two rare earth nitrate solutes was a function only of the total molality of the organic phase, when $(M_t)_{org.}$ was greater than 1.75, was found to give surprisingly reliable results. The reason for the validity of this assumption is not known, but it appears to be a good approximation.

3. The digital computer technique for deriving distribution coefficients from a series of arrays was accurate and convenient. The technique makes it possible to use experimentally determined equilibrium data directly in the computer solution rather than introduce the data in terms of a mathematical correlation.

4. The digital computer programs for stage by stage calculations should make it possible to carry out various studies on the effects of process variables, such as the effect of acidity of an internal feed stage on recovery in an

end stream, etc. Such studies without the use of machine calculations would be prohibitively time consuming.

5. The flame spectroscopic analytical technique developed by the analytical chemistry group headed by Dr. V. A. Fassel of the Ames Laboratory of the Atomic Energy Commission has been found to give reliable results for each of the rare earths used in this study. The fact that lanthanum can now be determined directly, rather than by difference, is a significant scientific advance in studies of this type.

RECOMMENDATIONS FOR FUTURE WORK

There are several logical extensions of the present work, the most straightforward being an incorporation into the calculation method of systems with a greater number of rare earth nitrate solutes.

Assuming that it was desired to incorporate a rare earth nitrate solute denoted $\text{RE}(\text{NO}_3)_3$ into the method it would be necessary to acquire single stage equilibrium data for the systems $\text{RE}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ and $\text{RE}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ by the methods described by Sharp (47). These data could then be processed in the manner described in the Method of Calculation section, and the calculation for the six solute system $\text{La}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{Nd}(\text{NO}_3)_3 - \text{Sm}(\text{NO}_3)_3 - \text{RE}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ would follow exactly the steps also given in that section. Also, the modification of the computer programs for the six solute system would be completely straightforward, as no changes would be made in the logic flow as described in Appendix D.

Such incorporation might be a worthwhile program if it was desired to apply this work to the design of ore processing equipment.

An interesting computer extension would be the writing of a program for a center fed cascade, the calculation to

start from both ends from an initial assumption of end conditions, and, continuously modifying the end concentrations, repeat the calculation a large number of times, endeavoring to match all concentrations at the feed stage.

There are also possibilities of using the existing computer programs, plus others that could be written, in various optimization studies. Because of the large number of variables such a project would probably have to have a statistical basis, and would probably be primarily of academic interest.

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APPENDIX A. ANALYTICAL PROCEDURES

Weighed samples of each equilibrium phase were analyzed. The solutes in the organic samples were transferred to aqueous solution prior to analysis. This was accomplished by contacting the organic samples a minimum of three times with distilled water. The aqueous phases were combined and analyzed in the same manner as the aqueous phase samples.

For the determination of total rare earths the aqueous sample was diluted to approximately 200 ml. with distilled water, brought to a boil on a hot plate, and the rare earths completely precipitated with a saturated solution of oxalic acid. The oxalates were filtered and converted to the oxides at approximately 870° C. in a muffle furnace. The weight of the oxides was determined on an analytical balance.

The composition of the final rare earth oxide sample was determined by a flame photometric method developed by members of the analytical chemistry group headed by Dr. V. A. Fassel of the Ames Laboratory of the Atomic Energy Commission.

To determine the nitric acid content, the samples were diluted to approximately 200 ml. and the rare earths present precipitated by addition of an excess of saturated potassium ferrocyanide. The nitric acid content was then determined by titration with standardized sodium hydroxide. An automatic titrater was used and the end point was taken at a pH of 8.7.

It was found that the nitric acid content of aqueous solutions of nitric acid and potassium ferrocyanide diminishes with time. This was thought to be due to oxidation by the acid. To obtain satisfactory analyses for the nitric acid it was necessary to titrate the aqueous solutions of nitric acid, potassium ferrocyanide, and precipitated rare earth ferrocyanides within about 15 minutes after addition of the potassium ferrocyanide solution.

APPENDIX B. EQUILIBRIUM DATA

Table 5. Equilibrium data for the system $\text{La}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$

	Aqueous phase			Organic phase		
	Grams of $\text{La}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{La}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
1	0.127	0.065	0.808	0.026	0.075	0.899
2	0.170	0.087	0.743	0.035	0.095	0.871
3	0.204	0.112	0.684	0.037	0.113	0.849
4	0.258	0.147	0.595	0.037	0.143	0.820
5	0.309	0.173	0.519	0.035	0.161	0.804
6	0.169	0.036	0.796	0.051	0.054	0.896
7	0.214	0.050	0.736	0.061	0.070	0.869
8	0.278	0.064	0.658	0.074	0.087	0.839
9	0.351	0.082	0.567	0.078	0.112	0.810
10	0.419	0.093	0.488	0.078	0.134	0.788
11	0.070	0.099	0.831	0.011	0.090	0.899
12	0.089	0.131	0.781	0.014	0.115	0.871
13	0.111	0.173	0.716	0.015	0.140	0.845
14	0.142	0.229	0.629	0.013	0.170	0.817
15	0.162	0.283	0.555	0.012	0.191	0.798
16	0.032	0.126	0.842	0.004	0.097	0.898
17	0.046	0.166	0.789	0.006	0.121	0.873
18	0.055	0.232	0.713	0.005	0.154	0.841
19	0.072	0.288	0.640	0.006	0.177	0.817
20	0.089	0.343	0.568	0.005	0.194	0.801
21	0.211	0.013	0.776	0.094	0.027	0.880
22	0.272	0.020	0.709	0.114	0.037	0.849
23	0.342	0.025	0.633	0.131	0.049	0.819
24	0.432	0.031	0.537	0.145	0.066	0.789
25	0.226	0.006	0.768	0.116	0.014	0.869

Table 5 (Continued)

	Aqueous phase			Organic phase		
	Grams of $\text{La}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{La}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
26	0.287	0.009	0.704	0.140	0.021	0.839
27	0.360	0.010	0.631	0.169	0.024	0.807
28	0.457	0.012	0.531	0.191	0.034	0.776
29	0.091	0.399	0.511	0.006	0.195	0.799
30	0.102	0.444	0.454	0.008	0.213	0.779
31	0.180	0.332	0.488	0.016	0.209	0.775
32	0.195	0.363	0.443	0.020	0.223	0.757
33	0.110	0.507	0.383	0.016	0.267	0.717
34	0.338	0.210	0.453	0.038	0.187	0.775
35	0.511	0.036	0.453	0.143	0.089	0.768
36	0.531	0.019	0.450	0.177	0.061	0.763
37	0.457	0.111	0.432	0.071	0.156	0.773
38	0.529	0.051	0.420	0.120	0.115	0.765
39	0.358	0.229	0.413	0.042	0.198	0.760
40	0.461	0.138	0.402	0.065	0.170	0.765
41	0.208	0.432	0.360	0.035	0.253	0.712

Table 6. Equilibrium data for the system $\text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$

	Aqueous phase			Organic phase		
	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
1	0.079	0.134	0.787	0.022	0.108	0.870
2	0.099	0.179	0.721	0.027	0.133	0.841
3	0.130	0.237	0.634	0.028	0.160	0.812
4	0.158	0.287	0.554	0.030	0.179	0.792
5	0.173	0.332	0.495	0.034	0.195	0.771
6	0.146	0.087	0.766	0.050	0.087	0.864
7	0.187	0.113	0.700	0.061	0.103	0.836
8	0.245	0.150	0.605	0.067	0.130	0.803
9	0.294	0.184	0.522	0.065	0.153	0.782
10	0.328	0.211	0.461	0.069	0.168	0.763
11	0.230	0.041	0.729	0.102	0.055	0.842
12	0.268	0.065	0.667	0.108	0.075	0.817
13	0.336	0.085	0.579	0.116	0.095	0.789
14	0.409	0.101	0.489	0.116	0.117	0.768
15	0.455	0.115	0.430	0.116	0.133	0.752
16	0.467	0.143	0.390	0.113	0.151	0.763
17	0.258	0.022	0.720	0.137	0.036	0.828
18	0.328	0.027	0.646	0.167	0.040	0.793
19	0.416	0.032	0.552	0.185	0.050	0.765
20	0.491	0.040	0.470	0.183	0.067	0.750
21	0.536	0.051	0.412	0.170	0.088	0.742
22	0.269	0.011	0.720	0.164	0.020	0.816
23	0.343	0.012	0.645	0.198	0.021	0.781
24	0.437	0.019	0.544	0.211	0.032	0.757
25	0.522	0.018	0.459	0.219	0.038	0.743
26	0.184	0.372	0.444	0.043	0.209	0.749
27	0.349	0.241	0.410	0.081	0.180	0.739
28	0.195	0.401	0.404	0.055	0.220	0.725
29	0.352	0.270	0.378	0.091	0.192	0.717
30	0.064	0.103	0.834	0.017	0.094	0.889

Table 6 (Continued)

Aqueous phase			Organic phase		
Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
31	0.124	0.066	0.809	0.040	0.888
32	0.172	0.039	0.789	0.069	0.877
33	0.208	0.014	0.778	0.113	0.860
34	0.224	0.007	0.770	0.139	0.847
35	0.201	0.424	0.375	0.068	0.706

Table 7. Equilibrium data for the system $\text{Nd}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$

Aqueous phase			Organic phase		
Grams of $\text{Nd}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{Nd}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
1	0.301	0.017	0.681	0.185	0.790
2	0.352	0.021	0.627	0.201	0.770
3	0.377	0.023	0.600	0.207	0.762
4	0.355	0.019	0.626	0.205	0.767
5	0.458	0.023	0.519	0.222	0.742
6	0.483	0.026	0.491	0.218	0.739
7	0.454	0.093	0.454	0.142	0.748
8	0.427	0.076	0.498	0.151	0.757
9	0.397	0.081	0.522	0.144	0.764
10	0.370	0.074	0.556	0.146	0.773

Table 7 (Continued)

	Aqueous phase			Organic phase		
	Grams of $\text{Nd}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{Nd}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
11	0.348	0.071	0.581	0.145	0.078	0.778
12	0.325	0.068	0.607	0.141	0.073	0.786
13	0.295	0.060	0.645	0.135	0.068	0.797
14	0.287	0.060	0.653	0.134	0.068	0.798
15	0.350	0.207	0.444	0.093	0.163	0.744
16	0.346	0.178	0.476	0.093	0.150	0.757
17	0.312	0.178	0.510	0.085	0.147	0.768
18	0.295	0.164	0.591	0.087	0.138	0.776
19	0.284	0.159	0.557	0.085	0.135	0.780
20	0.262	0.152	0.586	0.083	0.124	0.793
21	0.238	0.134	0.628	0.084	0.113	0.804
22	0.225	0.130	0.644	0.082	0.109	0.809
23	0.204	0.384	0.411	0.073	0.206	0.722
24	0.200	0.341	0.459	0.059	0.198	0.744
25	0.183	0.324	0.493	0.049	0.191	0.761
26	0.172	0.290	0.538	0.043	0.179	0.778
27	0.169	0.286	0.545	0.042	0.177	0.781
28	0.154	0.264	0.582	0.040	0.167	0.794
29	0.142	0.236	0.622	0.040	0.156	0.804
30	0.133	0.227	0.640	0.038	0.152	0.809
31	0.151	0.446	0.404	0.064	0.227	0.709
32	0.151	0.398	0.451	0.050	0.211	0.740
33	0.140	0.376	0.485	0.040	0.202	0.758
34	0.134	0.343	0.523	0.034	0.192	0.774
35	0.129	0.331	0.541	0.032	0.187	0.781
36	0.119	0.306	0.576	0.029	0.179	0.792
37	0.111	0.277	0.612	0.028	0.168	0.804
38	0.100	0.254	0.645	0.028	0.162	0.811
39	0.144	0.353	0.503	0.036	0.195	0.768
40	0.270	0.236	0.494	0.066	0.167	0.767

Table 7 (Continued)

	Aqueous phase			Organic phase		
	Grams of $\text{Nd}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{Nd}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
41	0.330	0.191	0.479	0.084	0.152	0.764
42	0.463	0.057	0.480	0.173	0.078	0.749
43	0.453	0.055	0.492	0.176	0.077	0.747
44	0.367	0.125	0.508	0.112	0.124	0.764
45	0.265	0.217	0.518	0.068	0.160	0.772
46	0.143	0.331	0.527	0.036	0.189	0.775
47	0.535	0.062	0.403	0.179	0.096	0.726
48	0.468	0.138	0.394	0.133	0.144	0.724
49	0.404	0.183	0.413	0.120	0.155	0.725
50	0.211	0.423	0.366	0.091	0.226	0.683
51	0.238	0.475	0.287	0.132	0.250	0.618
52	0.596	0.005	0.399	0.273	0.007	0.720
53	0.512	0.055	0.434	0.182	0.085	0.733
54	0.436	0.147	0.417	0.121	0.146	0.733
55	0.273	0.339	0.388	0.091	0.205	0.704
56	0.231	0.441	0.328	0.112	0.235	0.653
57	0.335	0.257	0.408	0.096	0.182	0.723
58	0.473	0.115	0.412	0.140	0.132	0.728
59	0.529	0.047	0.424	0.194	0.079	0.727
60	0.223	0.478	0.299	0.125	0.242	0.633
61	0.201	0.009	0.790	0.124	0.018	0.858
62	0.175	0.030	0.795	0.082	0.043	0.875
63	0.126	0.059	0.815	0.046	0.066	0.888
64	0.061	0.097	0.843	0.018	0.088	0.894
65	0.265	0.014	0.721	0.166	0.023	0.811
66	0.225	0.043	0.732	0.112	0.055	0.834
67	0.163	0.085	0.752	0.064	0.083	0.853
68	0.079	0.137	0.784	0.026	0.107	0.867
69	0.202	0.111	0.687	0.073	0.102	0.825
70	0.100	0.181	0.719	0.035	0.128	0.837

Table 8. Equilibrium data for the system $\text{Sm}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$

	Aqueous phase			Organic phase		
	Grams of $\text{Sm}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{Sm}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
1	0.487	0.029	0.484	0.226	0.047	0.727
2	0.447	0.030	0.523	0.228	0.037	0.735
3	0.386	0.027	0.587	0.225	0.031	0.744
4	0.341	0.023	0.637	0.217	0.027	0.756
5	0.307	0.020	0.672	0.207	0.026	0.767
6	0.313	0.022	0.665	0.208	0.026	0.766
7	0.277	0.018	0.705	0.194	0.023	0.783
8	0.248	0.016	0.737	0.177	0.018	0.805
9	0.400	0.108	0.492	0.160	0.098	0.742
10	0.376	0.096	0.528	0.163	0.086	0.751
11	0.324	0.087	0.589	0.159	0.076	0.765
12	0.282	0.072	0.646	0.154	0.066	0.781
13	0.261	0.063	0.676	0.148	0.063	0.789
14	0.259	0.071	0.670	0.146	0.063	0.791
15	0.234	0.059	0.707	0.136	0.057	0.808
16	0.178	0.043	0.779	0.102	0.049	0.850
17	0.269	0.283	0.448	0.113	0.161	0.726
18	0.261	0.260	0.480	0.104	0.156	0.740
19	0.230	0.228	0.542	0.092	0.142	0.766
20	0.205	0.196	0.599	0.088	0.129	0.783
21	0.188	0.179	0.633	0.088	0.123	0.790
22	0.176	0.174	0.650	0.083	0.120	0.798
23	0.162	0.159	0.680	0.081	0.113	0.807
24	0.142	0.140	0.718	0.072	0.102	0.826
25	0.129	0.432	0.439	0.090	0.197	0.657
26	0.123	0.402	0.475	0.074	0.189	0.684
27	0.119	0.344	0.537	0.056	0.176	0.768
28	0.103	0.294	0.604	0.047	0.164	0.789
29	0.099	0.283	0.618	0.046	0.160	0.794
30	0.094	0.271	0.636	0.044	0.153	0.803

Table 8 (Continued)

	Aqueous phase			Organic phase		
	Grams of $\text{Sm}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{Sm}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
31	0.085	0.243	0.672	0.041	0.148	0.811
32	0.055	0.142	0.804	0.026	0.108	0.869
33	0.222	0.291	0.487	0.097	0.165	0.739
34	0.217	0.280	0.503	0.093	0.160	0.747
35	0.213	0.269	0.518	0.089	0.156	0.754
36	0.202	0.245	0.553	0.085	0.147	0.769
37	0.222	0.292	0.486	0.095	0.166	0.739
38	0.219	0.285	0.497	0.092	0.162	0.746
39	0.214	0.270	0.516	0.088	0.158	0.754
40	0.204	0.244	0.553	0.082	0.151	0.767
41	0.129	0.526	0.345	0.126	0.222	0.653
42	0.200	0.383	0.418	0.114	0.188	0.698
43	0.278	0.268	0.454	0.116	0.161	0.723
44	0.422	0.130	0.448	0.156	0.116	0.728
45	0.484	0.064	0.452	0.202	0.073	0.725
46	0.541	0.043	0.416	0.222	0.065	0.713
47	0.579	0.007	0.416	0.277	0.009	0.714
48	0.101	0.597	0.302	0.138	0.248	0.614
49	0.075	0.088	0.837	0.032	0.080	0.888
50	0.113	0.066	0.821	0.052	0.067	0.882
51	0.163	0.034	0.803	0.092	0.047	0.862
52	0.194	0.014	0.792	0.132	0.022	0.847
53	0.144	0.093	0.763	0.075	0.081	0.844

Table 9. Equilibrium data for the system $\text{La}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$

