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NITRATES - NITRIC ACID - WATER - TRI-
BUTYL PHOSPHATE.

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

by

Brooks Martin Sharp

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Signature was redacted for privacy.

In Charge of ~~Major~~ Work

Signature was redacted for privacy.

Head of Major Department

Signature was redacted for privacy.

Dean of ~~Graduate~~ College

Iowa State University
Of Science and Technology
Ames, Iowa

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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. H_2O /unit time
- F - flow rate of solvent in a feed stream, kgm. H_2O /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
- HNO_3 - 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

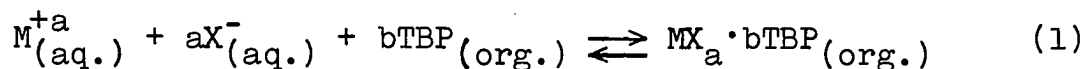
The first study of solvent extraction separation of the rare earths was made in 1937 by Fischer et al. (9). Since that time a large number of systems have been investigated, primarily by single stage "shakeups", and often using radioactive rare earth tracers. Typical studies are (10,11,12,13, 14,15).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

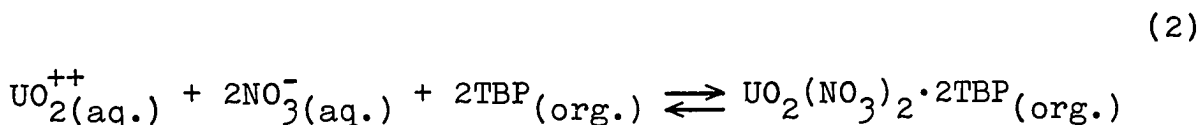
Many thermodynamic studies have been reported in the literature, typical studies being (20,21,22,23,24,25). In general, the conclusions were that the extraction of many

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

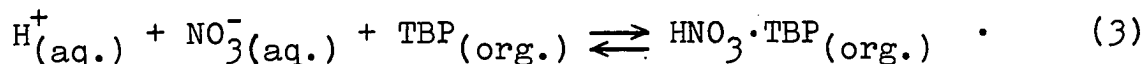


where b is the solvation number, that is, the number of TBP molecules complexed with one molecule of the extracted compound. For the rare earth nitrates b has been established to be three, and for nitric acid b is usually taken as one, although for nitric acid solubility considerations show such a simple 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 thesis 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

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

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

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

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

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

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

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

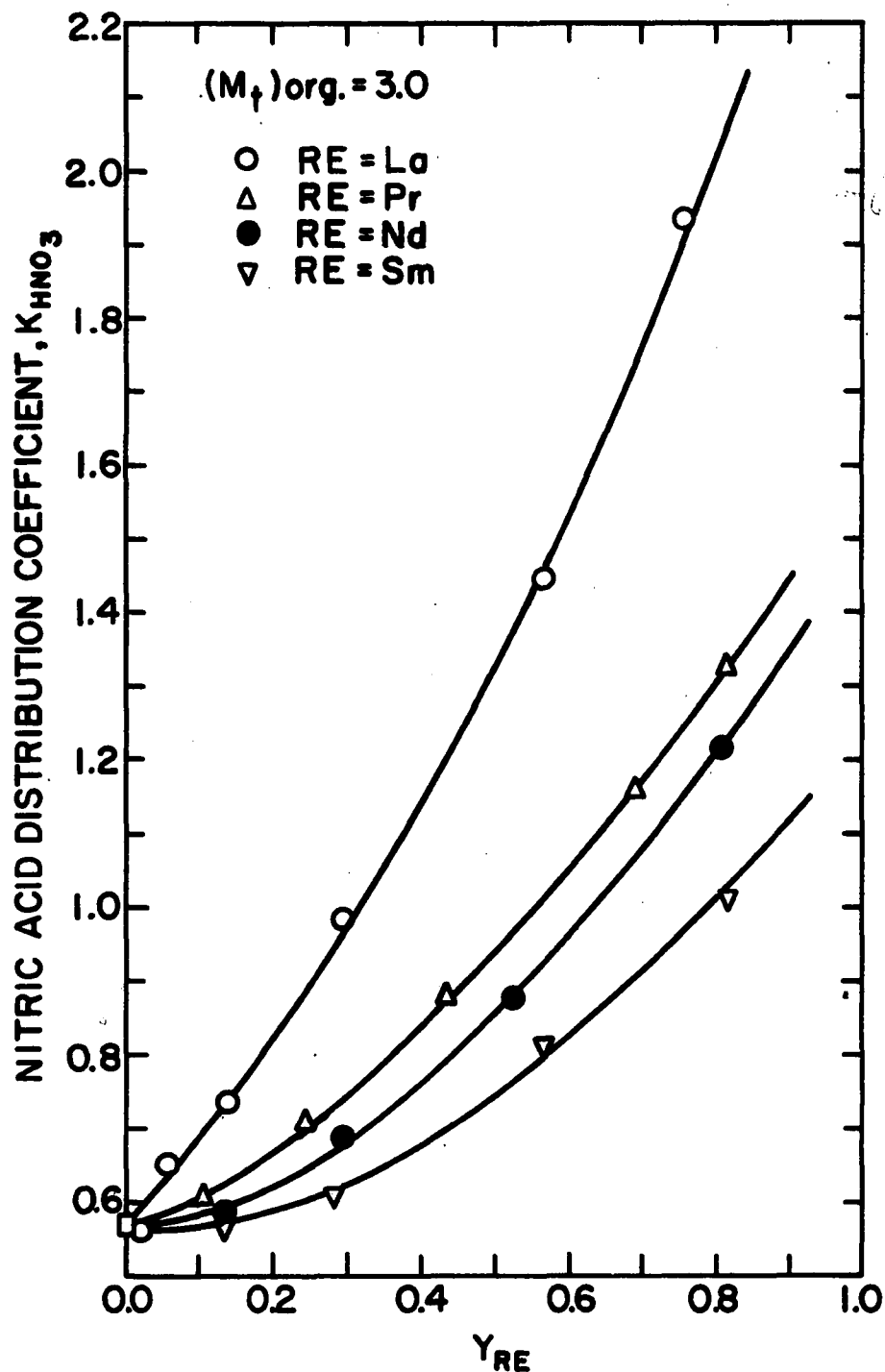


Figure 1. Nitric acid distribution coefficient for $RE(NO_3)_3 - HNO_3 - TBP - H_2O$ systems as a function of the composition of the organic phase at $(M_t)_{org.}$ equal to 3.0