	Aqueous phase				Organic phase			
	Grams of $\text{La}(\text{NO}_3)_3$ per gram of solution	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{La}(\text{NO}_3)_3$ per gram of solution	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
1	0.075	0.130	0.019	0.776	0.025	0.069	0.036	0.870
2	0.142	0.065	0.19	0.774	0.054	0.035	0.037	0.873
3	0.057	0.096	0.051	0.796	0.014	0.036	0.066	0.885
4	0.106	0.049	0.049	0.797	0.027	0.018	0.067	0.887
5	0.029	0.055	0.093	0.824	0.005	0.015	0.087	0.893
6	0.057	0.027	0.089	0.827	0.010	0.008	0.087	0.895
7	0.119	0.205	0.036	0.639	0.031	0.108	0.056	0.805
8	0.233	0.098	0.033	0.636	0.072	0.059	0.058	0.811
9	0.086	0.152	0.089	0.673	0.017	0.058	0.098	0.828
10	0.168	0.074	0.087	0.671	0.034	0.031	0.102	0.833
11	0.052	0.080	0.161	0.707	0.007	0.024	0.131	0.838
12	0.092	0.040	0.160	0.707	0.013	0.013	0.131	0.843
13	0.178	0.300	0.054	0.468	0.026	0.127	0.091	0.757

Table 9 (Continued)

	Aqueous phase				Organic phase			
	Grams of $\text{La}(\text{NO}_3)_3$ per gram of solution	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{La}(\text{NO}_3)_3$ per gram of solution	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
14	0.334	0.145	0.050	0.417	0.064	0.078	0.096	0.763
15	0.126	0.233	0.142	0.500	0.013	0.065	0.143	0.779
16	0.247	0.112	0.138	0.503	0.031	0.036	0.148	0.785
17	0.069	0.132	0.256	0.544	0.006	0.026	0.176	0.792
18	0.144	0.273	0.176	0.407	0.013	0.072	0.167	0.748
19	0.289	0.130	0.171	0.409	0.031	0.041	0.171	0.757
20	0.086	0.154	0.328	0.433	0.007	0.039	0.203	0.752
21	0.167	0.076	0.325	0.433	0.015	0.021	0.207	0.756

Table 10. Equilibrium data for the system $\text{Nd}(\text{NO}_3)_3$ - $\text{Pr}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O

	Aqueous phase				Organic phase			
	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of $\text{Nd}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of $\text{Nd}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
1	0.074	0.126	0.021	0.780	0.032	0.071	0.035	0.861
2	0.064	0.033	0.087	0.816	0.018	0.012	0.083	0.888
3	0.211	0.105	0.039	0.645	0.092	0.060	0.053	0.795
4	0.048	0.102	0.151	0.699	0.014	0.036	0.119	0.830
5	0.146	0.328	0.059	0.467	0.042	0.130	0.083	0.745
6	0.148	0.079	0.236	0.538	0.028	0.022	0.167	0.783
7	0.266	0.137	0.195	0.402	0.055	0.045	0.166	0.734
8	0.088	0.182	0.301	0.429	0.017	0.056	0.190	0.737

Table 11. Equilibrium data for the system $\text{Sm}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$

	Aqueous phase				Organic phase			
	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of $\text{Sm}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of $\text{Sm}(\text{NO}_3)_3$ per gram of solution	Grams of HNO_3 per gram of solution	Grams of solvent per gram of solution
1	0.073	0.118	0.022	0.787	0.033	0.079	0.033	0.855
2	0.064	0.025	0.088	0.824	0.020	0.010	0.082	0.888
3	0.221	0.087	0.040	0.652	0.090	0.072	0.049	0.789
4	0.052	0.083	0.154	0.711	0.013	0.047	0.116	0.825
5	0.176	0.288	0.062	0.474	0.031	0.159	0.075	0.735
6	0.158	0.062	0.236	0.545	0.027	0.035	0.159	0.779
7	0.265	0.108	0.220	0.408	0.043	0.071	0.162	0.724
8	0.102	0.154	0.311	0.433	0.013	0.090	0.173	0.723

APPENDIX C. MATHEMATICAL ANALYSIS OF PINCH

In this section an attempt to determine mathematically the generality of the "pinch" properties of the multicomponent, multistage calculation discussed in the body of this report is presented. The treatment is quite incomplete, however, the results indicate that the "pinch" of solute concentrations may be general over a wide range of system parameters. The cascade portrayed in Figure 10 was considered.

The approach used was to combine the defining equation of separation factor with a material balance and write an equation for the molality of solute j in organic stream S_n . Remember that the calculation to be considered is applied to the end of the cascade, first defining the solvent (S_0), the raffinate (R_1), and the flow ratio (α), and then working back through the cascade toward the feed.

By definition

$$(\beta_{j-Pr})_n = \frac{(M_j)_{S_n} / (M_j)_{R_n}}{(K_{Pr})_n} \quad (14)$$

or

$$(K_{Pr})_n (\beta_{j-Pr})_n (M_j)_{R_n} = (M_j)_{S_n} \quad (15)$$

Summing each side of Equation 15 over the solutes in the system get

$$(K_{Pr})_n \sum_{i=1}^T (\beta_{i-Pr})_n (M_i)_{R_n} = \sum_{i=1}^T (M_i)_{S_n} = (M_t)_{S_n} \quad (16)$$

Substituting Equation 16 into 15 get

$$(M_j)S_n = \frac{(M_t)S_n (\beta_{j-Pr})_n (M_j)_{R_n}}{\sum_{i=1}^T (\beta_{i-Pr})_n (M_i)_{R_n}} \quad (17)$$

Writing a material balance over the right hand end of the cascade gives

$$\begin{aligned} & \left[(M_j)_{R_1} \times R_1 \right] + \left[(M_j)_{S_{n-1}} \times S_{n-1} \right] = \\ & \left[(M_j)_{S_0} \times S_0 \right] + \left[(M_j)_{R_n} \times R_n \right] \end{aligned} \quad (18)$$

and assuming immiscible solvents

$$(M_j)_{R_n} = \alpha(M_j)_{S_{n-1}} + (M_j)_{R_1} - \alpha(M_j)_{S_0} \quad (19)$$

Substituting into Equation 17 get

$$(M_j)S_n = \frac{(M_t)S_n (\beta_{j-Pr})_n \left[\alpha(M_j)_{S_{n-1}} + (M_j)_{R_1} - \alpha(M_j)_{S_0} \right]}{\sum_{i=1}^T (\beta_{i-Pr})_n \left[\alpha(M_i)_{S_{n-1}} + (M_i)_{R_1} - \alpha(M_i)_{S_0} \right]} \quad (20)$$

The assumptions of "pinched" total molality and constant separation factors were now applied. The general situation in which the total molality is "pinched" at a high value is shown on a McCabe Thiele diagram in Figure 32. The equations to be considered below apply to the circled section on the drawing, that is to the "pinched" stages. The fact that the following equations assume a "pinch" in stage 1 causes no loss in generality, as in a case in which the total molality of

Figure 32. McCabe-Thiele representation of "pinched" total molality

several of the right hand stages is not constant stage 1 may be chosen as the first stage in which the organic molality attains its "pinch" value.

For this equilibrium model the stream and stage designations of the total molalities and separation factors may be deleted, and also, for convenience $(M_i)_n$ will be inserted for $(M_i)_{S_n}$ and so

$$(M_j)_n = \frac{\alpha M_t \beta_{j-Pr} (M_j)_{n-1} + M_t \beta_{j-Pr} \left[(M_j)_{R_1} - \alpha (M_j)_{S_0} \right]}{\alpha \sum_{i=1}^T \beta_{i-Pr} (M_i)_{n-1} + \sum_{i=1}^T \beta_{i-Pr} \left[(M_i)_{R_1} - \alpha (M_i)_{S_0} \right]} \quad (21)$$

Note that for specified end conditions and a specified "pinch" value of the total molality Equation 21 gives the molality of solute j in stream S_n as a function of the molalities of all solutes in stream S_{n-1} . By letting $n = 1, 2, 3, \dots$, a sequence was generated which gives the molality of solute j in successive organic streams in terms of the system parameters. If the sequence could be shown to converge to a non-zero value the "pinch" would be proven general. The author has written a large number of terms of the sequence but has not been able to write the general term.

For the special case of $T = 2$, that is two solutes, an analytical treatment of the general equation was developed and the limit taken. This case is now discussed. For convenience it was assumed that stream S_0 is pure solvent. This is not

necessary but simplifies the following equations algebraically. For this case, denoting quantities that pertain to the two solutes by the subscripts 1 and 2

$$(M_1)_n = \frac{M_t \beta_{1-Pr}(M_1)_{n-1} + (M_t/\alpha) \beta_{1-Pr}(M_1)_{R_1}}{\left[\beta_{1-Pr}(M_1)_{n-1} + \beta_{2-Pr}(M_2)_{n-1} \right] + (1/\alpha) \sum_{i=1}^2 \beta_{i-Pr}(M_i)_{R_1}}, \quad (22)$$

and

$$(M_2)_n = \frac{M_t \beta_{2-Pr}(M_2)_{n-1} + (M_t/\alpha) \beta_{2-Pr}(M_2)_{R_1}}{\left[\beta_{1-Pr}(M_1)_{n-1} + \beta_{2-Pr}(M_2)_{n-1} \right] + (1/\alpha) \sum_{i=1}^2 \beta_{i-Pr}(M_i)_{R_1}}. \quad (23)$$

These equations are of exactly the same form. By use of finite difference techniques they were solved for the molalities of the solutes as a function of the system parameters and stage number, and the limit taken as n becomes large. This technique is now illustrated by solving Equation 22 and then a numerical example given.

For the two solute case with "pinched" total molality

$$(M_1)_{n-1} + (M_2)_{n-1} = M_t, \quad (24)$$

and so substituting into Equation 22 get

$$(M_1)_n = \frac{M_t \beta_{1-Pr}(M_1)_{n-1} + (M_t/\alpha) \beta_{1-Pr}(M_1)_{R_1}}{(\beta_{1-Pr} - \beta_{2-Pr})(M_1)_{n-1} + \beta_{2-Pr} M_t + (1/\alpha) \sum_{i=1}^2 \beta_{i-Pr}(M_i)_{R_1}}. \quad (25)$$

Now let

$$\begin{aligned} a_1 &= M_t \beta_{1-Pr} \quad , \\ b_1 &= (M_t/\alpha) \beta_{1-Pr} (M_1)_{R_1} \quad , \\ c_1 &= \beta_{1-Pr} - \beta_{2-Pr} \quad , \\ d_1 &= \beta_{2-Pr} M_t + (1/\alpha) \sum_{i=1}^2 \beta_{i-Pr} (M_i)_{R_1} \quad . \end{aligned}$$

Substitution into Equation 25 and simplification gives

$$(M_1)_n (M_1)_{n-1} + \alpha_1 (M_1)_n + \theta_1 (M_1)_{n-1} + \gamma_1 = 0 \quad , \quad (26)$$

with

$$\begin{aligned} \alpha_1 &= d_1/c_1 \quad , \\ \theta_1 &= -a_1/c_1 \quad , \\ \gamma_1 &= -b_1/c_1 \quad . \end{aligned}$$

At this point it is to be noted that the limit of $(M_1)_n$ as n becomes large can be determined without solving Equation 26. This can be done by recognizing that if a "pinch" takes place $(M_1)_n = (M_1)_{n-1}$. If this substitution is made in Equation 26 and the resulting quadratic solved for $(M_1)_n$ two roots are obtained, one of which must be discarded on physical grounds.

Alternatively, Equation 26 is a Ricatti difference equation and may be reduced to a linear difference equation with constant coefficients by the substitution

$$(M_1)_{n-1} = (V_1)_n (V_1)_{n-1} - \alpha_1 \quad . \quad (27)$$

For the methods of solution the reader is referred to Boole (53) and Brand (54).

After substitution and simplification get

$$(V_1)_{n+1} + E_1(V_1)_n + F_1(V_1)_{n-1} = 0 \quad (28)$$

with

$$E_1 = \theta_1 - \alpha_1 \quad ,$$

$$F_1 = \gamma_1 - \alpha_1 \theta_1 \quad .$$

A trial solution of the form $(V_1)_n = Z^n$ gives the characteristic equation

$$Z^2 + E_1 Z + F_1 = 0 \quad , \quad (29)$$

and so

$$Z = \frac{-E_1 \pm (E_1^2 - 4F_1)^{0.5}}{2} \quad . \quad (30)$$

To complete the solution it was necessary to know the nature of the roots of the characteristic quadratic. For all calculations considered the roots were real and distinct. The author has attempted to prove that the discriminant of the quadratic is positive by expanding it in terms of the original system parameters. A proof has not been possible and so it was assumed that this is the case and the roots are real and distinct.

Let

$$G_{1\pm} = \frac{-E_1 \pm (E_1^2 - 4F_1)^{0.5}}{2}$$

and

$$G_{1-} = \frac{-E_1 - (E_1^2 - 4F_1)^{0.5}}{2}$$

Then the solution of Equation 28 is

$$(V_1)_n = C_1 G_{1+}^n + C_2 G_{1-}^n \quad (31)$$

with C_1 and C_2 constants, and the solution of Equation 26 is

$$(M_1)_n = \frac{C_1 G_{1+}^{n+1} + C_2 G_{1-}^{n+1}}{C_1 G_{1+}^n + C_2 G_{1-}^n} - \alpha_1 \quad (32)$$

The limit of Equation 32 was taken by noting that the roots are real and distinct. Then necessarily either $|G_{1+}| > |G_{1-}|$ or $|G_{1+}| < |G_{1-}|$. Assuming that $|G_{1+}| > |G_{1-}|$ the numerator and denominator of the fraction on the right hand side of Equation 32 was divided by G_{1+}^n giving

$$(M_1)_n = \frac{C_1 G_{1+} + C_2 G_{1-} (G_{1-}/G_{1+})^n}{C_1 + C_2 (G_{1-}/G_{1+})^n} - \alpha_1 \quad , \quad (33)$$

and so

$$\lim_{n \rightarrow \infty} (M_1)_n = G_{1+} - \alpha_1 \quad (34)$$

It should be noted at this point that the algebraic combinations of system parameters $a_1, b_1, c_1, d_1, \alpha_1, \theta_1, \gamma_1, E_1, F_1, G_{1+}, G_{1-}$ all refer to solute 1. Corresponding expressions for solute 2 may be obtained by interchanging the solute subscripts in the defining equations. Exactly the same treatment was applied to Equation 23. Alternatively, the limit of the differences of the molalities in successive

stages, that is $\left[(M_1)_{n+1} - (M_1)_n\right]$ and $\left[(M_2)_{n+1} - (M_2)_n\right]$ may be shown to approach zero as n becomes large.

As a numerical example the following values were chosen:

$$\alpha = 1.0 \quad ,$$

$$M_t = 3.50 \quad ,$$

$$\beta_{1-Pr} = 0.43 \quad ,$$

$$\beta_{2-Pr} = 1.00 \quad ,$$

$$(M_t)_{R_1} = 8.00 \quad ,$$

$$(M_1)_{R_1} = 4.00 \quad ,$$

$$(M_2)_{R_2} = 4.00 \quad .$$

Using these values

$$G_{1+} = -3.472 \quad ,$$

$$G_{1-} = -15.344 \quad ,$$

$$\alpha_1 = -16.175 \quad ,$$

$$G_{2+} = 15.344 \quad ,$$

$$G_{2-} = 3.472 \quad ,$$

$$\alpha_2 = 12.675 \quad ,$$

were calculated. The limits of $(M_1)_n$ and $(M_2)_n$ were then calculated to be

$$\lim_{n \rightarrow \infty} (M_1)_n = -15.344 + 16.175 = 0.831 \quad ,$$

$$\lim_{n \rightarrow \infty} (M_2)_n = 15.344 - 12.675 = 2.669 \quad .$$

Using alternate material balances and the chosen equilibrium model the stagewise values shown in Table 12 were calculated for this numerical example.

Table 12. Molalities of solutes 1 and 2 in organic streams of ideal cascade

	S_0	S_1	S_2	S_3	S_4	S_5	S_6	S_7
M_1	0.0000	1.0520	0.8820	0.8429	0.8340	0.8320	0.8315	0.8314
M_2	0.0000	2.4480	2.6180	2.6571	2.6660	2.6680	2.6685	2.6686

The stagewise concentrations "pinch" rather rapidly to the limiting values. Note however that this is not an independent check of the validity of the process, as the equation which was used to solve for and take the limit of the molalities is simply a generalization of the stage by stage calculation used to determine the stagewise concentrations in the preceeding table. This result indicates only that the solution of Equations 22 and 23 by finite difference techniques and the limiting process were carried out correctly.

Two comments should be made concerning the preceeding treatment. First the form of the solution is dependent on the

assumption of real and distinct roots of the characteristic quadratic. As pointed out previously, this has been true in all specific cases studied but no proof has been given. Secondly, it may be that the derived result, that is "pinched" concentrations of the individual solutes under the assumptions made and the situations considered, is or should be intuitively obvious from simple material balance considerations. No definite conclusion has been reached concerning this second statement.

APPENDIX D. DIGITAL COMPUTER PROGRAMS

The calculation which is discussed in the body of this thesis to give the stagewise conditions in a cascade of equilibrium stages was programmed in the Full Fortran Language for the IBM 7074 digital computer for four cascades of interest. These cascades are shown in Figures 33, 34, 35, and 36 with the direction of calculation denoted by dashed arrows.

In the computer operation the values of K_t and K_{HNO_3} were derived by straight line interpolation in two dimensional arrays prepared from the parametric plots of K_t and K_{HNO_3} versus equilibrium phase composition discussed in the Method of Calculation section. These two dimensional arrays are shown in Tables 13 through 28. All non-zero values in these arrays were taken from plots of the type depicted in Figures 1 through 8. The zero values have no physical meaning but were inserted for convenience in making "branches" in the programs.

The principal variable names used in the programs are given in Figure 37. A compilation of the four programs is given in Figures 38 through 45. In each case the logic flow is diagrammed and is followed by the Fortran program. The program designation corresponds to the cascade designation in Figures 33, 34, 35, and 36.

Figure 33. Cascade I

Figure 34. Cascade II

Figure 35. Cascade III

Figure 36. Cascade IV

Table 13. Array of values of K_t for the system $\text{La}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{aq.}}$ and X_{La}

X_{La}	$(M_t)_{\text{aq.}}$						
	3.0	4.0	5.0	7.0	10.0	13.0	16.0
0.00	0.713	0.640	0.580	0.478	0.382	0.330	0.296
0.05	0.695	0.626	0.569	0.475	0.382	0.329	0.298
0.10	0.676	0.612	0.560	0.471	0.382	0.328	0.299
0.15	0.659	0.598	0.550	0.468	0.382	0.326	0.299
0.20	0.643	0.586	0.541	0.464	0.382	0.325	0.299
0.25	0.628	0.575	0.533	0.460	0.381	0.324	0.298
0.30	0.614	0.564	0.524	0.456	0.380	0.322	0.297
0.35	0.601	0.554	0.516	0.452	0.378	0.320	0.295
0.40	0.589	0.545	0.508	0.448	0.376	0.318	0.293
0.45	0.578	0.537	0.501	0.443	0.374	0.316	0.289
0.50	0.568	0.529	0.494	0.438	0.371	0.314	0.285
0.55	0.559	0.523	0.487	0.433	0.369	0.311	0.281
0.60	0.549	0.516	0.481	0.428	0.366	0.308	0.276
0.65	0.541	0.511	0.474	0.423	0.363	0.306	0.271
0.70	0.533	0.506	0.469	0.417	0.359	0.303	0.266
0.75	0.526	0.500	0.464	0.412	0.355	0.301	0.259
0.80	0.521	0.495	0.460	0.407	0.349	0.296	0.252
0.85	0.518	0.491	0.456	0.401	0.336	0.288	0.244
0.90	0.519	0.489	0.455	0.396	0.331	0.278	0.236
0.95	0.524	0.491	0.454	0.389	0.319	0.266	0.226
1.00	0.534	0.497	0.456	0.384	0.303	0.248	0.217

Table 14. Array of values of K_t for the system $\text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{aq.}}$ and X_{Pr}

X_{Pr}	$(M_t)_{\text{aq.}}$						
	3.0	4.0	5.0	7.0	10.0	13.0	16.0
0.00	0.713	0.640	0.580	0.478	0.382	0.330	0.296
0.05	0.702	0.628	0.571	0.476	0.388	0.331	0.298
0.10	0.690	0.617	0.564	0.474	0.383	0.332	0.299
0.15	0.679	0.608	0.556	0.470	0.383	0.332	0.299
0.20	0.668	0.601	0.550	0.468	0.385	0.331	0.299
0.25	0.659	0.595	0.545	0.465	0.384	0.330	0.298
0.30	0.650	0.588	0.540	0.462	0.383	0.330	0.297
0.35	0.642	0.583	0.535	0.460	0.382	0.328	0.296
0.40	0.634	0.578	0.532	0.458	0.381	0.327	0.295
0.45	0.627	0.574	0.529	0.455	0.380	0.325	0.294
0.50	0.622	0.570	0.526	0.453	0.378	0.324	0.292
0.55	0.616	0.566	0.525	0.451	0.376	0.322	0.290
0.60	0.612	0.565	0.523	0.450	0.374	0.320	0.288
0.65	0.608	0.563	0.523	0.450	0.373	0.317	0.285
0.70	0.605	0.562	0.523	0.449	0.370	0.315	0.282
0.75	0.600	0.562	0.523	0.449	0.368	0.312	0.000
0.80	0.601	0.564	0.524	0.448	0.365	0.309	0.000
0.85	0.605	0.570	0.527	0.449	0.361	0.306	0.000
0.90	0.615	0.582	0.535	0.450	0.358	0.302	0.000
0.95	0.631	0.599	0.547	0.451	0.354	0.298	0.000
1.00	0.657	0.619	0.567	0.454	0.350	0.294	0.000

Table 15. Array of values of K_t for the system $\text{Nd}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{aq.}}$ and X_{Nd}

X_{Nd}	$(M_t)_{\text{aq.}}$						
	3.0	4.0	5.0	7.0	10.0	13.0	16.0
0.00	0.713	0.640	0.580	0.478	0.382	0.330	0.296
0.05	0.702	0.626	0.570	0.476	0.383	0.332	0.301
0.10	0.693	0.615	0.562	0.474	0.385	0.335	0.303
0.15	0.683	0.605	0.555	0.471	0.386	0.337	0.305
0.20	0.673	0.597	0.550	0.469	0.387	0.338	0.305
0.25	0.664	0.593	0.547	0.467	0.387	0.338	0.306
0.30	0.656	0.587	0.544	0.465	0.388	0.338	0.306
0.35	0.649	0.585	0.542	0.463	0.388	0.338	0.306
0.40	0.643	0.583	0.541	0.461	0.388	0.337	0.305
0.45	0.637	0.582	0.540	0.460	0.387	0.336	0.305
0.50	0.631	0.582	0.540	0.459	0.386	0.335	0.303
0.55	0.626	0.582	0.540	0.458	0.385	0.335	0.302
0.60	0.622	0.583	0.542	0.457	0.382	0.333	0.300
0.65	0.620	0.585	0.544	0.457	0.380	0.330	0.298
0.70	0.620	0.587	0.546	0.457	0.337	0.329	0.295
0.75	0.620	0.591	0.548	0.457	0.374	0.326	0.000
0.80	0.623	0.597	0.552	0.460	0.370	0.324	0.000
0.85	0.628	0.605	0.556	0.463	0.366	0.320	0.000
0.90	0.640	0.615	0.562	0.466	0.362	0.314	0.000
0.95	0.660	0.627	0.568	0.464	0.358	0.307	0.000
1.00	0.697	0.643	0.577	0.457	0.352	0.000	0.000

Table 16. Array of values of K_t for the system $\text{Sm}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O as a function of $(M_t)_{\text{aq.}}$ and X_{Sm}

X_{Sm}	$(M_t)_{\text{aq.}}$						
	3.0	4.0	5.0	7.0	10.0	13.0	16.0
0.00	0.713	0.640	0.580	0.478	0.382	0.330	0.296
0.05	0.706	0.635	0.576	0.480	0.388	0.335	0.309
0.10	0.699	0.630	0.573	0.479	0.391	0.339	0.316
0.15	0.693	0.628	0.570	0.479	0.394	0.342	0.323
0.20	0.687	0.625	0.569	0.479	0.396	0.345	0.327
0.25	0.681	0.622	0.567	0.479	0.398	0.348	0.332
0.30	0.675	0.620	0.566	0.480	0.399	0.350	0.335
0.35	0.672	0.619	0.565	0.480	0.399	0.350	0.338
0.40	0.668	0.618	0.566	0.480	0.399	0.351	0.341
0.45	0.666	0.619	0.566	0.481	0.398	0.351	0.343
0.50	0.665	0.619	0.568	0.483	0.396	0.351	0.344
0.55	0.665	0.621	0.570	0.480	0.395	0.350	0.000
0.60	0.667	0.623	0.573	0.486	0.394	0.348	0.000
0.65	0.670	0.625	0.577	0.488	0.393	0.346	0.000
0.70	0.674	0.630	0.581	0.490	0.390	0.343	0.000
0.75	0.681	0.637	0.586	0.492	0.389	0.340	0.000
0.80	0.688	0.648	0.591	0.494	0.387	0.335	0.000
0.85	0.697	0.666	0.598	0.496	0.384	0.328	0.000
0.90	0.708	0.682	0.604	0.498	0.380	0.319	0.000
0.95	0.731	0.693	0.612	0.501	0.375	0.307	0.000
1.00	0.770	0.700	0.620	0.504	0.370	0.290	0.000

[illegible]

[illegible]

[illegible]

[illegible]

Table 21. Array of values of K_t for the system $\text{La}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{org.}}$ and Y_{La}

Y_{La}	$(M_t)_{\text{org.}}$					
	2.0	2.5	3.0	3.5	4.0	4.5
0.00	0.769	0.667	0.566	0.441	0.358	0.314
0.05	0.610	0.547	0.484	0.394	0.344	0.304
0.10	0.568	0.505	0.452	0.370	0.329	0.295
0.15	0.545	0.482	0.430	0.354	0.314	0.283
0.20	0.529	0.466	0.413	0.345	0.300	0.270
0.25	0.516	0.457	0.399	0.337	0.284	0.254
0.30	0.505	0.450	0.389	0.329	0.269	0.000
0.35	0.498	0.445	0.380	0.320	0.254	0.000
0.40	0.492	0.442	0.374	0.312	0.239	0.000
0.45	0.486	0.438	0.370	0.303	0.000	0.000
0.50	0.484	0.435	0.367	0.295	0.000	0.000
0.55	0.482	0.432	0.365	0.286	0.000	0.000
0.60	0.480	0.430	0.364	0.278	0.000	0.000
0.65	0.480	0.427	0.361	0.270	0.000	0.000
0.70	0.481	0.425	0.357	0.262	0.000	0.000
0.75	0.483	0.424	0.352	0.253	0.000	0.000
0.80	0.485	0.422	0.346	0.245	0.000	0.000
0.85	0.487	0.420	0.339	0.237	0.000	0.000
0.90	0.490	0.419	0.331	0.228	0.000	0.000
0.95	0.494	0.417	0.322	0.220	0.000	0.000
1.00	0.498	0.415	0.313	0.212	0.000	0.000

Table 22. Array of values of K_t for the system $\text{Pr}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O as a function of $(M_t)_{\text{org.}}$ and Y_{Pr}

Y_{Pr}	$(M_t)_{\text{org.}}$					
	2.0	2.5	3.0	3.5	4.0	4.5
0.00	0.769	0.667	0.566	0.441	0.358	0.314
0.05	0.693	0.603	0.531	0.437	0.358	0.315
0.10	0.662	0.575	0.509	0.433	0.355	0.314
0.15	0.639	0.559	0.495	0.426	0.351	0.310
0.20	0.620	0.549	0.484	0.420	0.346	0.305
0.25	0.605	0.544	0.475	0.413	0.340	0.298
0.30	0.595	0.540	0.469	0.406	0.331	0.290
0.35	0.588	0.537	0.464	0.398	0.323	0.280
0.40	0.584	0.535	0.461	0.389	0.314	0.269
0.45	0.582	0.533	0.459	0.379	0.304	0.000
0.50	0.583	0.533	0.456	0.368	0.000	0.000
0.55	0.584	0.534	0.455	0.359	0.000	0.000
0.60	0.588	0.535	0.455	0.352	0.000	0.000
0.65	0.593	0.539	0.455	0.349	0.000	0.000
0.70	0.599	0.544	0.458	0.346	0.000	0.000
0.75	0.607	0.551	0.461	0.345	0.000	0.000
0.80	0.616	0.561	0.467	0.345	0.000	0.000
0.85	0.625	0.574	0.475	0.345	0.000	0.000
0.90	0.636	0.588	0.485	0.346	0.000	0.000
0.95	0.648	0.602	0.499	0.349	0.000	0.000
1.00	0.660	0.619	0.519	0.351	0.000	0.000

Table 23. Array of values of K_t for the system $\text{Nd}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{org.}}$ and Y_{Nd}

Y_{Nd}	$(M_t)_{\text{org.}}$					
	2.0	2.5	3.0	3.5	4.0	4.5
0.00	0.769	0.667	0.566	0.441	0.358	0.314
0.05	0.700	0.611	0.540	0.445	0.368	0.321
0.10	0.665	0.584	0.522	0.445	0.374	0.326
0.15	0.643	0.569	0.508	0.442	0.378	0.329
0.20	0.627	0.564	0.499	0.435	0.377	0.329
0.25	0.618	0.562	0.492	0.424	0.375	0.326
0.30	0.612	0.564	0.487	0.415	0.368	0.321
0.35	0.611	0.565	0.485	0.408	0.357	0.315
0.40	0.610	0.566	0.485	0.403	0.345	0.306
0.45	0.611	0.569	0.488	0.400	0.327	0.000
0.50	0.614	0.572	0.490	0.400	0.307	0.000
0.55	0.616	0.575	0.494	0.401	0.000	0.000
0.60	0.620	0.580	0.500	0.404	0.000	0.000
0.65	0.625	0.584	0.508	0.405	0.000	0.000
0.70	0.630	0.590	0.519	0.405	0.000	0.000
0.75	0.636	0.596	0.527	0.403	0.000	0.000
0.80	0.645	0.603	0.533	0.400	0.000	0.000
0.85	0.655	0.613	0.537	0.398	0.000	0.000
0.90	0.669	0.624	0.540	0.395	0.000	0.000
0.95	0.684	0.637	0.542	0.390	0.000	0.000
1.00	0.702	0.653	0.543	0.386	0.000	0.000

Table 24. Array of values of K_t for the system $\text{Sm}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{org.}}$ and Y_{Sm}

Y_{Sm}	$(M_t)_{\text{org.}}$					
	2.0	2.5	3.0	3.5	4.0	4.5
0.00	0.769	0.667	0.566	0.441	0.358	0.314
0.05	0.724	0.641	0.555	0.449	0.370	0.328
0.10	0.700	0.626	0.548	0.454	0.377	0.339
0.15	0.684	0.615	0.543	0.458	0.383	0.345
0.20	0.672	0.608	0.541	0.460	0.388	0.349
0.25	0.665	0.605	0.541	0.461	0.390	0.350
0.30	0.660	0.603	0.544	0.462	0.390	0.349
0.35	0.659	0.604	0.548	0.461	0.388	0.346
0.40	0.659	0.606	0.553	0.461	0.386	0.341
0.45	0.660	0.610	0.560	0.460	0.382	0.000
0.50	0.664	0.616	0.567	0.459	0.377	0.000
0.55	0.669	0.623	0.575	0.475	0.372	0.000
0.60	0.676	0.630	0.582	0.455	0.365	0.000
0.65	0.685	0.640	0.590	0.450	0.359	0.000
0.70	0.695	0.652	0.598	0.450	0.351	0.000
0.75	0.707	0.665	0.605	0.449	0.343	0.000
0.80	0.720	0.679	0.614	0.450	0.000	0.000
0.85	0.733	0.694	0.622	0.455	0.000	0.000
0.90	0.748	0.710	0.630	0.463	0.000	0.000
0.95	0.763	0.727	0.638	0.475	0.000	0.000
1.00	0.780	0.746	0.646	0.492	0.000	0.000

Table 25. Array of values of K_{HNO_3} for the system $\text{La}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{org.}}$ and Y_{La}

Y_{Sm}	$(M_t)_{\text{org.}}$					
	2.0	2.5	3.0	3.5	4.0	4.5
0.00	0.769	0.667	0.566	0.441	0.358	0.314
0.05	0.802	0.701	0.617	0.523	0.464	0.399
0.10	0.845	0.749	0.681	0.612	0.566	0.474
0.15	0.895	0.804	0.756	0.701	0.668	0.546
0.20	0.950	0.867	0.831	0.797	0.767	0.617
0.25	1.016	0.937	0.910	0.895	0.863	0.685
0.30	1.087	1.009	0.991	0.995	0.963	0.000
0.35	1.160	1.083	1.071	1.101	1.068	0.000
0.40	1.234	1.161	1.157	1.218	0.000	0.000
0.45	1.307	1.244	1.245	1.331	0.000	0.000
0.50	1.384	1.331	1.337	1.452	0.000	0.000
0.55	1.467	1.423	1.434	1.574	0.000	0.000
0.60	1.548	1.520	1.539	1.697	0.000	0.000
0.65	1.637	1.618	1.649	1.825	0.000	0.000
0.70	1.732	1.718	1.769	1.956	0.000	0.000
0.75	1.829	1.823	1.900	2.087	0.000	0.000
0.80	1.933	1.929	2.037	2.222	0.000	0.000
0.85	2.041	2.041	2.186	0.000	0.000	0.000
0.90	2.157	2.156	2.348	0.000	0.000	0.000
0.95	2.275	2.276	0.000	0.000	0.000	0.000
1.00	0.000	0.000	0.000	0.000	0.000	0.000

Table 26. Array of values of K_{HNO_3} for the system $\text{Pr}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O as a function of $(M_t)_{\text{org.}}$ and Y_{Pr}

Y_{Pr}	$(M_t)_{\text{org.}}$					
	2.0	2.5	3.0	3.5	4.0	4.5
0.00	0.769	0.667	0.566	0.441	0.358	0.314
0.05	0.785	0.678	0.581	0.479	0.399	0.346
0.10	0.809	0.697	0.601	0.521	0.442	0.380
0.15	0.839	0.723	0.628	0.563	0.487	0.418
0.20	0.872	0.760	0.661	0.607	0.534	0.458
0.25	0.912	0.802	0.700	0.653	0.584	0.507
0.30	0.959	0.848	0.748	0.701	0.638	0.571
0.35	1.011	0.894	0.795	0.750	0.697	0.640
0.40	1.067	0.940	0.844	0.799	0.756	0.722
0.45	1.133	0.991	0.892	0.854	0.819	0.000
0.50	1.207	1.044	0.945	0.911	0.886	0.000
0.55	1.280	1.099	0.999	0.971	0.000	0.000
0.60	1.358	1.157	1.055	1.035	0.000	0.000
0.65	1.437	1.221	1.112	1.099	0.000	0.000
0.70	1.523	1.291	1.173	1.167	0.000	0.000
0.75	1.613	1.370	1.237	1.234	0.000	0.000
0.80	1.709	1.454	1.301	1.303	0.000	0.000
0.85	1.810	1.547	1.371	1.376	0.000	0.000
0.90	1.913	1.643	1.442	1.449	0.000	0.000
0.95	2.021	1.752	0.000	0.000	0.000	0.000
1.00	0.000	0.000	0.000	0.000	0.000	0.000

Table 27. Array of values of K_{HNO_3} for the system $\text{Nd}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{org.}}$ and Y_{Nd}