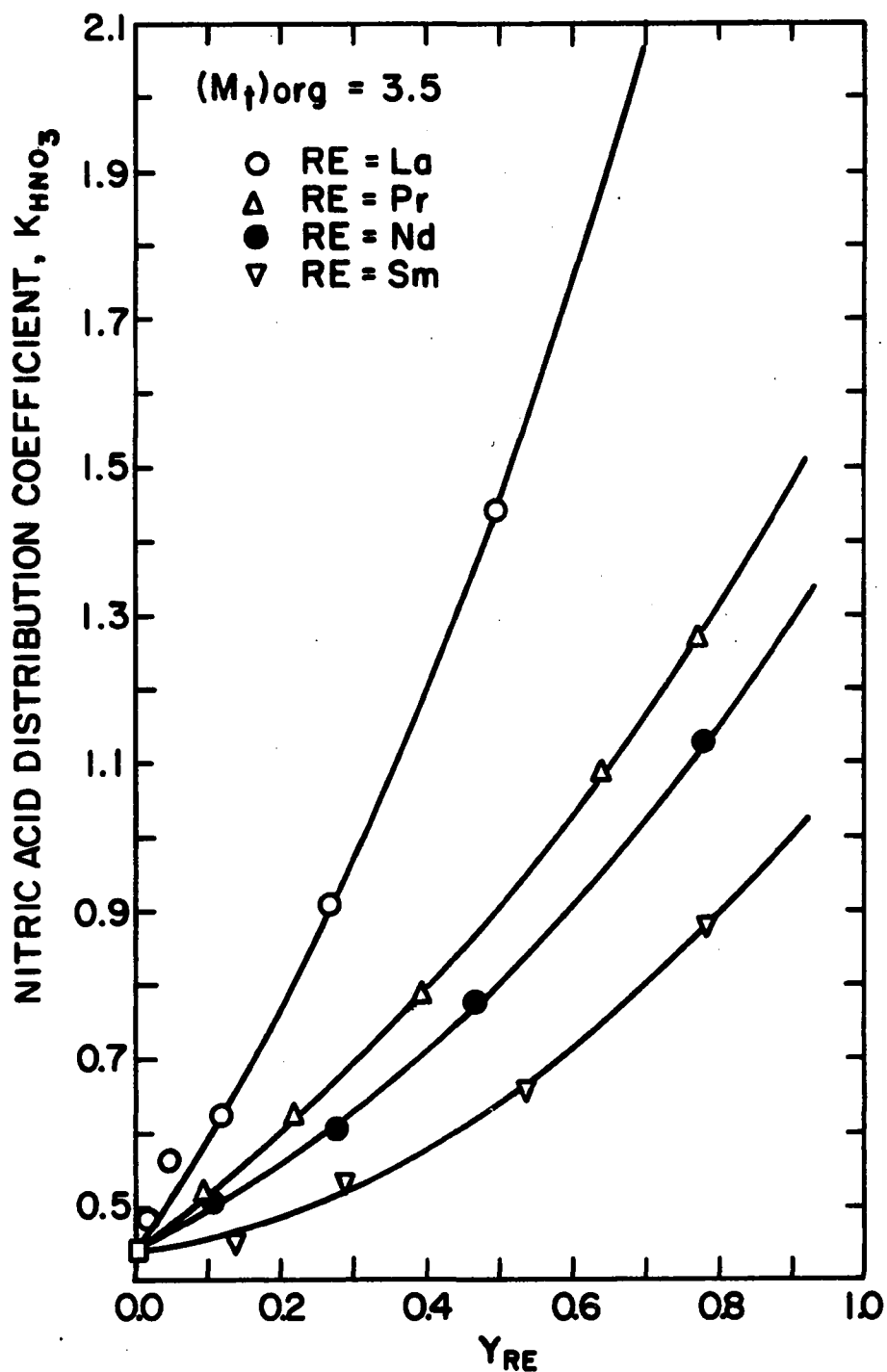
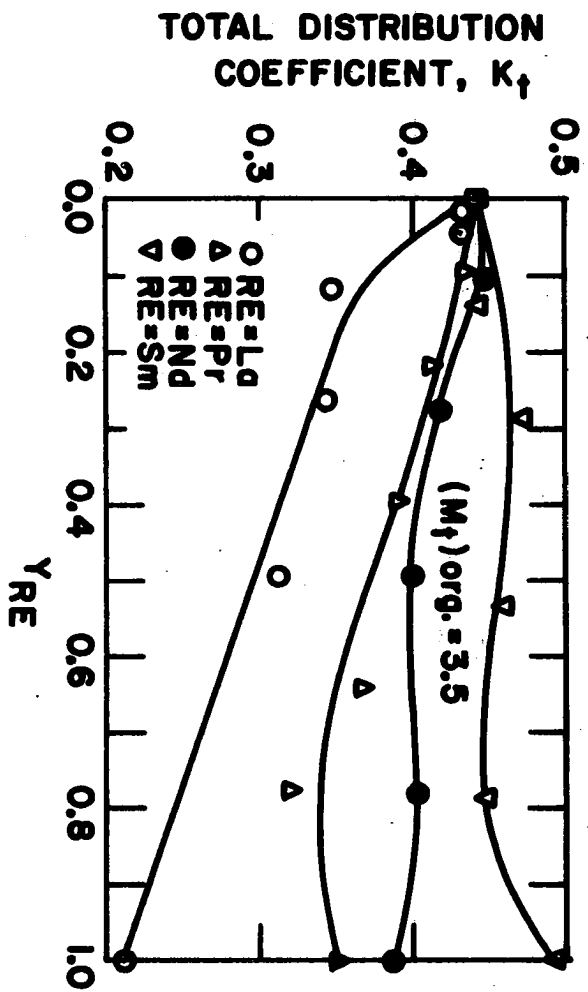
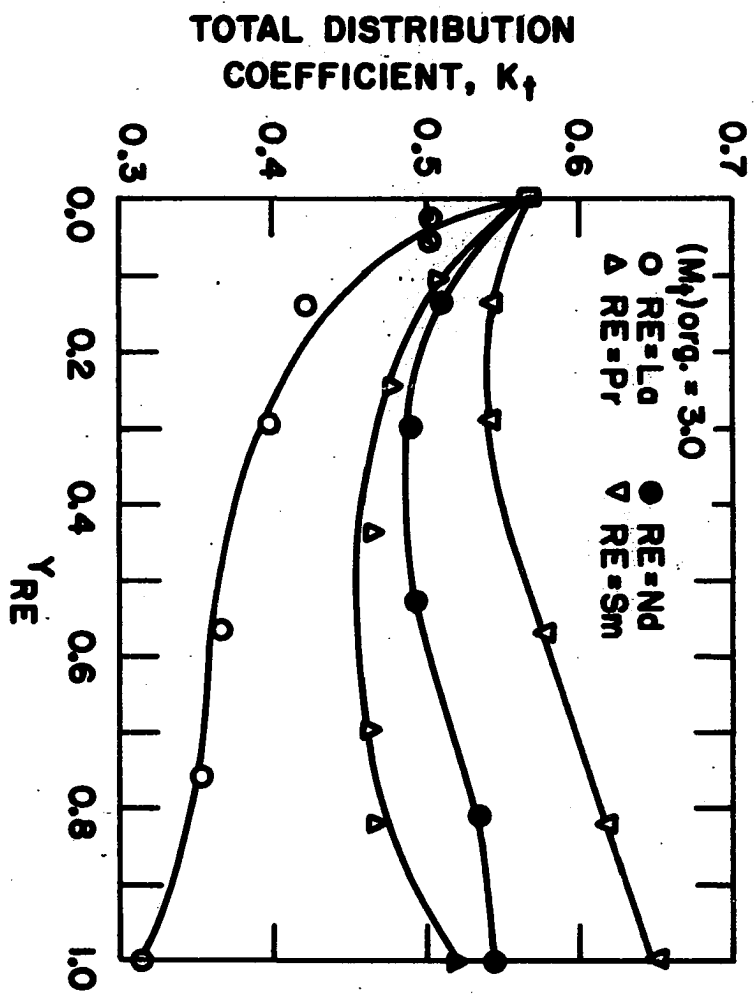