Y_{Nd}	$(M_t)_{\text{org.}}$					
	2.0	2.5	3.0	3.5	4.0	4.5
0.00	0.769	0.667	0.566	0.441	0.358	0.314
0.05	0.772	0.678	0.566	0.461	0.385	0.336
0.10	0.780	0.696	0.573	0.488	0.423	0.366
0.15	0.802	0.716	0.589	0.520	0.469	0.399
0.20	0.836	0.740	0.612	0.557	0.516	0.439
0.25	0.876	0.773	0.641	0.597	0.561	0.490
0.30	0.924	0.816	0.680	0.637	0.608	0.542
0.35	0.977	0.857	0.721	0.680	0.655	0.600
0.40	1.033	0.900	0.764	0.725	0.701	0.663
0.45	1.090	0.946	0.808	0.770	0.748	0.000
0.50	1.151	0.993	0.855	0.819	0.795	0.000
0.55	1.220	1.042	0.901	0.869	0.843	0.000
0.60	1.291	1.093	0.956	0.920	0.891	0.000
0.65	1.371	1.148	0.013	0.975	0.000	0.000
0.70	1.455	1.207	1.075	1.030	0.000	0.000
0.75	1.545	1.268	1.136	1.089	0.000	0.000
0.80	1.642	1.329	1.207	1.150	0.000	0.000
0.85	1.746	1.396	1.279	1.211	0.000	0.000
0.90	1.857	1.466	1.353	1.273	0.000	0.000
0.95	1.977	1.537	0.000	0.000	0.000	0.000
1.00	0.000	0.000	0.000	0.000	0.000	0.000

Table 28. Array of values of K_{HNO_3} for the system $\text{Sm}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{org.}}$ and Y_{Sm}

Y_{Sm}	$(M_t)_{\text{org.}}$					
	2.0	2.5	3.0	3.5	4.0	4.5
0.00	0.769	0.667	0.566	0.441	0.358	0.314
0.05	0.769	0.658	0.560	0.448	0.367	0.336
0.10	0.773	0.656	0.564	0.456	0.380	0.336
0.15	0.787	0.664	0.571	0.467	0.395	0.350
0.20	0.804	0.677	0.584	0.482	0.413	0.368
0.25	0.829	0.696	0.600	0.500	0.435	0.388
0.30	0.859	0.716	0.619	0.523	0.461	0.410
0.35	0.892	0.738	0.641	0.550	0.493	0.437
0.40	0.928	0.767	0.668	0.580	0.531	0.464
0.45	0.963	0.797	0.700	0.612	0.573	0.000
0.50	0.1003	0.831	0.735	0.648	0.623	0.000
0.55	1.047	0.869	0.776	0.684	0.690	0.000
0.60	1.092	0.907	0.817	0.722	0.772	0.000
0.65	1.139	0.947	0.863	0.762	0.878	0.000
0.70	1.191	0.988	0.911	0.805	1.018	0.000
0.75	1.245	1.032	0.961	0.850	0.000	0.000
0.80	1.301	1.079	1.015	0.897	0.000	0.000
0.85	1.360	1.129	1.072	0.947	0.000	0.000
0.90	1.421	1.179	1.131	0.998	0.000	0.000
0.95	1.488	1.231	0.000	0.000	0.000	0.000
1.00	0.000	0.000	0.000	0.000	0.000	0.000

N	- total number of stages in an extraction cascade
M	- feed stage in an extraction cascade with internal feed
S	- flow rate of solvent in organic streams, kgm. TBP/ unit time
F	- flow rate of solvent in a feed stream, kgm. H ₂ O/ unit time
SOVR	- flow rate ratio, S/R
ROVS	- flow rate ratio, R/S
REX	- flow rate of solvent in aqueous streams on extract side of internally fed cascade, kgm. H ₂ O/unit time
RSC	- flow rate of solvent in aqueous streams on scrub side of internally fed cascade
TMAQ	- (M_t) _{aq.}
AMAAQ	- (M_{HNO_3}) _{aq.}
XLAMAAQ	- (M_{La}) _{aq.}
PRMAQ	- (M_{Pr}) _{aq.}
XNDMAQ	- (M_{Nd}) _{aq.}
SMMAQ	- (M_{Sm}) _{aq.}
REMAQ	- (M_{RE}) _{aq.}
XHNO3	- X_{HNO_3}
XLA	- X_{La}
XPR	- X_{Pr}
XND	- X_{Nd}
XSM	- X_{Sm}

Figure 37. Principal variable names

XRE	- X_{RE}
XLASF	- x_{La}
XPRSF	- x_{Pr}
XNDSF	- x_{Nd}
XSMSF	- x_{Sm}
TMOR	- $(M_t)_{org.}$
AMOR	- $(M_{HNO_3})_{org.}$
XLAMOR	- $(M_{La})_{org.}$
PRMOR	- $(M_{Pr})_{org.}$
XNDMOR	- $(M_{Nd})_{org.}$
SMMOR	- $(M_{Sm})_{org.}$
REMOR	- $(M_{RE})_{org.}$
YHNO3	- Y_{HNO_3}
YLA	- Y_{La}
YPR	- Y_{Pr}
YND	- Y_{Nd}
YSM	- Y_{Sm}
YRE	- Y_{RE}
YLASF	- y_{La}
YPRSF	- y_{Pr}
YNDSF	- y_{Nd}
YSMSF	- y_{Sm}

Figure 37. (Continued)

XKTRE	- K_t for the system $\text{RE}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{aq.}}$ and X_{RE} ; RE = La, Pr, Nd, Sm
XKARE	- K_{HNO_3} for the system $\text{RE}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{aq.}}$ and X_{RE} ; RE = La, Pr, Nd, Sm
YKTRE	- K_t for the system $\text{RE}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{org.}}$ and Y_{RE} ; RE = La, Pr, Nd, Sm
YKARE	- K_{HNO_3} for the system $\text{RE}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ as a function of $(M_t)_{\text{org.}}$ and Y_{RE} ; RE = La, Pr, Nd, Sm
BLAPR	- $\beta_{\text{La-Pr}}$
BPRPR	- $\beta_{\text{Pr-Pr}}$
BNDPR	- $\beta_{\text{Nd-Pr}}$
BSMPR	- $\beta_{\text{Sm-Pr}}$
TOTK	- K_t
HNO3K	- K_{HNO_3}
FTM	- $(M_t)_F$
FAM	- $(M_{\text{HNO}_3})_F$
FLAM	- $(M_{\text{La}})_F$
FPRM	- $(M_{\text{Pr}})_F$
FNDM	- $(M_{\text{Nd}})_F$
FSMM	- $(M_{\text{Sm}})_F$
FREM	- $(M_{\text{RE}})_F$
XAF	- $(X_{\text{HNO}_3})_F$

Figure 37. (Continued)

XLAF	- $(X_{La})_F$
XPRF	- $(X_{Pr})_F$
XNDF	- $(X_{Nd})_F$
XSMF	- $(X_{Sm})_F$
XREF	- $(X_{RE})_F$
XLASFF	- $(x_{La})_F$
XPRSFF	- $(x_{Pr})_F$
XNDSFF	- $(x_{Nd})_F$
XSMSFF	- $(x_{Sm})_F$

For Programs 1 and 3:

RLTM	- $(M_t)_{R_1}$
RLAM	- $(M_{HNO_3})_{R_1}$
RLLAM	- $(M_{La})_{R_1}$
RLPRM	- $(M_{Pr})_{R_1}$
RLNDM	- $(M_{Nd})_{R_1}$
RLSMM	- $(M_{Sm})_{R_1}$
SOTM	- $(M_t)_{S_0}$
SOAM	- $(M_{HNO_3})_{S_0}$
SOLAM	- $(M_{La})_{S_0}$
SOPRM	- $(M_{Pr})_{S_0}$

Figure 37. (Continued)

SONDM - $(M_{\text{Nd}})S_0$

SOSMM - $(M_{\text{Sm}})S_0$

For Programs 2 and 4:

ROTM - $(M_t)R_0$

ROAM - $(M_{\text{HNO}_3})R_0$

ROLAM - $(M_{\text{La}})R_0$

ROPRM - $(M_{\text{Pr}})R_0$

RONDM - $(M_{\text{Nd}})R_0$

ROSMM - $(M_{\text{Sm}})R_0$

SlTM - $(M_t)S_1$

SlAM - $(M_{\text{HNO}_3})S_1$

SlLAM - $(M_{\text{La}})S_1$

SlPRM - $(M_{\text{Pr}})S_1$

SlNDM - $(M_{\text{Nd}})S_1$

SlSMM - $(M_{\text{Sm}})S_1$

Figure 37. (Continued)

Fig. 38. Flow diagram, Program I

Fig. 38. (cont.)

Fig. 38. (cont.)

Fig. 38. (cont.)

Fig. 38. (cont.)

```

        DIMENSION XKTLA(21,7),XKTPR(21,7),XKTND(21,7),XKTSM(21,7),XKALA(21,7)
        DO 5 I = 1,21
5      READ INPUT TAPE 5, 500, (XKTLA(I,J),J = 1,7)
        DO 10 I = 1,21
10     READ INPUT TAPE 5, 500, (XKTPR(I,J),J = 1,7)
        DO 15 I = 1,21
15     READ INPUT TAPE 5, 500, (XKTND(I,J),J = 1,7)
        DO 20 I = 1,21
20     READ INPUT TAPE 5, 500, (XKTSM(I,J),J = 1,7)
        DO 25 I = 1,21
25     READ INPUT TAPE 5, 500, (XKALA(I,J),J = 1,7)
        DO 30 I = 1,21
30     READ INPUT TAPE 5, 500, (XKAPR(I,J),J = 1,7)
        DO 35 I = 1,21
35     READ INPUT TAPE 5, 500, (XKAND(I,J),J = 1,7)
        DO 40 I = 1,21
40     READ INPUT TAPE 5, 500, (XKASM(I,J),J = 1,7)
45     READ INPUT TAPE 5, 501, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SMMAQ, REMAQ
        READ INPUT TAPE 5, 502, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR,
1 SOVR, N, K
        PRINT 503, SOVR, N
        PRINT 504
        XHNO3 = AMAQ/TMAQ
        XLA = XLAMAQ/TMAQ
        XPR = PRMAQ/TMAQ
        XND = XNDMAQ/TMAQ
        XSM = SMMAQ/TMAQ
        XRE = REMAQ/TMAQ
        SXA = XHNO3 + XLA + XPR + XND + XSM
        XLASF = XLAMAQ/REMAQ
        XPRSF = PRMAQ/REMAQ
        XNDSF = XNDMAQ/REMAQ
        XSMSF = SMMAQ/REMAQ
        SXREA = XLASF + XPRSF + XNDSF + XSMSF
        YHNO3 = AMOR/TMOR
        YLA = XLAMOR/TMOR
        YPR = PRMOR/TMOR
        YND = XNDMOR/TMOR
        YSM = SMMOR/TMOR
        YRE = REMOR/TMOR
        SYO = YHNO3 + YLA + YPR + YND + YSM
        YLASF = XLAMOR/REMOR
        YPRSF = PRMOR/REMOR
        YNDSF = XNDMOR/REMOR
        YSMSF = SMMOR/REMOR
        SYREO = YLASF + YPRSF + YNDSF + YSMSF
        PRINT 505, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR, YHNO3, YLA, YPR
1, YND, YSM, YRE, YLASF, YPRSF, YNDSF, YSMSF, SYO, SYREO
        PRINT 506, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SMMAQ, REMAQ, XHNO3, XLA, XPR
1, XND, XSM, XRE, XLASF, XPRSF, XNDSF, XSMSF, SXA, SXREA
        RITM = TMAQ
        RIAM = AMAQ
        RILAM = XLAMAQ
        RIPRM = PRMAQ
        RINDM = XNDMAQ
        RISMM = SMMAQ
        SOTM = TMOR
        SOAM = AMOR
        SOLAM = XLAMOR
        SOPRM = PRMOR
        SONDM = XNDMOR

```

Figure 39. Fortran statements, Program I

```

50      SOSMM = SMMOR                                BMS1 079
      DO 150 L = 1,N                                BMS1 080
      XREI = (XRE*100.0 + 5.0)/5.0                  BMS1 081
      IX = XREI                                       BMS1 082
      XI = IX                                         BMS1 083
      FRX = XREI - XI                                 BMS1 084
55      IF(5.0 - TMAQ) 60,70,65                      BMS1 085
60      IF(7.0 - TMAQ) 75,75,70                      BMS1 086
65      Z = TMAQ - 2.0                                BMS1 087
      GO TO 80                                         BMS1 088
70      Z = (TMAQ + 1.0)/2.0                          BMS1 089
      GO TO 80                                         BMS1 090
75      Z = (TMAQ + 5.0)/3.0                          BMS1 091
80      KZ = Z                                         BMS1 092
      ZK = KZ                                         BMS1 093
      FRZ = Z - ZK                                    BMS1 094
      SKT = MIN1F(XKTLA(IX,KZ),XKTLA(IX+1,KZ),XKTLA(IX,KZ+1),XKTLA(IX+1,
1KZ+1),XKTPR(IX,KZ),XKTPR(IX+1,KZ),XKTPR(IX,KZ+1),XKTPR(IX+1,KZ+1),BMS1 095
2XKTND(IX,KZ),XKTND(IX+1,KZ),XKTND(IX,KZ+1),XKTND(IX+1,KZ+1),XKTSM(BMS1 096
3IX,KZ),XKTSM(IX+1,KZ),XKTSM(IX,KZ+1),XKTSM(IX+1,KZ+1))    BMS1 097
      IF(SKT) 85,85,90                                BMS1 098
85      PRINT 507, XKTLA(IX,KZ),XKTLA(IX+1,KZ),XKTLA(IX,KZ+1),XKTLA(IX+1,
1Z+1),XKTPR(IX,KZ),XKTPR(IX+1,KZ),XKTPR(IX,KZ+1),XKTPR(IX+1,KZ+1),XBMS1 100
2KTND(IX,KZ),XKTND(IX+1,KZ),XKTND(IX,KZ+1),XKTND(IX+1,KZ+1),XKTSM(BMS1 101
3X,KZ),XKTSM(IX+1,KZ),XKTSM(IX,KZ+1),XKTSM(IX+1,KZ+1),TMAQ,XRE    BMS1 102
      IF(K) 495,495,45                                BMS1 103
90      XKTLA1 = XKTLA(IX,KZ)*(1.0 - FRX) + XKTLA(IX+1,KZ)*FRX    BMS1 104
      XKTLA2 = XKTLA(IX,KZ+1)*(1.0 - FRX) + XKTLA(IX+1,KZ+1)*FRX    BMS1 105
      XKTLA3 = XKTLA1*(1.0 - FRZ) + XKTLA2*FRZ          BMS1 106
      CKTLA = XKTLA3 * XLASF                             BMS1 107
      XKTPR1 = XKTPR(IX,KZ)*(1.0 - FRX) + XKTPR(IX+1,KZ)*FRX    BMS1 108
      XKTPR2 = XKTPR(IX,KZ+1)*(1.0 - FRX) + XKTPR(IX+1,KZ+1)*FRX    BMS1 109
      XKTPR3 = XKTPR1*(1.0 - FRZ) + XKTPR2*FRZ          BMS1 110
      CKTPR = XKTPR3 * XPRSF                             BMS1 111
      XKTND1 = XKTND(IX,KZ)*(1.0 - FRX) + XKTND(IX+1,KZ)*FRX    BMS1 112
      XKTND2 = XKTND(IX,KZ+1)*(1.0 - FRX) + XKTND(IX+1,KZ+1)*FRX    BMS1 113
      XKTND3 = XKTND1*(1.0 - FRZ) + XKTND2*FRZ          BMS1 114
      CKTND = XKTND3 * XNDSF                             BMS1 115
      XKTSM1 = XKTSM(IX,KZ)*(1.0 - FRX) + XKTSM(IX+1,KZ)*FRX    BMS1 116
      XKTSM2 = XKTSM(IX,KZ+1)*(1.0 - FRX) + XKTSM(IX+1,KZ+1)*FRX    BMS1 117
      XKTSM3 = XKTSM1*(1.0 - FRZ) + XKTSM2*FRZ          BMS1 118
      CKTSM = XKTSM3 * XSMSF                             BMS1 119
      SKA = MIN1F(XKALA(IX,KZ),XKALA(IX+1,KZ),XKALA(IX,KZ+1),XKALA(IX+1,
1KZ+1),XKAPR(IX,KZ),XKAPR(IX+1,KZ),XKAPR(IX,KZ+1),XKAPR(IX+1,KZ+1),XBMS1 120
2XKAND(IX,KZ),XKAND(IX+1,KZ),XKAND(IX,KZ+1),XKAND(IX+1,KZ+1),XKASM(BMS1 121
3IX,KZ),XKASM(IX+1,KZ),XKASM(IX,KZ+1),XKASM(IX+1,KZ+1))    BMS1 122
      IF(SKA) 95,95,100                                BMS1 123
95      PRINT 508, XKALA(IX,KZ),XKALA(IX+1,KZ),XKALA(IX,KZ+1),XKALA(IX+1,
1Z+1),XKAPR(IX,KZ),XKAPR(IX+1,KZ),XKAPR(IX,KZ+1),XKAPR(IX+1,KZ+1),XBMS1 124
2KAND(IX,KZ),XKAND(IX+1,KZ),XKAND(IX,KZ+1),XKAND(IX+1,KZ+1),XKASM(BMS1 125
3X,KZ),XKASM(IX+1,KZ),XKASM(IX,KZ+1),XKASM(IX+1,KZ+1),TMAQ,XRE    BMS1 126
      IF(K) 495,495,45                                BMS1 127
100     XKALA1 = XKALA(IX,KZ)*(1.0 - FRX) + XKALA(IX+1,KZ)*FRX    BMS1 128
      XKALA2 = XKALA(IX,KZ+1)*(1.0 - FRX) + XKALA(IX+1,KZ+1)*FRX    BMS1 129
      XKALA3 = XKALA1*(1.0 - FRZ) + XKALA2*FRZ          BMS1 130
      CKALA = XKALA3 * XLASF                             BMS1 131
      XKAPR1 = XKAPR(IX,KZ)*(1.0 - FRX) + XKAPR(IX+1,KZ)*FRX    BMS1 132
      XKAPR2 = XKAPR(IX,KZ+1)*(1.0 - FRX) + XKAPR(IX+1,KZ+1)*FRX    BMS1 133
      XKAPR3 = XKAPR1*(1.0 - FRZ) + XKAPR2*FRZ          BMS1 134
      CKAPR = XKAPR3 * XPRSF                             BMS1 135
      XKAND1 = XKAND(IX,KZ)*(1.0 - FRX) + XKAND(IX+1,KZ)*FRX    BMS1 136
      XKAND2 = XKAND(IX,KZ+1)*(1.0 - FRX) + XKAND(IX+1,KZ+1)*FRX    BMS1 137

```

Figure 39. (Continued)

```

XKAND3 = XKAND1*(1.0 - FRZ) + XKAND2*FRZ      BMS1 141
CKAND = XKAND3 * XNDSF                          BMS1 142
XKASM1 = XKASM(IX,KZ)*(1.0 - FRX) + XKASM(IX+1,KZ)*FRX      BMS1 143
XKASM2 = XKASM(IX,KZ+1)*(1.0 - FRX) + XKASM(IX+1,KZ+1)*FRX  BMS1 144
XKASM3 = XKASM1*(1.0 - FRZ) + XKASM2*FRZ          BMS1 145
CKASM = XKASM3 * XSMSF                          BMS1 146
TOTK = CKTLA + CKTPR + CKTND + CKTSM            BMS1 147
HNO3K = CKALA + CKAPR + CKAND + CKASM            BMS1 148
TMOR = TMAQ*TOTK                                BMS1 149
IF(TMOR - 1.75) 105,110,110                      BMS1 150
105 PRINT 509, TMOR,TMAQ,TOTK                     BMS1 151
    IF(K) 495,495,45                             BMS1 152
110 AMOR = AMAQ*HNO3K                             BMS1 153
    REMOR = TMOR - AMOR                           BMS1 154
    IF(REMOR) 115,115,120                         BMS1 155
115 PRINT 510, TMOR,AMOR,REMOR,HNO3K              BMS1 156
    IF(K) 495,495,45                             BMS1 157
120 BLAPR = 0.8187 - 0.1106*TMOR                 BMS1 158
    BPRPR = 1.0                                   BMS1 159
    BNDPR = 1.0448 + 0.09874*TMOR                 BMS1 160
    BSMPR = -0.3795 + 0.9214*TMOR                 BMS1 161
    DEMS = XLAMAQ*BLAPR + PRMAQ*BPRPR + XNDMAQ*BNDPR + SMMAQ*BSMPR BMS1 162
    XLAMOR = REMOR*BLAPR*XLAMAQ/DEMS              BMS1 163
    PRMOR = REMOR*BPRPR*PRMAQ/DEMS                BMS1 164
    XNDMOR = REMOR*BNDPR*XNDMAQ/DEMS              BMS1 165
    SMMOR = REMOR*BSMPR*SMMAQ/DEMS                BMS1 166
    YHNO3 = AMOR/TMOR                             BMS1 167
    YLA = XLAMOR/TMOR                             BMS1 168
    YPR = PRMOR/TMOR                              BMS1 169
    YND = XNDMOR/TMOR                             BMS1 170
    YSM = SMMOR/TMOR                              BMS1 171
    YRE = REMOR/TMOR                              BMS1 172
    SYO = YHNO3 + YLA + YPR + YND + YSM           BMS1 173
    YLASF = XLAMOR/REMOR                          BMS1 174
    YPRSF = PRMOR/REMOR                           BMS1 175
    YNDSF = XNDMOR/REMOR                          BMS1 176
    YSMSF = SMMOR/REMOR                           BMS1 177
    SYREO = YLASF + YPRSF + YNDSF + YSMSF         BMS1 178
    PRINT 511,L, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,YHNO3,YLA,YPBMS1 179
1R,YND,YSM,YRE,YLASF,YPRSF,YNDSF,YSMSF,SYO,SYREO      BMS1 180
    TMAQ = TMOR*SOVR - SOTM*SOVR + R1TM           BMS1 181
    AMAQ = AMOR*SOVR - SOAM*SOVR + R1AM           BMS1 182
    XLAMAQ = XLAMOR*SOVR - SOLAM*SOVR + R1LAM      BMS1 183
    PRMAQ = PRMOR*SOVR - SOPRM*SOVR + R1PRM       BMS1 184
    XNDMAQ = XNDMOR*SOVR - SONDM*SOVR + R1NDM     BMS1 185
    SMMAQ = SMMOR*SOVR - SOSMM*SOVR + R1SMM       BMS1 186
    REMAQ = TMAQ - AMAQ                           BMS1 187
    SAM = MIN1F(TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ) BMS1 188
    IF(SAM) 125,125,130                          BMS1 189
125 PRINT 512,TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ BMS1 190
    IF(K) 495,495,45                             BMS1 191
130 XHNO3 = AMAQ/TMAQ                             BMS1 192
    XLA = XLAMAQ/TMAQ                             BMS1 193
    XPR = PRMAQ/TMAQ                              BMS1 194
    XND = XNDMAQ/TMAQ                             BMS1 195
    XSM = SMMAQ/TMAQ                              BMS1 196
    XRE = REMAQ/TMAQ                              BMS1 197
    SXA = XHNO3 + XLA + XPR + XND + XSM           BMS1 198
    XLASF = XLAMAQ/REMAQ                          BMS1 199
    XPRSF = PRMAQ/REMAQ                          BMS1 200
    XNDSF = XNDMAQ/REMAQ                         BMS1 201
    XSMSF = SMMAQ/REMAQ                         BMS1 202

```

Figure 39. (Continued)


```

      SXREA = XLASF + XPRSF + XNDSF + XSMSF                      BMS1 203
      LL = L+1                                                    BMS1 204
      PRINT 513,LL,TMAQ,AM AQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ,XHNO3,XLA,XBMS1 205
1PR,XND,XSM,XRE,XLASF,XPRSF,XNDSF,XSMSF,SXA,SXREA              BMS1 206
      IF(TMAQ - 3.0) 135,140,140                                  BMS1 207
135  PRINT 514, TMAQ                                              BMS1 208
      IF(K) 495,495,45                                           BMS1 209
140  IF(TMAQ - 16.0) 150,145,145                                  BMS1 210
145  PRINT 514,TMAQ                                              BMS1 211
      IF(K) 495,495,45                                           BMS1 212
150  CONTINUE                                                    BMS1 213
      IF(K)495,495,45                                           BMS1 214
500  FORMAT (7F10.3)                                             BMS1 217
501  FORMAT (7F9.4)                                              BMS1 218
502  FORMAT (7F7.4,F8.4,I3,I3)                                   BMS1 219
503  FORMAT (31H1EXTRACT SIDE CALCULATION SOVR= F8.4,4H N= 13) BMS1 220
504  FORMAT (120HJ TOTALMOLHNO3 MOL LA MOL PR MOL NO MOL SM MOL BMS1 221
1RE MOL ACFR LAFR PRFR NDFR SMFR REFRLA/REPR/REND/RESM/RE STFRSREFRDBMS1 222
2)                                                                BMS1 223
505  FORMAT (4HJS 0 7F8.4,12F5.3)                               BMS1 224
506  FORMAT (4H R 1 7F8.4,12F5.3)                               BMS1 225
507  FORMAT (8HJXKTRE=0 16F6.3,F8.4,F6.3)                      BMS1 226
508  FORMAT (8HJXKARE=0 16F6.3,F8.4,F6.3)                      BMS1 227
509  FORMAT (6HJTMOR= F10.4,6H TMAQ= F8.4,6H TOTK= F8.4)       BMS1 228
510  FORMAT (6HJTMOR= F10.4,6H AMOR= F10.8,7H REMOR= F10.8,7H HNO3K= F18BMS1 229
10.8)                                                            BMS1 230
511  FORMAT (2HJS 12,7F8.4,12F5.3)                               BMS1 231
512  FORMAT (6HJTMAQ= F10.4,6H AMAQ= F10.4,8H XLAMAQ= F10.4,7H PRMAQ= FBMS1 232
110.4,8H XNDMAQ= F10.4,7H SMMAQ= F10.4,7H REMAQ= F10.4)        BMS1 233
513  FORMAT (2H R 12,7F8.4,12F5.3)                               BMS1 234
514  FORMAT (6HJTMAQ= F10.4)                                     BMS1 235
495  STOP 89                                                     BMS1 215
      END                                                         BMS1 216

```

Figure 39. (Continued)

Fig. 40. Flow diagram, Program II.

Fig. 40. (cont.)

Fig. 40. (cont.)

Fig. 40. (cont.)

Fig. 40. (cont.)

```

      DIMENSION YKTLA(21,6),YKTPR(21,6),YKTND(21,6),YKTSM(21,6),YKALA(21,6)
      1,6),YKAPR(21,6),YKAND(21,6),YKASM(21,6)
      DO 5 I = 1,21
5      READ INPUT TAPE 5, 500, (YKTLA(I,J),J = 1,6)
      DO 10 I = 1,21
10     READ INPUT TAPE 5, 500, (YKTPR(I,J),J = 1,6)
      DO 15 I = 1,21
15     READ INPUT TAPE 5, 500, (YKTND(I,J),J = 1,6)
      DO 20 I = 1,21
20     READ INPUT TAPE 5, 500, (YKTSM(I,J),J = 1,6)
      DO 25 I = 1,21
25     READ INPUT TAPE 5, 500, (YKALA(I,J),J = 1,6)
      DO 30 I = 1,21
30     READ INPUT TAPE 5, 500, (YKAPR(I,J),J = 1,6)
      DO 35 I = 1,21
35     READ INPUT TAPE 5, 500, (YKAND(I,J),J = 1,6)
      DO 40 I = 1,21
40     READ INPUT TAPE 5, 500, (YKASM(I,J),J = 1,6)
45     READ INPUT TAPE 5, 501, TMAQ,AM AQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ
      READ INPUT TAPE 5, 502, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,
1,ROVS,N,K
      PRINT 503, ROVS,N
      PRINT 504
      IF(TMAQ) 600,65,50
50     XHNO3 = AMAQ/TMAQ
      XLA = XLAMAQ/TMAQ
      XPR = PRMAQ/TMAQ
      XND = XNDMAQ/TMAQ
      XSM = SMMAQ/TMAQ
      XRE = REMAQ/TMAQ
      IF(REMAQ) 600,60,55
55     XLASF = XLAMAQ/REMAQ
      XPRSF = PRMAQ/REMAQ
      XNDSF = XNDMAQ/REMAQ
      XSMSF = SMMAQ/REMAQ
      PRINT 505, TMAQ,AM AQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ,XHNO3,XLA,XPR
1,XND,XSM,XRE,XLASF,XPRSF,XNDSF,XSMSF
      GO TO 70
60     PRINT 506, TMAQ,AM AQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ,XHNO3,XLA,XPR
1,XND,XSM,XRE
      GO TO 70
65     PRINT 507, TMAQ,AM AQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ
70     YHNO3 = AMOR/TMOR
      YLA = XLAMOR/TMOR
      YPR = PRMOR/TMOR
      YND = XNDMOR/TMOR
      YSM = SMMOR/TMOR
      YRE = REMOR/TMOR
      YLASF = XLAMOR/REMOR
      YPRSF = PRMOR/REMOR
      YNDSF = XNDMOR/REMOR
      YSMSF = SMMOR/REMOR
      PRINT 508, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,YHNO3,YLA,YPR
1,YND,YSM,YRE,YLASF,YPRSF,YNDSF,YSMSF
      ROTM = TMAQ
      ROAM = AMAQ
      RCLAM = XLAMAQ
      ROPRM = PRMAQ
      RONDM = XNDMAQ
      ROSMM = SMMAQ
      SITM = TMOR
      SIAM = AMOR

```

Figure 41. Fortran statements, Program II

```

SILAM = XLAMOR                                BMS2 063
SIPRM = PRMOR                                  BMS2 064
SINDM = XNDMOR                                BMS2 065
SISMM = SMOR                                  BMS2 066
DO 185 L = 1,N                                BMS2 067
YREI = (YRE*100.0 + 5.0)/5.0                  BMS2 068
IY = YREI                                      BMS2 069
YI = IY                                        BMS2 070
FRY = YREI - YI                                BMS2 071
Z = (IMOR*10.0 - 15.0)/5.0                    BMS2 072
KZ = Z                                         BMS2 073
ZK = KZ                                        BMS2 074
FRZ = Z - ZK                                  BMS2 075
SKT = MINIF(YKTLA(IY,KZ),YKTLA(IY+1,KZ),YKTLA(IY,KZ+1),YKTLA(IY+1,KZ+1),YKTPR(IY,KZ),YKTPR(IY+1,KZ),YKTPR(IY,KZ+1),YKTPR(IY+1,KZ+1),YKTND(IY,KZ),YKTND(IY+1,KZ),YKTND(IY,KZ+1),YKTND(IY+1,KZ+1),YKTSM(IY,KZ),YKTSM(IY+1,KZ),YKTSM(IY,KZ+1),YKTSM(IY+1,KZ+1)) BMS2 076
IF (SKT) 75,75,80                                BMS2 080
75 PRINT 509, YKTLA(IY,KZ),YKTLA(IY+1,KZ),YKTLA(IY,KZ+1),YKTLA(IY+1,KZ+1),YKTPR(IY,KZ),YKTPR(IY+1,KZ),YKTPR(IY,KZ+1),YKTPR(IY+1,KZ+1),YKTND(IY,KZ),YKTND(IY+1,KZ),YKTND(IY,KZ+1),YKTND(IY+1,KZ+1),YKTSM(IY,KZ),YKTSM(IY+1,KZ),YKTSM(IY,KZ+1),YKTSM(IY+1,KZ+1),TMOR,YRE BMS2 081
IF (K) 600,600,45                                BMS2 085
80 YKTLA1 = YKTLA(IY,KZ)*(1.0 - FRY) + YKTLA(IY+1,KZ)*FRY BMS2 086
YKTLA2 = YKTLA(IY,KZ+1)*(1.0 - FRY) + YKTLA(IY+1,KZ+1)*FRY BMS2 087
YKTLA3 = YKTLA1*(1.0 - FRZ) + YKTLA2*FRZ          BMS2 088
CKTLA = YKTLA3 * YLASF                            BMS2 089
YKTPR1 = YKTPR(IY,KZ)*(1.0 - FRY) + YKTPR(IY+1,KZ)*FRY BMS2 090
YKTPR2 = YKTPR(IY,KZ+1)*(1.0 - FRY) + YKTPR(IY+1,KZ+1)*FRY BMS2 091
YKTPR3 = YKTPR1*(1.0 - FRZ) + YKTPR2*FRZ          BMS2 092
CKTPR = YKTPR3 * YPRSF                            BMS2 093
YKTND1 = YKTND(IY,KZ)*(1.0 - FRY) + YKTND(IY+1,KZ)*FRY BMS2 094
YKTND2 = YKTND(IY,KZ+1)*(1.0 - FRY) + YKTND(IY+1,KZ+1)*FRY BMS2 095
YKTND3 = YKTND1*(1.0 - FRZ) + YKTND2*FRZ          BMS2 096
CKTND = YKTND3 * YNDSF                            BMS2 097
YKTSM1 = YKTSM(IY,KZ)*(1.0 - FRY) + YKTSM(IY+1,KZ)*FRY BMS2 098
YKTSM2 = YKTSM(IY,KZ+1)*(1.0 - FRY) + YKTSM(IY+1,KZ+1)*FRY BMS2 099
YKTSM3 = YKTSM1*(1.0 - FRZ) + YKTSM2*FRZ          BMS2 100
CKTSM = YKTSM3 * YSMSF                            BMS2 101
SKA = MINIF(YKALA(IY,KZ),YKALA(IY+1,KZ),YKALA(IY,KZ+1),YKALA(IY+1,KZ+1),YKAPR(IY,KZ),YKAPR(IY+1,KZ),YKAPR(IY,KZ+1),YKAPR(IY+1,KZ+1),YKAND(IY,KZ),YKAND(IY+1,KZ),YKAND(IY,KZ+1),YKAND(IY+1,KZ+1),YKASM(IY,KZ),YKASM(IY+1,KZ),YKASM(IY,KZ+1),YKASM(IY+1,KZ+1)) BMS2 102
IF (SKA) 85,85,90                                BMS2 106
85 PRINT 510, YKALA(IY,KZ),YKALA(IY+1,KZ),YKALA(IY,KZ+1),YKALA(IY+1,KZ+1),YKAPR(IY,KZ),YKAPR(IY+1,KZ),YKAPR(IY,KZ+1),YKAPR(IY+1,KZ+1),YKAND(IY,KZ),YKAND(IY+1,KZ),YKAND(IY,KZ+1),YKAND(IY+1,KZ+1),YKASM(IY,KZ),YKASM(IY+1,KZ),YKASM(IY,KZ+1),YKASM(IY+1,KZ+1),TMOR,YRE BMS2 107
IF (K) 600,600,45                                BMS2 111
90 YKALA1 = YKALA(IY,KZ)*(1.0 - FRY) + YKALA(IY+1,KZ)*FRY BMS2 112
YKALA2 = YKALA(IY,KZ+1)*(1.0 - FRY) + YKALA(IY+1,KZ+1)*FRY BMS2 113
YKALA3 = YKALA1*(1.0 - FRZ) + YKALA2*FRZ          BMS2 114
CKALA = YKALA3 * YLASF                            BMS2 115
YKAPR1 = YKAPR(IY,KZ)*(1.0 - FRY) + YKAPR(IY+1,KZ)*FRY BMS2 116
YKAPR2 = YKAPR(IY,KZ+1)*(1.0 - FRY) + YKAPR(IY+1,KZ+1)*FRY BMS2 117
YKAPR3 = YKAPR1*(1.0 - FRZ) + YKAPR2*FRZ          BMS2 118
CKAPR = YKAPR3 * YPRSF                            BMS2 119
YKAND1 = YKAND(IY,KZ)*(1.0 - FRY) + YKAND(IY+1,KZ)*FRY BMS2 120
YKAND2 = YKAND(IY,KZ+1)*(1.0 - FRY) + YKAND(IY+1,KZ+1)*FRY BMS2 121
YKAND3 = YKAND1*(1.0 - FRZ) + YKAND2*FRZ          BMS2 122
CKAND = YKAND3 * YNDSF                            BMS2 123
YKASM1 = YKASM(IY,KZ)*(1.0 - FRY) + YKASM(IY+1,KZ)*FRY BMS2 124