Figure 2. Nitric acid distribution coefficient for $\text{RE}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ systems as a function of the composition of the organic phase at $(M_t)_{\text{org}}$ equal to 3.5

Figure 3. Total distribution coefficient for $\text{RE}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O systems as a function of the composition of the organic phase at $(M_t)_{\text{org}}$ equal to 3.0

Figure 4. Total 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



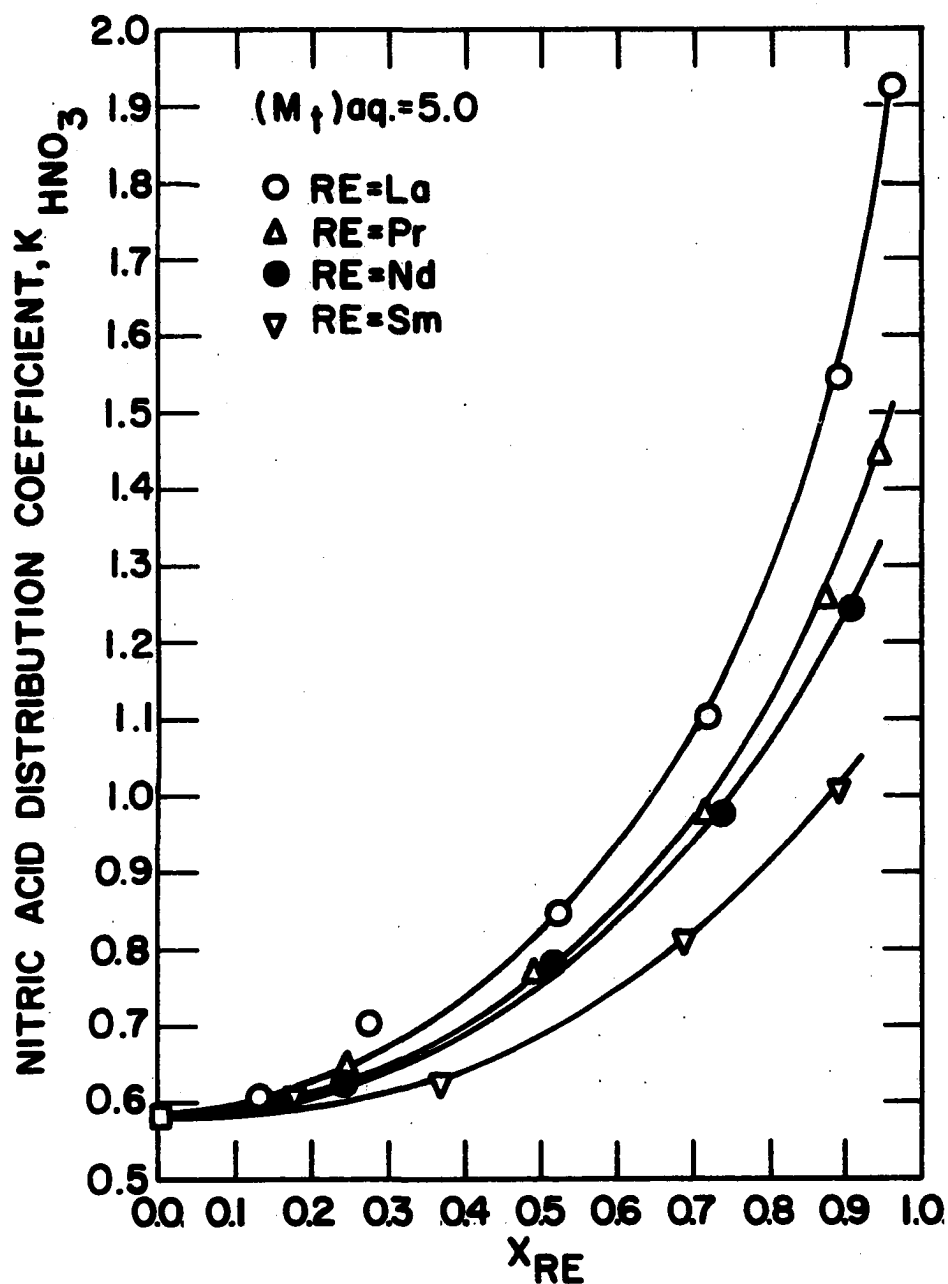


Figure 5. Nitric acid distribution coefficient for $RE(NO_3)_3 - HNO_3 - TBP - H_2O$ systems as a function of the composition of the aqueous phase at $(M_t)_{aq.}$ equal to 5.0