```

Figure 41. (Continued)


```

YKASM2 = YKASM(IY,KZ+1)*(1.0 - FRY) + YKASM(IY+1,KZ+1)*FRY      BMS2 125
YKASM3 = YKASM1*(1.0 - FRZ) + YKASM2*FRZ                          BMS2 126
CKASM = YKASM3 * YSMSF                                           BMS2 127
TOTK = CKTLA + CKTPR + CKTND + CKTSM                             BMS2 128
HNO3K = CKALA + CKAPR + CKAND + CKASM                             BMS2 129
TMAQ = TMOR/TOTK                                                  BMS2 130
AMAO = AMOR/HNO3K                                                 BMS2 131
REMAQ = TMAQ - AMAQ                                               BMS2 132
IF (REMAQ) 95,95,100                                             BMS2 133
95  PRINT 511, TMAQ,AMAO,REMAQ,HNO3K                             BMS2 134
    IF (K) 600,600,45                                             BMS2 135
100 BLAPR = 0.8187 - 0.1106*TMOR                                  BMS2 136
    BPRPR = 1.0                                                  BMS2 137
    BNDPR = 1.0448 + 0.09874*TMOR                                 BMS2 138
    BSMPR = -0.3795 + 0.9214*TMOR                                 BMS2 139
    DEMS = XLAMOR/BLAPR + PRMOR/BPRPR + XNDMOR/BNDPR + SMMOR/BSMPR BMS2 140
    XLAMAO = XLAMOR*REMAQ/(BLAPR*DEMS)                           BMS2 141
    PRMAQ = PRMOR*REMAQ/(BPRPR*DEMS)                             BMS2 142
    XNDMAQ = XNDMOR*REMAQ/(BNDPR*DEMS)                           BMS2 143
    SMMAQ = SMMOR*REMAQ/(BSMPR*DEMS)                             BMS2 144
    XHNO3 = AMAQ/TMAQ                                              BMS2 145
    XLA = XLAMAO/TMAQ                                              BMS2 146
    XPR = PRMAQ/TMAQ                                              BMS2 147
    XND = XNDMAQ/TMAQ                                             BMS2 148
    XSM = SMMAQ/TMAQ                                              BMS2 149
    XRE = REMAQ/TMAQ                                              BMS2 150
    XLASF = XLAMAO/REMAQ                                           BMS2 151
    XPRSF = PRMAQ/REMAQ                                           BMS2 152
    XNDSF = XNDMAQ/REMAQ                                           BMS2 153
    XSMSF = SMMAQ/REMAQ                                           BMS2 154
    SXA = XHNO3 + XLA + XPR + XND + XSM                           BMS2 155
    IF (0.9999 - SXA) 105,115,110                                 BMS2 156
105 IF (1.0001 - SXA) 110,115,115                                 BMS2 157
110 PRINT 512, TMAQ,AMAO,XLAMAO,PRMAQ,XNDMAQ,SMMAQ,REMAQ        BMS2 158
    IF (K) 600,600,45                                             BMS2 159
115 SXREA = XLASF + XPRSF + XNDSF + XSMSF                         BMS2 160
    IF (0.9999 - SXREA) 120,130,125                               BMS2 161
120 IF (1.0001 - SXREA) 125,130,130                               BMS2 162
125 PRINT 513, TMAQ,AMAO,XLAMAO,PRMAQ,XNDMAQ,SMMAQ,REMAQ        BMS2 163
    IF (K) 600,600,45                                             BMS2 164
130 PRINT 514, L, TMAQ,AMAO,XLAMAO,PRMAQ,XNDMAQ,SMMAQ,REMAQ,XHNO3,XLA,XPR BMS2 165
    1,XND,XSM,XRE,XLASF,XPRSF,XNDSF,XSMSF                       BMS2 166
    TMOR = TMAQ * ROVS + S1TM - ROTM*ROVS                         BMS2 167
    AMOR = AMAQ*ROVS + S1AM - ROAM*ROVS                           BMS2 168
    XLAMOR = XLAMAO*ROVS + S1LAM - ROLAM*ROVS                     BMS2 169
    PRMOR = PRMAQ*ROVS + S1PRM - ROPRM*ROVS                       BMS2 170
    XNDMOR = XNDMAQ*ROVS + S1NDM - ROND*ROVS                      BMS2 171
    SMMOR = SMMAQ*ROVS + S1SMM - ROSMM*ROVS                       BMS2 172
    REMOR = TMOR - AMOR                                           BMS2 173
    SOM = MIN1(TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR)        BMS2 174
    IF (SOM) 135,135,140                                          BMS2 175
135 PRINT 515, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR        BMS2 176
    IF (K) 600,600,45                                             BMS2 177
140 YHNO3 = AMOR/TMOR                                              BMS2 178
    YLA = XLAMOR/TMOR                                              BMS2 179
    YPR = PRMOR/TMOR                                              BMS2 180
    YND = XNDMOR/TMOR                                              BMS2 181
    YSM = SMMOR/TMOR                                              BMS2 182
    YRE = REMOR/TMOR                                              BMS2 183
    YLASF = XLAMOR/REMOR                                           BMS2 184
    YPRSF = PRMOR/REMOR                                           BMS2 185
    YNDSF = XNDMOR/REMOR                                           BMS2 186

```

Figure 41. (Continued)

```

      YSMSF = SMMOR/REMOR                                BMS2 187
      SYO = YHNO3 + YLA + YPR + YND + YSM                BMS2 188
      IF (0.9999 - SYO) 145,155,150                      BMS2 189
145    IF (1.0001 - SYO) 150,155,155                      BMS2 190
150    PRINT 516, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR BMS2 191
      IF (K) 600,600,45                                    BMS2 192
155    SYREO = YLASF + YPRSF + YNDSF + YSMSF              BMS2 193
      IF (0.9999 - SYREO) 160,170,165                    BMS2 194
160    IF (1.0001 - SYREO) 165,170,170                    BMS2 195
165    PRINT 517, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR BMS2 196
      IF (K) 600,600,45                                    BMS2 197
170    LL = L + 1                                           BMS2 198
      PRINT 518, LL, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR, YHNO3, YLA, BMS2 199
      IYPR, YND, YSM, YRF, YLASF, YPRSF, YNDSF, YSMSF      BMS2 200
      IF (TMOR - 2.0) 175,180,180                          BMS2 201
175    PRINT 519, TMOR                                      BMS2 202
      IF (K) 600,600,45                                    BMS2 203
180    IF (TMOR 4.5) 185,175,175                          BMS2 204
185    CONTINUE                                             BMS2 205
      IF (K) 600,600,45                                    BMS2 206
500    FORMAT (6F10.3)                                     BMS2 207
501    FORMAT (7F9.4)                                       BMS2 208
502    FORMAT (7F7.4,F8.4,I3,I3)                          BMS2 209
503    FORMAT (29H1SCRUB SIDE CALCULATION ROVS=F8.4,4H N=13) BMS2 210
504    FORMAT (120HJ  TOTALMOLHNO3 MOL  LA MOL  PR MOL  ND MOL  SM MOL  BMS2 211
1RF MOL  ACFR  LAFR  PRFR  NDFR  SMFR  REFR LA/RE PR/RE ND/RE SM/RE BMS2 212
2)                                                         BMS2 213
505    FORMAT (4HJR 07F8.4,10F6.3)                        BMS2 214
506    FORMAT (4HJR 07F8.4,6F6.3)                         BMS2 215
507    FORMAT (4HJR 07F8.4)                               BMS2 216
508    FORMAT (4H S 17F8.4,10F6.3)                       BMS2 217
509    FORMAT (8HJYKTRF=016F6.3,F8.4,F6.3)               BMS2 218
510    FORMAT (8HJYKARE=016F6.3,F8.4,F6.3)               BMS2 219
511    FORMAT (18HJREMAQ LESS THAN 04F10.4)               BMS2 220
512    FORMAT (16HJSXA NOT EQUAL 17F10.4)                 BMS2 221
513    FORMAT (18HJSXREA NOT EQUAL 17F10.4)               BMS2 222
514    FORMAT (2HJRI2,7F8.4,10F6.3)                      BMS2 223
515    FORMAT (6HJTMOR=F10.4,6H AMOR=F10.4,8H XLAMOR=F10.4,7H PRMOR=F10.4 BMS2 224
1,8H XNDMOR=F10.4,7H SMMOR=F10.4,7H REMOR=F10.4)         BMS2 225
516    FORMAT (16HJSYO NOT FQUAL 17F10.4)                 BMS2 226
517    FORMAT (18HJSYREO NOT EQUAL 17F10.4)               BMS2 227
518    FORMAT (2H SI2,7F8.4,10F6.3)                      BMS2 228
519    FORMAT (6HJTMOR=F10.4)                             BMS2 229
600    STOP 89                                             BMS2 230
      END                                                  BMS2 231

```

Figure 41. (Continued)

Fig. 42. Flow diagram, Program III.

Fig. 42. (cont.)

Fig. 42. (cont.)

Fig. 42. (cont.)

```

      DIMENSION XKTLA(21,7),XKTPR(21,7),XKTND(21,7),XKTSM(21,7),XKALA(21,7) BMS3 001
      1,7),XKAPR(21,7),XKAND(21,7),XKASM(21,7) BMS3 002
      DO 5 I = 1,21 BMS3 003
5      READ INPUT TAPE 5, 500, (XKTLA(I,J),J = 1,7) BMS3 004
      DO 10 I = 1,21 BMS3 005
10     READ INPUT TAPE 5, 500, (XKTPR(I,J),J = 1,7) BMS3 006
      DO 15 I = 1,21 BMS3 007
15     READ INPUT TAPE 5, 500, (XKTND(I,J),J = 1,7) BMS3 008
      DO 20 I = 1,21 BMS3 009
20     READ INPUT TAPE 5, 500, (XKTSM(I,J),J = 1,7) BMS3 010
      DO 25 I = 1,21 BMS3 011
25     READ INPUT TAPE 5, 500, (XKALA(I,J),J = 1,7) BMS3 012
      DO 30 I = 1,21 BMS3 013
30     READ INPUT TAPE 5, 500, (XKAPR(I,J),J = 1,7) BMS3 014
      DO 35 I = 1,21 BMS3 015
35     READ INPUT TAPE 5, 500, (XKAND(I,J),J = 1,7) BMS3 016
      DO 40 I = 1,21 BMS3 017
40     READ INPUT TAPE 5, 500, (XKASM(I,J),J = 1,7) BMS3 018
45     READ INPUT TAPE 5, 501, TMAQ,AM AQ,XLAM AQ,PRMAQ,XNDMAQ,SMAQ,REMAQ BMS3 019
      READ INPUT TAPE 5, 501, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMR BMS3 020
      READ INPUT TAPE 5, 502, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM,S,F,REX,RBMS3 021
      1SC,N,M,K BMS3 022
      PRINT 503, S,F,REX,RSC,N,M BMS3 023
      PRINT 504 BMS3 024
      IF (FTM) 600,65,50 BMS3 025
50     XAF = FAM/FTM BMS3 026
      XLAF = FLAM/FTM BMS3 027
      XPRF = FPRM/FTM BMS3 028
      XNDF = FNDM/FTM BMS3 029
      XSME = FSMM/FTM BMS3 030
      XREF = FREM/FTM BMS3 031
      IF (FREM) 600,60,55 BMS3 032
55     XLASFF = FLAM/FREM BMS3 033
      XPRSFF = FPRM/FREM BMS3 034
      XNDSFF = FNDM/FREM BMS3 035
      XSMSFF = FSMM/FREM BMS3 036
      PRINT 505, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM,XAF,XLAF,XPRF,XNDF,XSMBMS3 037
      1F,XREF,XLASFF,XPRSFF,XNDSFF,XSMSFF BMS3 038
      GO TO 70 BMS3 039
60     PRINT 506, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM,XAF,XLAF,XPRF,XNDF,XSMBMS3 040
      1F,XREF BMS3 041
      GO TO 70 BMS3 042
65     PRINT 507, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM BMS3 043
70     IF(TMOR) 600,90,75 BMS3 044
75     YHNO3 = AMOR/TMOR BMS3 045
      YLA = XLAMOR/TMOR BMS3 046
      YPR = PRMOR/TMOR BMS3 047
      YND = XNDMOR/TMOR BMS3 048
      YSM = SMMOR/TMOR BMS3 049
      YRE = REMOR/TMOR BMS3 050
      IF (REMOR) 600,85,80 BMS3 051
80     YLASF = XLAMOR/REMOR BMS3 052
      YPRSF = PRMOR/REMOR BMS3 053
      YNDSF = XNDMOR/REMOR BMS3 054
      YSMSF = SMMOR/REMOR BMS3 055
      PRINT 508, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,YHNO3,YLA,YPRBMS3 056
      1,YND,YSM,YRE,YLASF,YPRSF,YNDSF,YSMSF BMS3 057
      GO TO 95 BMS3 058
85     PRINT 509, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,YHNO3,YLA,YPRBMS3 059
      1,YND,YSM,YRE BMS3 060
      GO TO 95 BMS3 061
90     PRINT 510, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR BMS3 062