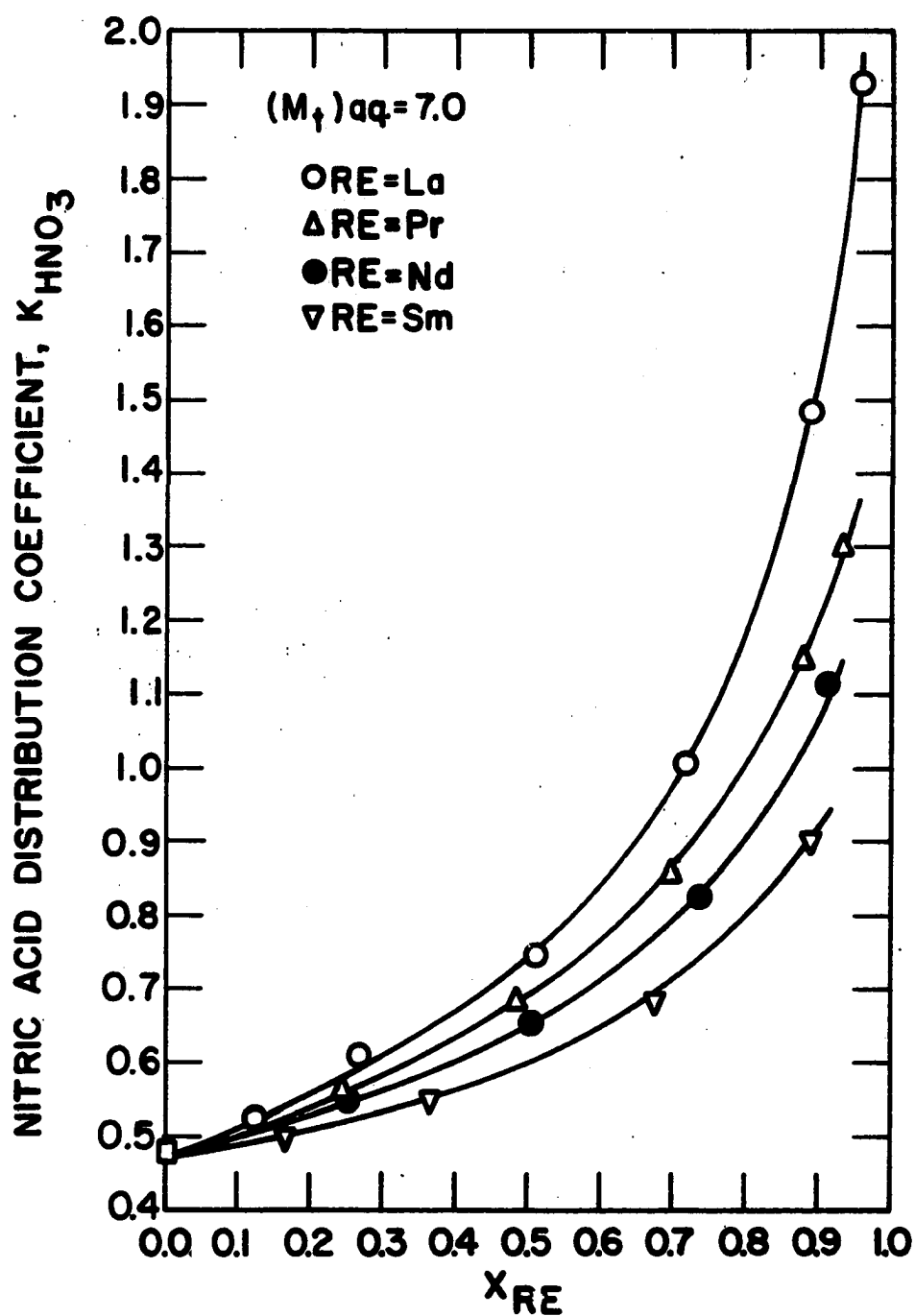
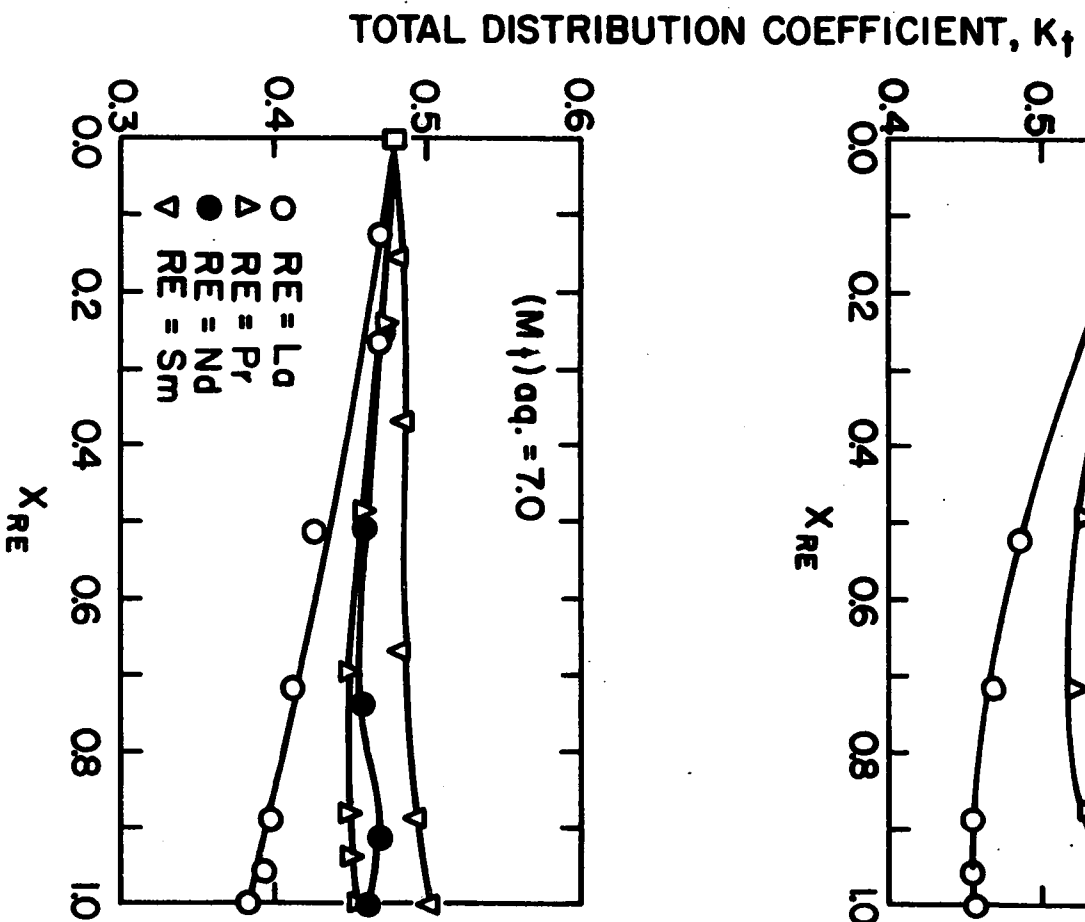
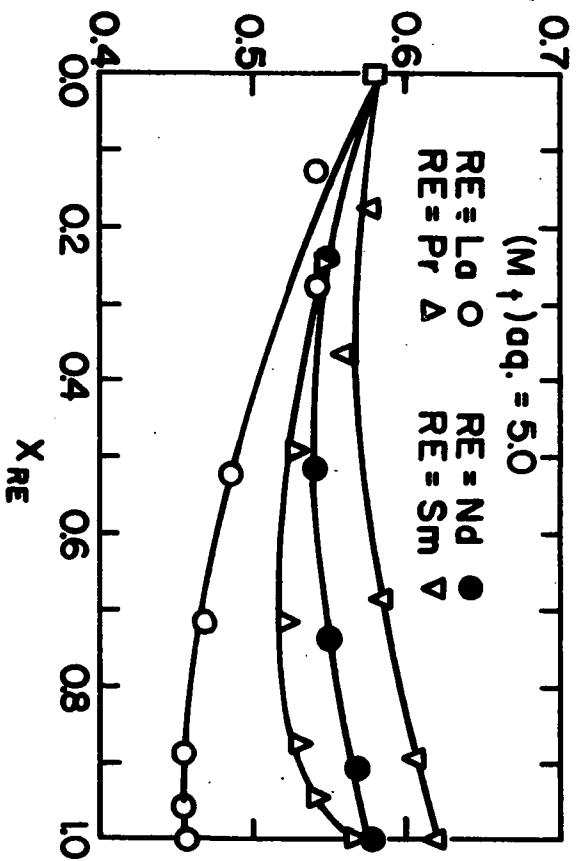


Figure 6. Nitric acid distribution coefficient for $\text{RE}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$ systems as a function of the composition of the aqueous phase at $(M_t)_{\text{aq}}$ equal to 7.0

Figure 7. Total distribution coefficient for $\text{RE}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O systems as a function of the composition of the aqueous phase at $(M_t)_{\text{aq}}$ equal to 5.0

Figure 8. Total distribution coefficient for $\text{RE}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O systems as a function of the composition of the aqueous phase at $(M_t)_{\text{aq}}$ equal to 7.0



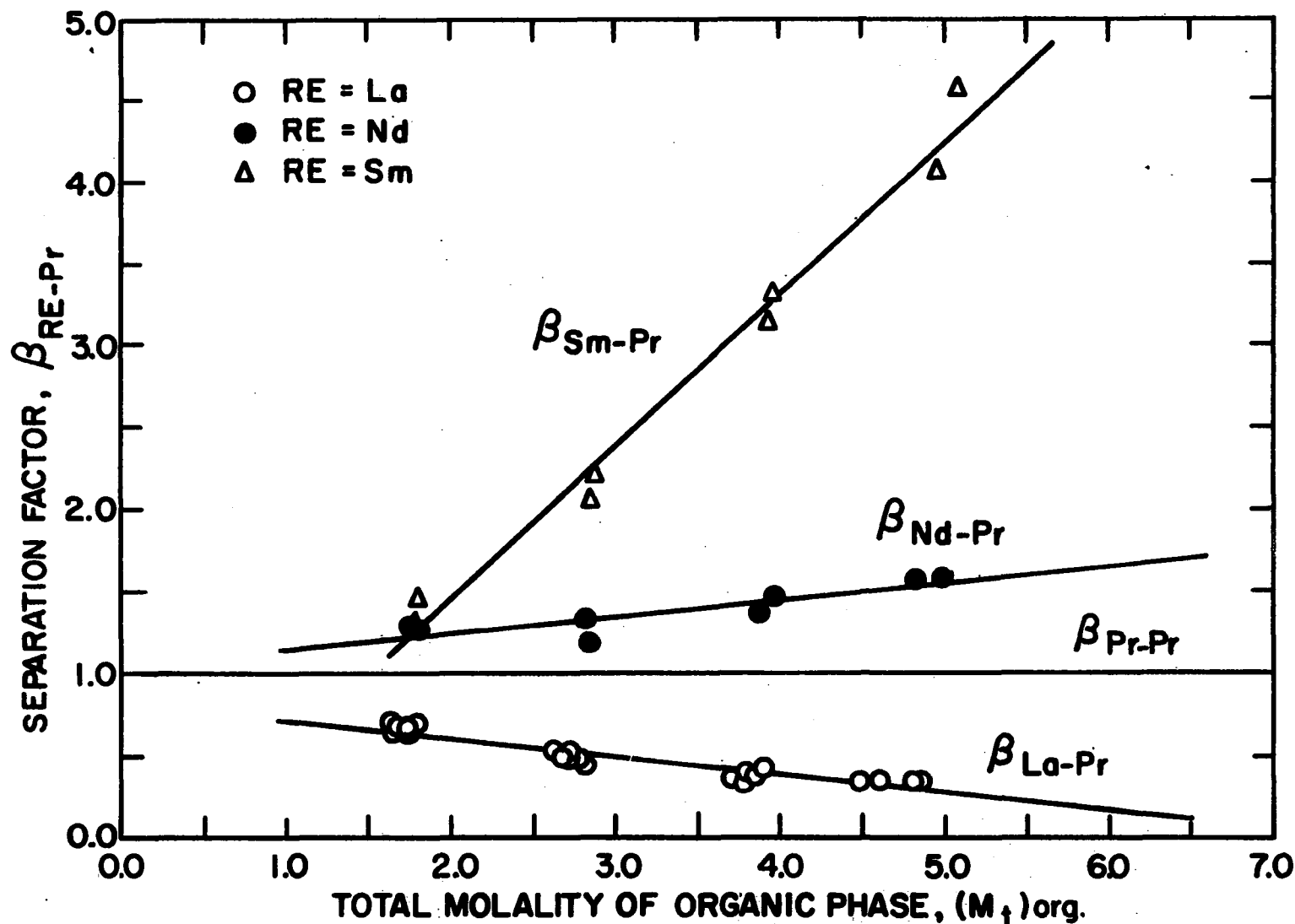


Figure 9. Separation factor between $RE(NO_3)_3$ and $Pr(NO_3)_3$ for $RE(NO_3)_3 - Pr(NO_3)_3 - HNO_3 - TBP - H_2O$ systems as a function of concentration of the organic phase