```

Figure 43. Fortran statements, Program III

```

95      XHNO3 = AMAQ /TMAQ                                BMS3 063
      XLA = XLAMAQ/TMAQ                                    BMS3 064
      XPR = PRMAQ/TMAQ                                    BMS3 065
      XND = XNDMAQ/TMAQ                                    BMS3 066
      XSM = SMMAQ/TMAQ                                    BMS3 067
      XRE = REMAQ/TMAQ                                    BMS3 068
      XLASF = XLAMAQ/REMAQ                                BMS3 069
      XPRSF = PRMAQ/REMAQ                                BMS3 070
      XNDSF = XNDMAQ/REMAQ                                BMS3 071
      XSMSF = SMMAQ/REMAQ                                BMS3 072
      PRINT 511, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SMMAQ, REMAQ, XHNO3, XLA, XPR, XND, XSM, XRE, XLASF, XPRSF, XNDSF, XSMSF BMS3 073
1      R1TM = TMAQ                                         BMS3 074
      R1AM = AMAQ                                         BMS3 075
      R1LAM = XLAMAQ                                       BMS3 076
      R1PRM = PRMAQ                                       BMS3 077
      R1NDM = XNDMAQ                                       BMS3 078
      R1SMM = SMMAQ                                       BMS3 079
      SOTM = TMOR                                          BMS3 080
      SOAM = AMOR                                          BMS3 081
      SOLAM = XLAMOR                                       BMS3 082
      SOPRM = PRMOR                                        BMS3 083
      SONDM = XNDMOR                                       BMS3 084
      SOSMM = SMMOR                                        BMS3 085
      DO 270 L = 1, N                                       BMS3 086
      XREI = (XRE*100.0 + 5.0)/5.0                         BMS3 087
      IX = XREI                                            BMS3 088
      XI = IX                                              BMS3 089
      FRX = XREI - XI                                       BMS3 090
      IF (5.0 - TMAQ) 100,110,105                          BMS3 091
100     IF (7.0 - TMAQ) 115,115,110                        BMS3 092
105     Z = TMAQ - 2.0                                       BMS3 093
      GO TO 120                                             BMS3 094
110     Z = (TMAQ + 1.0)/2.0                               BMS3 095
      GO TO 120                                             BMS3 096
115     Z = (TMAQ + 5.0)/3.0                               BMS3 097
120     KZ = Z                                              BMS3 098
      ZK = KZ                                              BMS3 099
      FRZ = Z - ZK                                         BMS3 100
      SKT = MIN1(XKTLA(IX,KZ),XKTLA(IX+1,KZ),XKTLA(IX,KZ+1),XKTLA(IX+1,KZ+1),XKTTPR(IX,KZ),XKTTPR(IX+1,KZ),XKTTPR(IX,KZ+1),XKTTPR(IX+1,KZ+1),XKTND(IX,KZ),XKTND(IX+1,KZ),XKTND(IX,KZ+1),XKTND(IX+1,KZ+1),XKTSM(IX,KZ),XKTSM(IX+1,KZ),XKTSM(IX,KZ+1),XKTSM(IX+1,KZ+1)) BMS3 101
      IF (SKT) 125,125,130                                  BMS3 102
125     PRINT 512, XKTLA(IX,KZ),XKTLA(IX+1,KZ),XKTLA(IX,KZ+1),XKTLA(IX+1,KZ+1),XKTTPR(IX,KZ),XKTTPR(IX+1,KZ),XKTTPR(IX,KZ+1),XKTTPR(IX+1,KZ+1),XKTND(IX,KZ),XKTND(IX+1,KZ),XKTND(IX,KZ+1),XKTND(IX+1,KZ+1),XKTSM(IX,KZ),XKTSM(IX+1,KZ),XKTSM(IX,KZ+1),XKTSM(IX+1,KZ+1),TMAQ,XRE BMS3 103
      IF (K) 600,600,45                                     BMS3 104
130     XKTLA1 = XKTLA(IX,KZ)*(1.0 - FRX) + XKTLA(IX+1,KZ)*FRX BMS3 105
      XKTLA2 = XKTLA(IX,KZ+1)*(1.0 - FRX) + XKTLA(IX+1,KZ+1)*FRX BMS3 106
      XKTLA3 = XKTLA1*(1.0-FRZ) + XKTLA2*FRZ              BMS3 107
      CKTLA = XKTLA3*XLASF                                 BMS3 108
      XKTTPR1 = XKTTPR(IX,KZ)*(1.0-FRX) + XKTTPR(IX+1,KZ)*FRX BMS3 109
      XKTTPR2 = XKTTPR(IX,KZ+1)*(1.0-FRX) + XKTTPR(IX+1,KZ+1)*FRX BMS3 110
      XKTTPR3 = XKTTPR1*(1.0-FRZ) + XKTTPR2 *FRZ         BMS3 111
      CKTPR = XKTTPR3 * XPRSF                             BMS3 112
      XKTND1 = XKTND(IX,KZ)*(1.0-FRX) + XKTND(IX+1,KZ)*FRX BMS3 113
      XKTND2 = XKTND(IX,KZ+1)*(1.0 - FRX) + XKTND(IX+1,KZ+1)*FRX BMS3 114
      XKTND3 = XKTND1*(1.0- FRZ) + XKTND2 * FRZ          BMS3 115
      CKTND = XKTND3 * XNDSF                              BMS3 116
      XKTSM1 = XKTSM(IX,KZ)*(1.0-FRX) + XKTSM(IX+1,KZ)*FRX BMS3 117

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Figure 43. (Continued)


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XKTSM2 = XKTSM(IX,KZ+1)*(1.0 -FRX) + XKTSM(IX+1,KZ+1)*FRX      BMS3 125
XKTSM3 = XKTSM1*(1.0 -FRZ) + XKTSM2 * FRZ                        BMS3 126
CKTSM = XKTSM3 * XSMSF                                           BMS3 127
SKA = MIN1F(XKALA(IX,KZ),XKALA(IX+1,KZ),XKALA(IX,KZ+1),XKALA(IX+1,KZ+1),XKAPR(IX,KZ),XKAPR(IX+1,KZ),XKAPR(IX,KZ+1),XKAPR(IX+1,KZ+1),XKAND(IX,KZ),XKAND(IX+1,KZ),XKAND(IX,KZ+1),XKAND(IX+1,KZ+1),XKASM(IX,KZ),XKASM(IX+1,KZ),XKASM(IX,KZ+1),XKASM(IX+1,KZ+1)) BMS3 128
IF (SKA) 135,135,140                                             BMS3 129
135 PRINT 513, XKALA(IX,KZ),XKALA(IX+1,KZ),XKALA(IX,KZ+1),XKALA(IX+1,KZ+1),XKAPR(IX,KZ),XKAPR(IX+1,KZ),XKAPR(IX,KZ+1),XKAPR(IX+1,KZ+1),XKAND(IX,KZ),XKAND(IX+1,KZ),XKAND(IX,KZ+1),XKAND(IX+1,KZ+1),XKASM(IX,KZ),XKASM(IX+1,KZ),XKASM(IX,KZ+1),XKASM(IX+1,KZ+1),TMAQ,XRE BMS3 130
IF (K) 135,135,140                                             BMS3 131
140 CKALA = XKALA3 * XLASF                                         BMS3 132
XKAPR1 = XKAPR(IX,KZ)*(1.0 -FRX) + XKAPR(IX+1,KZ)* FRX          BMS3 133
XKAPR2 = XKAPR(IX,KZ+1)*(1.0 -FRX) + XKAPR(IX+1,KZ+1)*FRX      BMS3 134
XKAPR3 = XKAPR1*(1.0 -FRZ) + XKAPR2 * FRZ                      BMS3 135
CKAPR = XKAPR3 * XPRSF                                           BMS3 136
XKAND1 = XKAND(IX,KZ)*(1.0 -FRX) + XKAND(IX+1,KZ)*FRX          BMS3 137
XKAND2 = XKAND(IX,KZ+1)*(1.0 -FRX) + XKAND(IX+1,KZ+1)*FRX      BMS3 138
XKAND3 = XKAND1*(1.0 -FRZ) + XKAND2 * FRZ                      BMS3 139
CKAND = XKAND3 * XNDSF                                           BMS3 140
XKASM1 = XKASM(IX,KZ)*(1.0 -FRX) + XKASM(IX+1,KZ)*FRX          BMS3 141
XKASM2 = XKASM(IX,KZ+1)*(1.0 -FRX) + XKASM(IX+1,KZ+1)*FRX      BMS3 142
XKASM3 = XKASM1*(1.0 -FRZ) + XKASM2 * FRZ                      BMS3 143
CKASM = XKASM3 * XSMSF                                           BMS3 144
TOTK = CKTLA + CKTPR + CKTND + CKTSM                            BMS3 145
HNO3K = CKALA + CKAPR + CKAND + CKASM                            BMS3 146
TMOR = TMAQ * TOTK                                               BMS3 147
IF (TMOR - 1.75) 145,150,150                                     BMS3 148
145 PRINT 514, TMOR,TMAQ,TOTK                                     BMS3 149
IF (K) 600,600,45                                               BMS3 150
150 AMOR = AMAQ * HNO3K                                           BMS3 151
REMOR = TMOR - AMOR                                              BMS3 152
IF (REMOR) 155,155,160                                          BMS3 153
155 PRINT 515, TMOR,AMOR,REMOR,HNO3K                             BMS3 154
IF (K) 600,600,45                                               BMS3 155
160 BLAPR = 0.8187 - 0.1106*TMOR                                 BMS3 156
BPRPR = 1.0                                                      BMS3 157
BNDPR = 1.0448 + 0.09874*TMOR                                    BMS3 158
BSMPR = -0.3795 + 0.9214*TMOR                                    BMS3 159
DEMS = XLAMAQ*BLAPR + PRMAQ*BPRPR + XNDMAQ*BNDPR + SMMAQ*BSMPR BMS3 160
XLAMOR = REMOR*BLAPR*XLAMAQ/DEMS                                 BMS3 161
PRMOR = REMOR*BPRPR*PRMAQ/DEMS                                   BMS3 162
XNDMOR = REMOR*BNDPR*XNDMAQ/DEMS                                 BMS3 163
SMMOR = REMOR*BSMPR*SMMAQ/DEMS                                   BMS3 164
YHNO3 = AMOR/TMOR                                                BMS3 165
YLA = XLAMOR/TMOR                                                BMS3 166
YPR = PRMOR/TMOR                                                 BMS3 167
YND = XNDMOR/TMOR                                                BMS3 168
YSM = SMMOR/TMOR                                                 BMS3 169
YRE = REMOR/TMOR                                                 BMS3 170
SYO = YHNO3 + YLA + YPR + YND + YSM                             BMS3 171
IF (0.9999 - SYO) 165,175,170                                    BMS3 172
165 IF (1.0001 - SYO) 170,175,175                                BMS3 173
170 PRINT 516, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR       BMS3 174
IF (K) 600,600,45                                               BMS3 175
175 YLASF = XLAMOR/REMOR                                          BMS3 176
YPRSF = PRMOR/REMOR                                              BMS3 177

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Figure 43. (Continued)

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YNSDF = XNDMOR/REMOR                                BMS3 187
YSMSF = SMMOR/REMOR                                BMS3 188
SYREO = YLASF + YPRSF + YNSDF + YSMSF              BMS3 189
IF (0.9999 - SYREO) 180,190,185                    BMS3 190
180 IF (1.0001 - SYREO) 185,190,190                  BMS3 191
185 PRINT 517, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR BMS3 192
IF (K) 600,600,45                                    BMS3 193
190 IF (L - M) 200,195,200                            BMS3 194
195 PRINT 518                                           BMS3 195
200 PRINT 519, L, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR, YHNO3, YLA, YPRMOR, YNSDF, YSMSF BMS3 196
IF (L-M) 205,210,210                                    BMS3 197
205 TMAQ = TMOR*S/REX - SOTM*S/REX + RITM              BMS3 199
    AMAQ = AMOR*S/REX - SOAM*S/REX + RIAM              BMS3 200
    XLAMAQ = XLAMOR*S/REX - SOLAM*S/REX + RILAM         BMS3 201
    PRMAQ = PRMOR*S/REX - SOPRM*S/REX + R1PRM          BMS3 202
    XNDMAQ = XNDMOR*S/REX - SONDM*S/REX + RINDM        BMS3 203
    SMMAQ = SMMOR*S/REX - SOSMM*S/REX + R1SMM          BMS3 204
    GO TO 215                                           BMS3 205
210 TMAQ = TMOR*S/RSC - SOTM*S/RSC - FTM*F/RSC + RITM*REX/RSC BMS3 206
    AMAQ = AMOR*S/RSC - SOAM*S/RSC - FAM*F/RSC + RIAM*REX/RSC BMS3 207
    XLAMAQ = XLAMOR*S/RSC - SOLAM*S/RSC - FLAM*F/RSC + RILAM*REX/RSC BMS3 208
    PRMAQ = PRMOR*S/RSC - SOPRM*S/RSC - FPRM*F/RSC + R1PRM*REX/RSC BMS3 209
    XNDMAQ = XNDMOR*S/RSC - SONDM*S/RSC - FNDM*F/RSC + RINDM*REX/RSC BMS3 210
    SMMAQ = SMMOR*S/RSC - SOSMM*S/RSC - FSMM*F/RSC + R1SMM*REX/RSC BMS3 211
215 REMAQ = TMAQ - AMAQ                                BMS3 212
    SAM = MINIF(TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SMMAQ, REMAQ) BMS3 213
    IF (SAM) 220,220,225                                BMS3 214
220 PRINT 520, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SMMAQ, REMAQ BMS3 215
IF (K) 600,600,45                                    BMS3 216
225 XHNO3 = AMAQ/TMAQ                                  BMS3 217
    XLA = XLAMAQ/TMAQ                                  BMS3 218
    XPR = PRMAQ/TMAQ                                  BMS3 219
    XND = XNDMAQ/TMAQ                                  BMS3 220
    XSM = SMMAQ/TMAQ                                  BMS3 221
    XRE = REMAQ/TMAQ                                  BMS3 222
    SXA = XHNO3 + XLA + XPR + XND + XSM                BMS3 223
    IF (0.9999 - SXA) 230,240,235                      BMS3 224
230 IF (1.0001 - SXA) 235,240,240                    BMS3 225
235 PRINT 521, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SMMAQ, REMAQ BMS3 226
IF (K) 600,600,45                                    BMS3 227
240 XLASF = XLAMAQ/REMAQ                              BMS3 228
    XPRSF = PRMAQ/REMAQ                              BMS3 229
    XNSDF = XNDMAQ/REMAQ                              BMS3 230
    XSMSF = SMMAQ/REMAQ                              BMS3 231
    SXREA = XLASF + XPRSF + XNSDF + XSMSF              BMS3 232
    IF (0.9999 - SXREA) 245,255,250                    BMS3 233
245 IF (1.0001 - SXREA) 250,255,255                  BMS3 234
250 PRINT 522, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SMMAQ, REMAQ BMS3 235
IF (K) 600,600,45                                    BMS3 236
255 LL = L+1                                           BMS3 237
    PRINT 523, LL, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SMMAQ, REMAQ, XHNO3, XLA, XPR, XND, XSM, XRE, XLASF, XPRSF, XNSDF, XSMSF BMS3 238
IF (TMAQ - 3.0) 260,265,265                            BMS3 239
260 PRINT 524, TMAQ                                    BMS3 241
IF (K) 600,600,45                                    BMS3 242
265 IF (TMAQ - 16.0) 270,260,260                      BMS3 243
270 CONTINUE                                           BMS3 244
IF (K) 600,600,45                                    BMS3 245
500 FORMAT (7F10.3)                                    BMS3 246
501 FORMAT (7F10.4)                                    BMS3 247
502 FORMAT (7F7.4,4F5.2,3I3)                          BMS3 248

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Figure 43. (Continued)

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503  FORMAT (36H1INTERNAL FEED,EXTRACT SIDE START S=F5.2,3H F=F5.2,5H RBMS3 249
      1EX=F5.2,5H RSC=F5.2,3H N=13,3H M=13) BMS3 250
504  FORMAT (120HJ TOTALMOLHNO3 MOL LA MOL PR MOL ND MOL SM MOL BMS3 251
      1RE MOL ACFR LAFR PRFR NDFR SMFR REFR LA/RE PR/RE ND/RE SM/REBMS3 252
      2) BMS3 253
505  FORMAT (4HJ F7F8.4,10F6.3) BMS3 254
506  FORMAT (4HJ F7F8.4,6F6.3) BMS3 255
507  FORMAT (4HJ F7F8.4) BMS3 256
508  FORMAT (4HJS 07F8.4,10F6.3) BMS3 257
509  FORMAT (4HJS 07F8.4,6F6.3) BMS3 258
510  FORMAT (4HJS 07F8.4) BMS3 259
511  FORMAT (4H R 17F8.4,10F6.3) BMS3 260
512  FORMAT (8HJXKTRE=016F6.3,F8.4,F6.3) BMS3 261
513  FORMAT (8HJXKARE=016F6.3,F8.4,F6.3) BMS3 262
514  FORMAT (6HJTMOR=F8.4,6H TMAQ=F8.4,6H TOTK=F8.4) BMS3 263
515  FORMAT (18HJREMOR LESS THAN 04F10.4) BMS3 264
516  FORMAT (16HJSYO NOT EQUAL 17F10.4) BMS3 265
517  FORMAT (18HJSYREO NOT EQUAL 17F10.4) BMS3 266
518  FORMAT (17HJFEED ENTRY POINT) BMS3 267
519  FORMAT (2HJSI2,7F8.4,10F6.3) BMS3 268
520  FORMAT (6HJTMAQ=F10.4,6H AMAQ=F10.4,8H XLAMAQ=F10.4,7H PRMAQ=F10.4BMS3 269
      1,8H XNDMAQ=F10.4,7H SMMAQ=F10.4,7H REMAQ=F10.4) BMS3 270
521  FORMAT (16HJSXA NOT EQUAL 17F10.4) BMS3 271
522  FORMAT (18HJSXREA NOT EQUAL 17F10.4) BMS3 272
523  FORMAT (2H RI2,7F8.4,10F6.3) BMS3 273
524  FORMAT (6HJTMAQ=F10.4) BMS3 274
600  STOP 89 BMS3 275
      END BMS3 276

```

Figure 43. (Continued)

Fig. 44. Flow diagram, Program IV.

Fig. 44. (cont.)

Fig. 44. (cont.)

Fig. 44. (cont.)

Fig. 44. (cont.)

Fig. 44. (cont.)

Fig. 44. (cont.)

Fig. 44. (cont.)

```

      DIMENSION YKTLA(21,6),YKTPR(21,6),YKTND(21,6),YKTSM(21,6),YKALA(21,6),YKAPR(21,6),YKAND(21,6),YKASM(21,6)
      DO 5 I = 1,21
5      READ INPUT TAPE 5, 500, (YKTLA(I,J),J = 1,6)
      DO 10 I = 1,21
10     READ INPUT TAPE 5, 500, (YKTPR(I,J),J = 1,6)
      DO 15 I = 1,21
15     READ INPUT TAPE 5, 500, (YKTND(I,J),J = 1,6)
      DO 20 I = 1,21
20     READ INPUT TAPE 5, 500, (YKTSM(I,J),J = 1,6)
      DO 25 I = 1,21
25     READ INPUT TAPE 5, 500, (YKALA(I,J),J = 1,6)
      DO 30 I = 1,21
30     READ INPUT TAPE 5, 500, (YKAPR(I,J),J = 1,6)
      DO 35 I = 1,21
35     READ INPUT TAPE 5, 500, (YKAND(I,J),J = 1,6)
      DO 40 I = 1,21
40     READ INPUT TAPE 5, 500, (YKASM(I,J),J = 1,6)
45     READ INPUT TAPE 5, 501, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ
      READ INPUT TAPE 5, 501, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REHOR
      READ INPUT TAPE 5, 502, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM,S,F,REX,RBMS4
1     SC,N,M,K
      PRINT 503, S,F,REX,RSC,N,M
      PRINT 504
      IF (FTM) 600,65,50
50     XAF = FAM/FTM
      XLAF = FLAM/FTM
      XPRF = FPRM/FTM
      XNDF = FNDM/FTM
      XSMF = FSMM/FTM
      XREF = FREM/FTM
      IF (FREM) 600,60,55
55     XLASFF = FLAM/FREM
      XPRSFF = FPRM/FREM
      XNDSFF = FNDM/FREM
      XSMSFF = FSMM/FREM
      PRINT 505, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM,XAF,XLAF,XPRF,XNDF,XSMBMS4
1     F,XREF,XLASFF,XPRSFF,XNDSFF,XSMSFF
      GO TO 70
60     PRINT 506, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM,XAF,XLAF,XPRF,XNDF,XSMBMS4
1     F,XREF
      GO TO 70
65     PRINT 507, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM
70     IF (TMAQ) 600,90,75
75     XHNO3 = AMAQ/TMAQ
      XLA = XLAMAQ/TMAQ
      XPR = PRMAQ/TMAQ
      XND = XNDMAQ/TMAQ
      XSM = SMMAQ/TMAQ
      XRE = REMAQ/TMAQ
      IF (REMAQ) 600,95,80
80     XLASF = XLAMAQ/REMAQ
      XPRSF = PRMAQ/REMAQ
      XNDSF = XNDMAQ/REMAQ
      XSMSF = SMMAQ/REMAQ
      PRINT 508, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ,XHNO3,XLA,XPRBMS4
1     XND,XSM,XRE,XLASF,XPRSF,XNDSF,XSMSF
      GO TO 95
85     PRINT 509, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ,XHNO3,XLA,XPRBMS4
1     XND,XSM,XRE
      GO TO 95
90     PRINT 510, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ