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

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

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

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

$$\begin{aligned}
 y_{\text{Pr}} &= (M_{\text{Pr}})_{\text{org.}} / (M_{\text{RE}})_{\text{org.}} = 0.0460 / 0.6671 = 0.0690 \quad , \\
 y_{\text{Nd}} &= (M_{\text{Nd}})_{\text{org.}} / (M_{\text{RE}})_{\text{org.}} = 0.0706 / 0.6671 = 0.1058 \quad , \\
 y_{\text{Sm}} &= (M_{\text{Sm}})_{\text{org.}} / (M_{\text{RE}})_{\text{org.}} = 0.5108 / 0.6671 = 0.7657 \quad .
 \end{aligned}$$

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:

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

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

$$\begin{aligned} (M_{\text{La}})_{\text{aq.}} &= \frac{(M_{\text{RE}})_{\text{aq.}} \times (M_{\text{La}})_{\text{org.}}}{\beta_{\text{La-Pr}} \times \sum_{i=1}^T ((M_i)_{\text{org.}} / \beta_{i-\text{Pr}})} \\ &= \frac{(1.9610)(0.0397)}{(0.4840)(0.3926)} = 0.4097 \end{aligned}$$

and in exactly the same manner

$$\begin{aligned} (M_{\text{Pr}})_{\text{aq.}} &= 0.2298 \quad , \\ (M_{\text{Nd}})_{\text{aq.}} &= 0.2625 \quad , \\ (M_{\text{Sm}})_{\text{aq.}} &= 1.0592 \quad . \end{aligned}$$

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

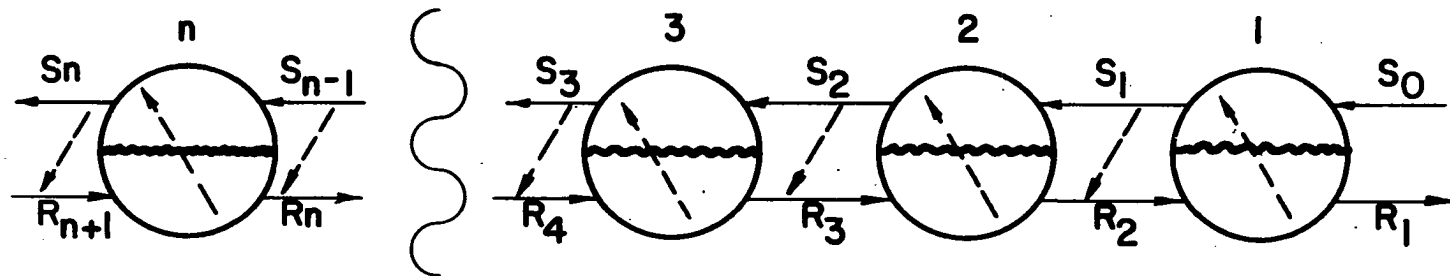


Figure 10. Cascade I

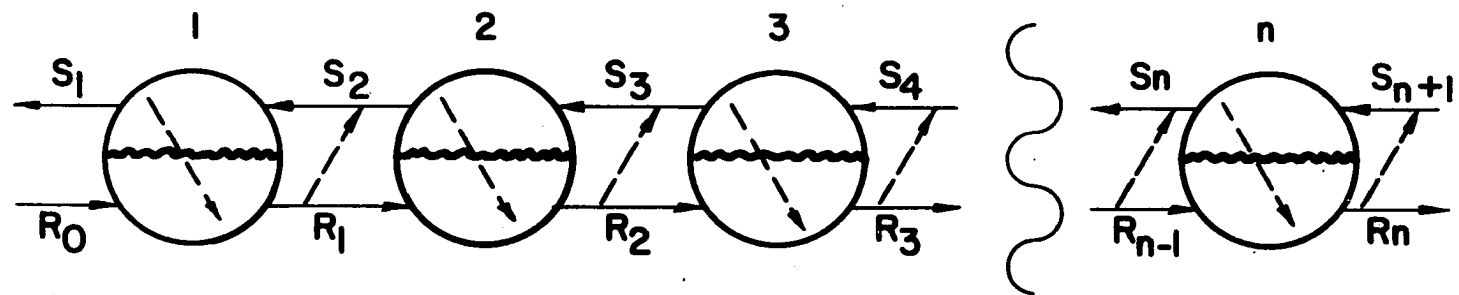


Figure 11. Cascade II

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).

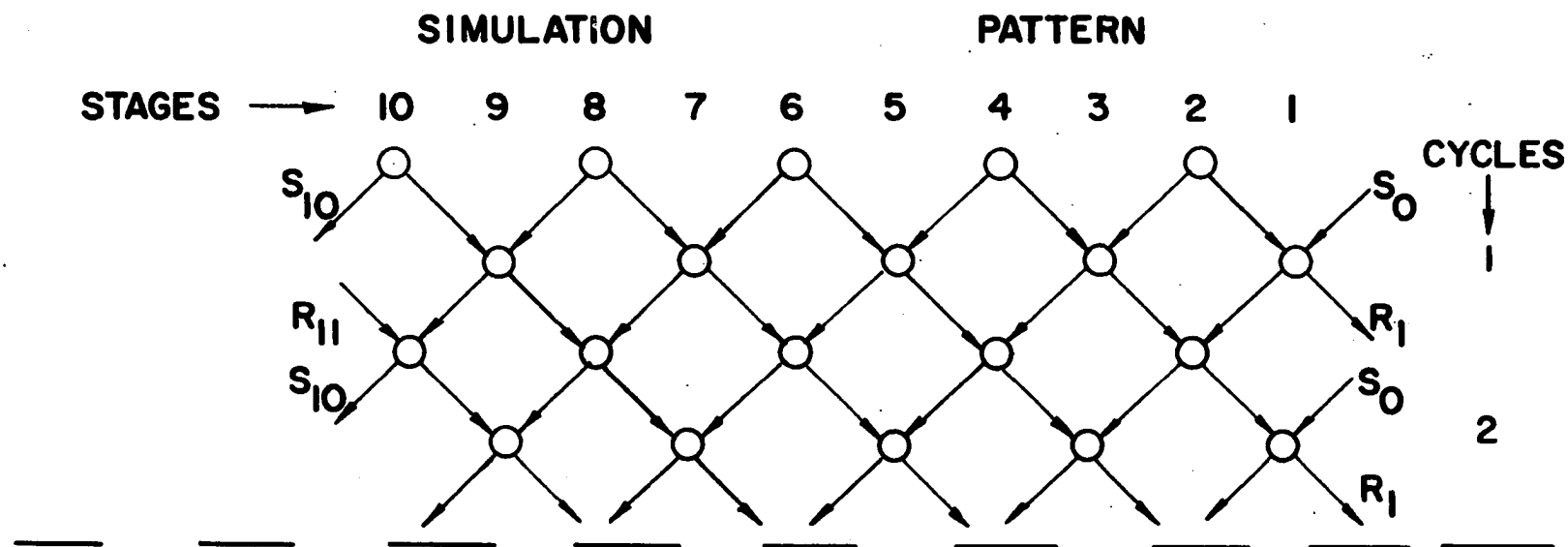
Four of the prediction calculations discussed in the Method of Calculation section were chosen for simulation. The experiments were carried out in laboratory glassware at room temperature, using 1/100 horsepower laboratory stirrers for the mixing steps. A minimum of two minutes mixing and three minutes 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 : $M_{HNO_3} = 0.00$, $M_{RE} = 0.00$