```

Figure 45. Fortran statements, Program IV

```

95  YHNO3 = AMOR/TMOR                      BMS4 063
    YLA = XLAMOR/TMOR                      BMS4 064
    YPR = PRMOR/TMOR                      BMS4 065
    YND = XNDMOR/TMOR                     BMS4 066
    YSM = SMMOR/TMOR                      BMS4 067
    YRE = REMOR/TMOR                      BMS4 068
    YLASF = XLAMOR/REMOR                  BMS4 069
    YPRSF = PRMOR/REMOR                  BMS4 070
    YNDSF = XNDMOR/REMOR                  BMS4 071
    YSMF = SMMOR/REMOR                   BMS4 072
    PRINT 511, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR, YHNO3, YLA, YPRBMS4 073
1  YND, YSM, YRE, YLASF, YPRSF, YNDSF, YSMF BMS4 074
    ROTM = TMAQ                           BMS4 075
    ROAM = AMAQ                           BMS4 076
    RGLAM = XLAMAQ                        BMS4 077
    ROPRM = PRMAQ                         BMS4 078
    RCNDM = XNDMAQ                       BMS4 079
    ROSMM = SMMAQ                        BMS4 080
    SITM = TMOR                          BMS4 081
    SIAM = AMOR                          BMS4 082
    SILAM = XLAMOR                       BMS4 083
    SIPRM = PRMOR                        BMS4 084
    SINDM = XNDMOR                       BMS4 085
    SISMM = SMMOR                        BMS4 086
    DO 235 L = 1, N                       BMS4 087
    YEI = (YRE*100.0 + 5.0)/5.0          BMS4 088
    IY = YEI                             BMS4 089
    YI = IY                              BMS4 090
    FRY = YREI - YI                      BMS4 091
    Z = (TMOR*10.0 - 15.0)/5.0           BMS4 092
    KZ = Z                               BMS4 093
    ZK = KZ                             BMS4 094
    FRZ = Z - ZK                         BMS4 095
    SKT = MIN1F(YKTLA(IY,KZ),YKTLA(IY+1,KZ),YKTLA(IY,KZ+1),YKTLA(IY+1,KZ+1),YKTPR(IY,KZ),YKTPR(IY+1,KZ),YKTPR(IY,KZ+1),YKTPR(IY+1,KZ+1),YKTND(IY,KZ),YKTND(IY+1,KZ),YKTND(IY,KZ+1),YKTND(IY+1,KZ+1),YKTSM(IY,KZ),YKTSM(IY+1,KZ),YKTSM(IY,KZ+1),YKTSM(IY+1,KZ+1)) BMS4 096
    IF (SKT) 100,100,105                  BMS4 097
100  PRINT 512, YKTLA(IY,KZ),YKTLA(IY+1,KZ),YKTLA(IY,KZ+1),YKTLA(IY+1,KZ+1),YKTPR(IY,KZ),YKTPR(IY+1,KZ),YKTPR(IY,KZ+1),YKTPR(IY+1,KZ+1),YKTND(IY,KZ),YKTND(IY+1,KZ),YKTND(IY,KZ+1),YKTND(IY+1,KZ+1),YKTSM(IY,KZ),YKTSM(IY+1,KZ),YKTSM(IY,KZ+1),YKTSM(IY+1,KZ+1),TMOR,YRE BMS4 098
    IF (K) 600,600,45                     BMS4 099
105  YKTLA1 = YKTLA(IY,KZ)*(1.0 - FRY) + YKTLA(IY+1,KZ)*FRY BMS4 100
    YKTLA2 = YKTLA(IY,KZ+1)*(1.0 - FRY) + YKTLA(IY+1,KZ+1)*FRY BMS4 101
    YKTLA3 = YKTLA1*(1.0 - FRZ) + YKTLA2*FRZ BMS4 102
    CKTLA = YKTLA3 * YLASF                 BMS4 103
    YKTPR1 = YKTPR(IY,KZ)*(1.0 - FRY) + YKTPR(IY+1,KZ)*FRY BMS4 104
    YKTPR2 = YKTPR(IY,KZ+1)*(1.0 - FRY) + YKTPR(IY+1,KZ+1)*FRY BMS4 105
    YKTPR3 = YKTPR1*(1.0 - FRZ) + YKTPR2*FRZ BMS4 106
    CKTPR = YKTPR3 * YPRSF                 BMS4 107
    YKTND1 = YKTND(IY,KZ)*(1.0 - FRY) + YKTND(IY+1,KZ)*FRY BMS4 108
    YKTND2 = YKTND(IY,KZ+1)*(1.0 - FRY) + YKTND(IY+1,KZ+1)*FRY BMS4 109
    YKTND3 = YKTND1*(1.0 - FRZ) + YKTND2*FRZ BMS4 110
    CKTND = YKTND3 * YNDSF                 BMS4 111
    YKTSM1 = YKTSM(IY,KZ)*(1.0 - FRY) + YKTSM(IY+1,KZ)*FRY BMS4 112
    YKTSM2 = YKTSM(IY,KZ+1)*(1.0 - FRY) + YKTSM(IY+1,KZ+1)*FRY BMS4 113
    YKTSM3 = YKTSM1*(1.0 - FRZ) + YKTSM2*FRZ BMS4 114
    CKTSM = YKTSM3 * YSMF                  BMS4 115
    SKA = MIN1F(YKALA(IY,KZ),YKALA(IY+1,KZ),YKALA(IY,KZ+1),YKALA(IY+1,KZ+1),YKAPR(IY,KZ),YKAPR(IY+1,KZ),YKAPR(IY,KZ+1),YKAPR(IY+1,KZ+1),YKAND(IY,KZ),YKAND(IY+1,KZ),YKAND(IY,KZ+1),YKAND(IY+1,KZ+1),YKASM(IY,KZ),YKASM(IY+1,KZ),YKASM(IY,KZ+1),YKASM(IY+1,KZ+1)) BMS4 116
    2YKAND(IY,KZ),YKAND(IY+1,KZ),YKAND(IY,KZ+1),YKAND(IY+1,KZ+1),YKASM(IY,KZ),YKASM(IY+1,KZ),YKASM(IY,KZ+1),YKASM(IY+1,KZ+1)) BMS4 117
    BMS4 118
    BMS4 119
    BMS4 120
    BMS4 121
    BMS4 122
    BMS4 123
    BMS4 124

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Figure 45. (Continued)

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3 IY,KZ),YKASM(IY+1,KZ),YKASM(IY,KZ+1),YKASM(IY+1,KZ+1))      BMS4 125
  IF (SKA) 110,110,115      BMS4 126
110 PRINT 513, YKALA(IY,KZ),YKALA(IY+1,KZ),YKALA(IY,KZ+1),YKALA(IY+1,KZ+1),YKAPR(IY,KZ),YKAPR(IY+1,KZ),YKAPR(IY,KZ+1),YKAPR(IY+1,KZ+1),YKAND(IY,KZ),YKAND(IY+1,KZ),YKAND(IY,KZ+1),YKAND(IY+1,KZ+1),YKASM(IY,KZ),YKASM(IY+1,KZ),YKASM(IY,KZ+1),YKASM(IY+1,KZ+1),TMOR,YRE      BMS4 127
  IF (K) 600,600,45      BMS4 128
115 YKALA1 = YKALA(IY,KZ)*(1.0 - FRY) + YKALA(IY+1,KZ)*FRY      BMS4 129
  YKALA2 = YKALA(IY,KZ+1)*(1.0 - FRY) + YKALA(IY+1,KZ+1)*FRY      BMS4 130
  YKALA3 = YKALA1*(1.0 - FRZ) + YKALA2*FRZ      BMS4 131
  CKALA = YKALA3 * YLASF      BMS4 132
  YKAPR1 = YKAPR(IY,KZ)*(1.0 - FRY) + YKAPR(IY+1,KZ)*FRY      BMS4 133
  YKAPR2 = YKAPR(IY,KZ+1)*(1.0 - FRY) + YKAPR(IY+1,KZ+1)*FRY      BMS4 134
  YKAPR3 = YKAPR1*(1.0 - FRZ) + YKAPR2*FRZ      BMS4 135
  CKAPR = YKAPR3 * YPRSF      BMS4 136
  YKAND1 = YKAND(IY,KZ)*(1.0 - FRY) + YKAND(IY+1,KZ)*FRY      BMS4 137
  YKAND2 = YKAND(IY,KZ+1)*(1.0 - FRY) + YKAND(IY+1,KZ+1)*FRY      BMS4 138
  YKAND3 = YKAND1*(1.0 - FRZ) + YKAND2*FRZ      BMS4 139
  CKAND = YKAND3 * YNDSF      BMS4 140
  YKASM1 = YKASM(IY,KZ)*(1.0 - FRY) + YKASM(IY+1,KZ)*FRY      BMS4 141
  YKASM2 = YKASM(IY,KZ+1)*(1.0 - FRY) + YKASM(IY+1,KZ+1)*FRY      BMS4 142
  YKASM3 = YKASM1*(1.0 - FRZ) + YKASM2*FRZ      BMS4 143
  CKASM = YKASM3 * YSMSF      BMS4 144
  TOTK = CKTLA + CKTPR + CKTND + CKTSM      BMS4 145
  HNO3K = CKALA + CKAPR + CKAND + CKASM      BMS4 146
  TMAQ = TMOR/TOTK      BMS4 147
  AMAQ = AMOR/HNO3K      BMS4 148
  REMAQ = TMAQ - AMAQ      BMS4 149
  IF (REMAQ) 120,120,125      BMS4 150
120 PRINT 514, TMAQ,AMAQ,REMAQ,HNO3K      BMS4 151
  IF (K) 600,600,45      BMS4 152
125 BLAPR = 0.8187 - 0.1106*TMOR      BMS4 153
  BPRPR = 1.0      BMS4 154
  BNDPR = 1.0448 + 0.09874*TMOR      BMS4 155
  BSMPR = -0.3795 + 0.9214*TMOR      BMS4 156
  DEMS = XLAMOR/BLAPR + PRMOR/BPRPR + XNDMOR/BNDPR + SMMOR/BSMPR      BMS4 157
  XLAMAQ = XLAMOR*REMAQ/(BLAPR*DEMS)      BMS4 158
  PRMAQ = PRMOR*REMAQ/(BPRPR*DEMS)      BMS4 159
  XNDMAQ = XNDMOR*REMAQ/(BNDPR*DEMS)      BMS4 160
  SMMAQ = SMMOR*REMAQ/(BSMPR*DEMS)      BMS4 161
  XHNO3 = AMAQ/TMAQ      BMS4 162
  XLA = XLAMAQ/TMAQ      BMS4 163
  XPR = PRMAQ/TMAQ      BMS4 164
  XND = XNDMAQ/TMAQ      BMS4 165
  XSM = SMMAQ/TMAQ      BMS4 166
  XRE = REMAQ/TMAQ      BMS4 167
  XLASF = XLAMAQ/REMAQ      BMS4 168
  XPRSF = PRMAQ/REMAQ      BMS4 169
  XNDSF = XNDMAQ/REMAQ      BMS4 170
  XSMSF = SMMAQ/REMAQ      BMS4 171
  SXA = XHNO3 + XLA + XPR + XND + XSM      BMS4 172
  IF (0.9999 - SXA) 130,140,135      BMS4 173
130 IF (1.0001 - SXA) 135,140,140      BMS4 174
135 PRINT 515, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ      BMS4 175
  IF (K) 600,600,45      BMS4 176
140 SXREA = XLASF + XPRSF + XNDSF + XSMSF      BMS4 177
  IF (0.9999 - SXREA) 145,155,150      BMS4 178
145 IF (1.0001 - SXREA) 150,155,155      BMS4 179
150 PRINT 516, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ      BMS4 180
  IF (K) 600,600,45      BMS4 181
155 IF (L - M) 165,160,165      BMS4 182
160 PRINT 517      BMS4 183

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Figure 45. (Continued)

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165  PRINT 518,L,TMAQ,AMAO,XLAMAQ,PRMAQ,XNDMAQ,SMMMAQ,REMAQ,XHNO3,XLA,XPRBMS4 187
IR,XND,XSM,XRL,XLASF,XPRSF,XNDSF,XSMSF BMS4 188
IF (L - M) 170,175,175 BMS4 189
170  TMOR = ((TMAQ - ROTM)*RSC/S) + S1TM BMS4 190
AMOR = ((AMAO - ROAM)*RSC/S) + S1AM BMS4 191
XLAMOR = ((XLAMAQ - ROLAM)*RSC/S) + S1LAM BMS4 192
PRMOR = ((PRMAQ - ROPRM)*RSC/S) + S1PRM BMS4 193
XNDMOR = ((XNDMAQ - RONDM)*RSC/S) + S1NDM BMS4 194
SMMOR = ((SMMMAQ - ROSMM)*RSC/S) + S1SMM BMS4 195
GO TO 180 BMS4 196
175  TMOR = TMAQ*REX/S FTM*F/S ROTM*RSC/S + S1TM BMS4 197
AMOR = AMAQ*REX/S FAM*F/S - ROAM*RSC/S + S1AM BMS4 198
XLAMOR = XLAMAQ*REX/S - FLAM*F/S ROLAM*RSC/S + S1LAM BMS4 199
PRMOR = PRMAQ*REX/S - FPRM*F/S - ROPRM*RSC/S + S1PRM BMS4 200
XNDMOR = XNDMAQ*REX/S - FNDM*F/S - RONDM*RSC/S + S1NDM BMS4 201
SMMOR = SMMMAQ*REX/S FSMM*F/S - ROSMM*RSC/S + S1SMM BMS4 202
180  REMOR = TMOR - AMOR BMS4 203
SOM = MIN1F(TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR) BMS4 204
IF (SOM) 185,185,190 BMS4 205
185  PRINT 519, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR BMS4 206
IF (K) 600,600,45 BMS4 207
190  YHNO3 = AMOR/TMOR BMS4 208
YLA = XLAMOR/TMOR BMS4 209
YPR = PRMOR/TMOR BMS4 210
YND = XNDMOR/TMOR BMS4 211
YSM = SMMOR/TMOR BMS4 212
YRE = REMOR/TMOR BMS4 213
YLASF = XLAMOR/REMOR BMS4 214
YPRSF = PRMOR/REMOR BMS4 215
YNDSE = XNDMOR/REMOR BMS4 216
YSMSF = SMMOR/REMOR BMS4 217
SYO = YHNO3 + YLA + YPR + YND + YSM BMS4 218
IF (0.9999 - SYO) 195,205,200 BMS4 219
195  IF (1.0001 - SYO) 200,205,205 BMS4 220
200  PRINT 520, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR BMS4 221
IF (K) 600,600,45 BMS4 222
205  SYREO = YLASF + YPRSF + YNDSE + YSMSF BMS4 223
IF (0.9999 - SYREO) 210,220,215 BMS4 224
210  IF (1.0001 - SYREO) 215,220,220 BMS4 225
215  PRINT 521, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR BMS4 226
IF (K) 600,600,45 BMS4 227
220  LL = L + 1 BMS4 228
PRINT 522, LL, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,YHNO3,YLA, BMS4 229
1YPR,YND,YSM,YRE,YLASF,YPRSF,YNDSE,YSMSF BMS4 230
IF (TMOR - 2.0) 225,230,230 BMS4 231
225  PRINT 523, TMOR BMS4 232
IF (K) 600,600,45 BMS4 233
230  IF (TMOR - 4.5) 235,225,225 BMS4 234
235  CONTINUE BMS4 235
IF (K) 600,600,45 BMS4 236
500  FORMAT (6F10.3) BMS4 237
501  FORMAT (7F10.4) BMS4 238
502  FORMAT (7F7.4,4F5.2,3I3) BMS4 239
503  FORMAT (34H1INTERNAL FEED,SCRUB SIDE START S=F5.2,3H F=F5.2,5H REX BMS4 240
1=F5.2,5H RSC=F5.2,3H N=13,3H M=13) BMS4 241
504  FORMAT (120HJ TOTALMOLHNQ3 MOL LA MOL PR MOL ND MOL SM MOL BMS4 242
1RE MOL ACFR LAFR PRFR NDFR SMFR REFR LA/RE PR/RE ND/RE SM/RE BMS4 243
2) BMS4 244
505  FORMAT (4HJ F7F8.4,10F6.3) BMS4 245
506  FORMAT (4HJ F7F8.4,6F6.3) BMS4 246
507  FORMAT (4HJ F7F8.4) BMS4 247
508  FORMAT (4HJR 07F8.4,10F6.3) BMS4 248

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Figure 45. (Continued)

509	FORMAT (4HJR 07F8.4,6F6.3)	BMS4 249
510	FORMAT (4HJR 07F8.4)	BMS4 250
511	FORMAT (4H S 17F8.4,10F6.3)	BMS4 251
512	FORMAT (8HJYKTRE=016F6.3,F8.4,F6.3)	BMS4 252
513	FORMAT (8HJYKARE=016F6.3,F8.4,F6.3)	BMS4 253
514	FORMAT (18HJREMAQ LESS THAN 04F10.4)	BMS4 254
515	FORMAT (16HJSXA NOT EQUAL 17F10.4)	BMS4 255
516	FORMAT (18HJSXREA NOT EQUAL 17F10.4)	BMS4 256
517	FORMAT (17HJFEED ENTRY PDINT)	BMS4 257
518	FORMAT (2HJR12,7F8.4,10F6.3)	BMS4 258
519	FORMAT (6HJTMOR=F10.4,6H AMOR=F10.4,8H XLAMOR=F10.4,7H PRMOR=F10.4,1,8H XNDMOR=F10.4,7H SMMOR=F10.4,7H REMOR=F10.4)	BMS4 259
520	FORMAT (16HJSYO NOT EQUAL 17F10.4)	BMS4 260
521	FORMAT (18HJSYRED NOT EQUAL 17F10.4)	BMS4 261
522	FORMAT (2H SI2,7F8.4,10F6.3)	BMS4 262
523	FORMAT (6HJTMOR=F10.4)	BMS4 263
600	STOP 89	BMS4 264
	END	BMS4 265
		BMS4 266

Figure 45. (Continued)