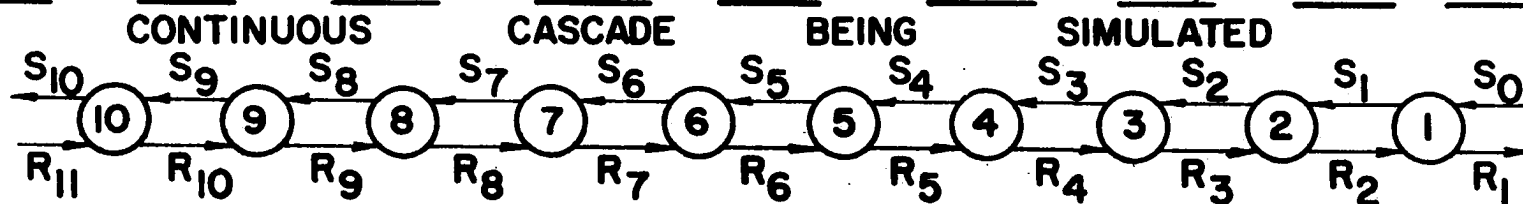


Figure 12. General information pertaining to Simulated Column Experiment I

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

	Weight % La ₂ O ₃ in total oxides		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.
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_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 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

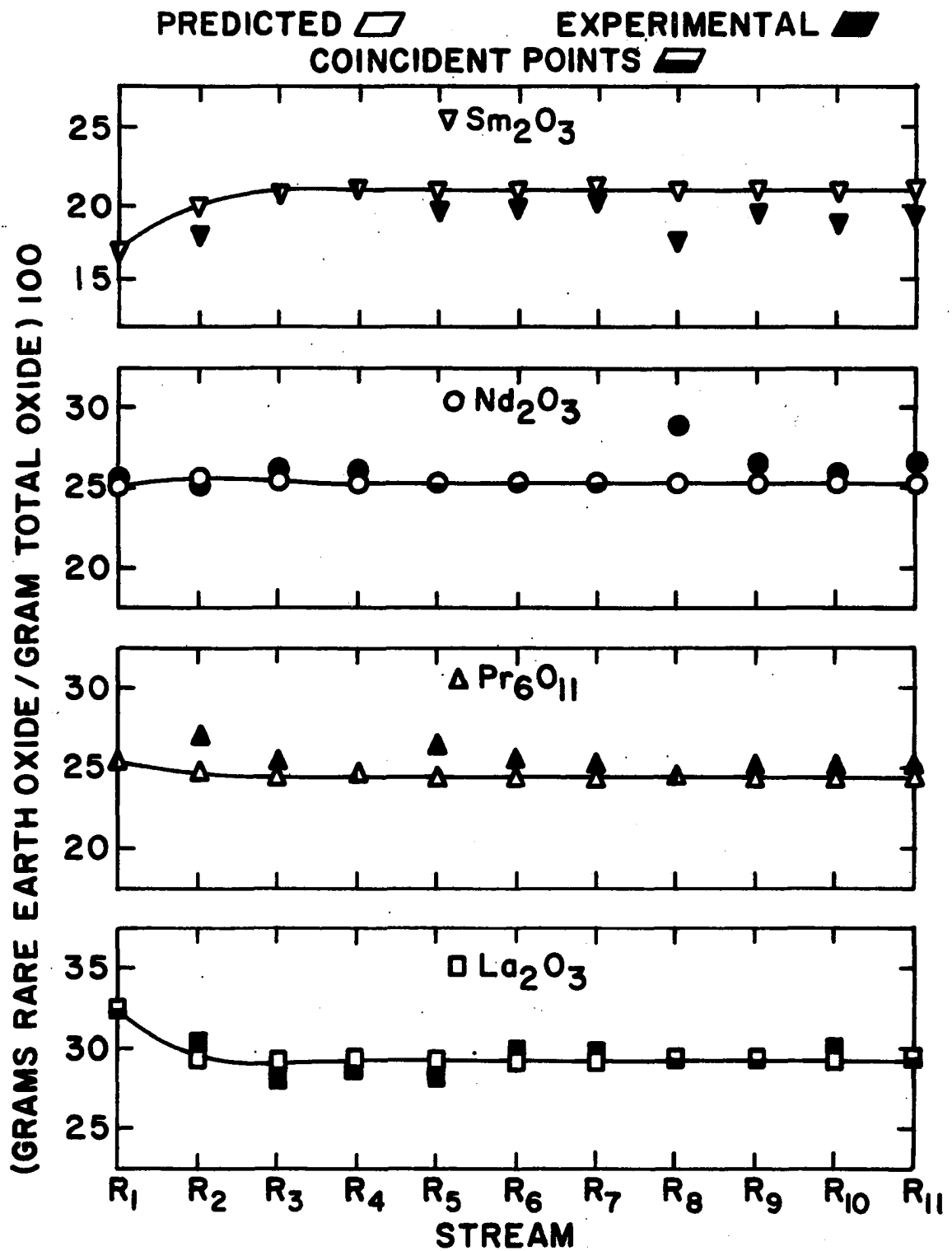


Figure 13. Stagewise aqueous rare earth oxide composition for Simulated Column Experiment I

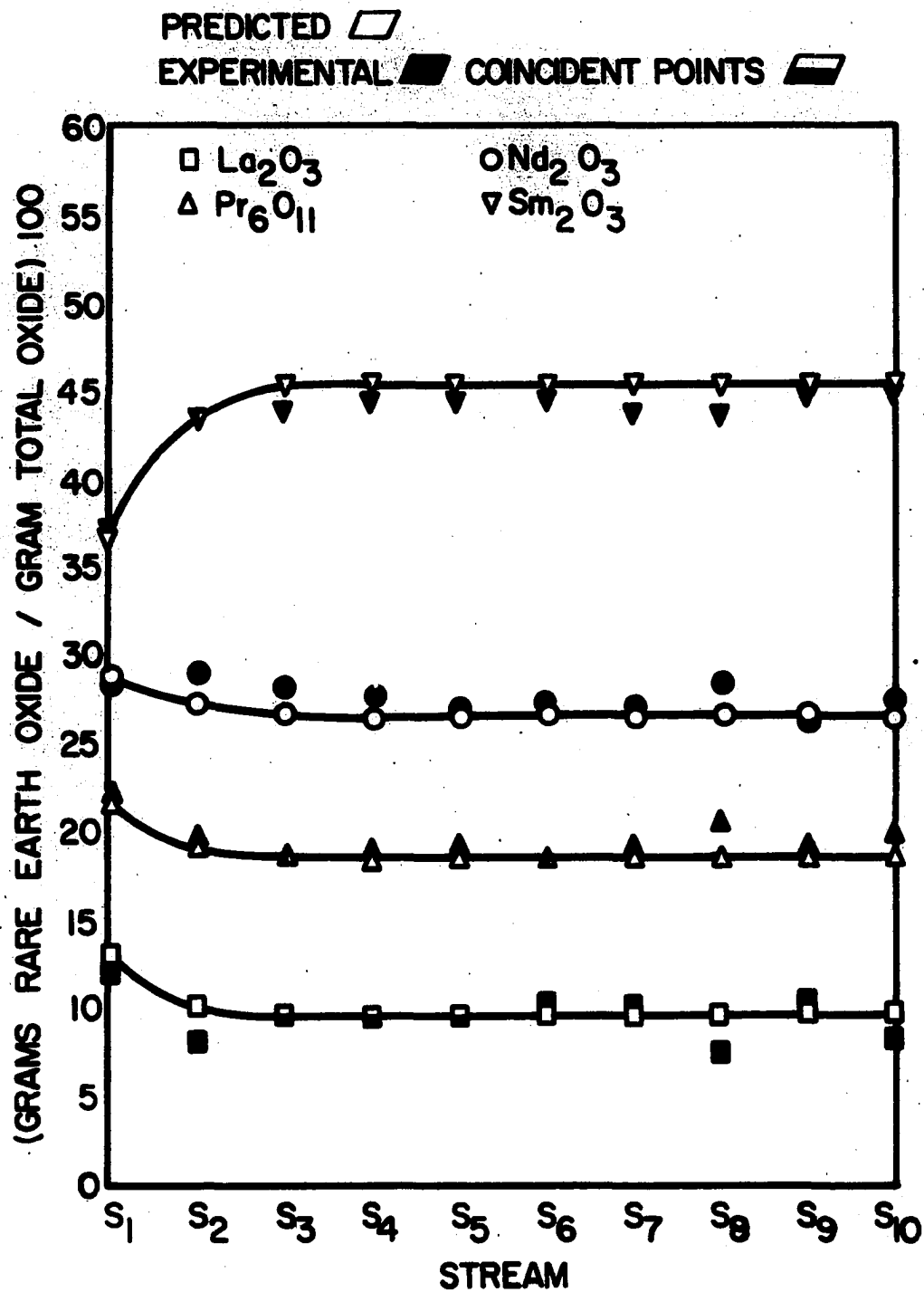


Figure 14. Stagewise organic rare earth oxide composition for Simulated Column Experiment I

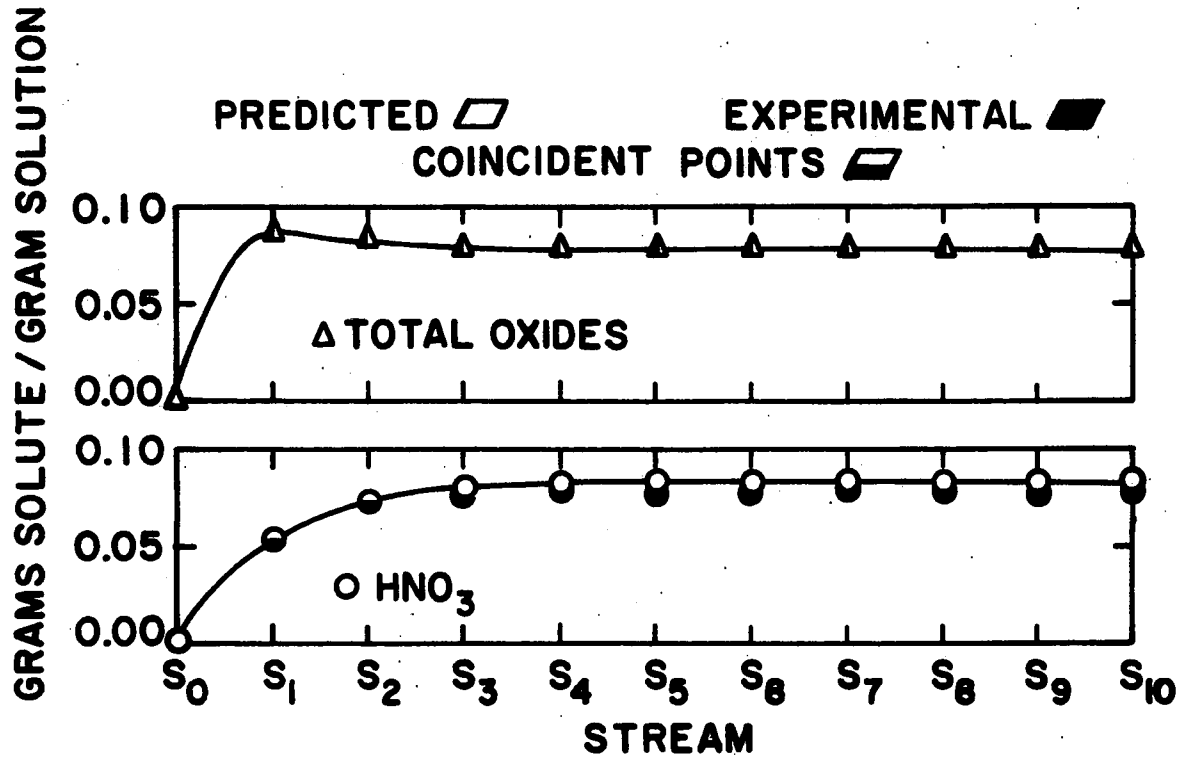


Figure 15. Stagewise organic rare earth oxide and nitric acid concentrations for Simulated Column Experiment I

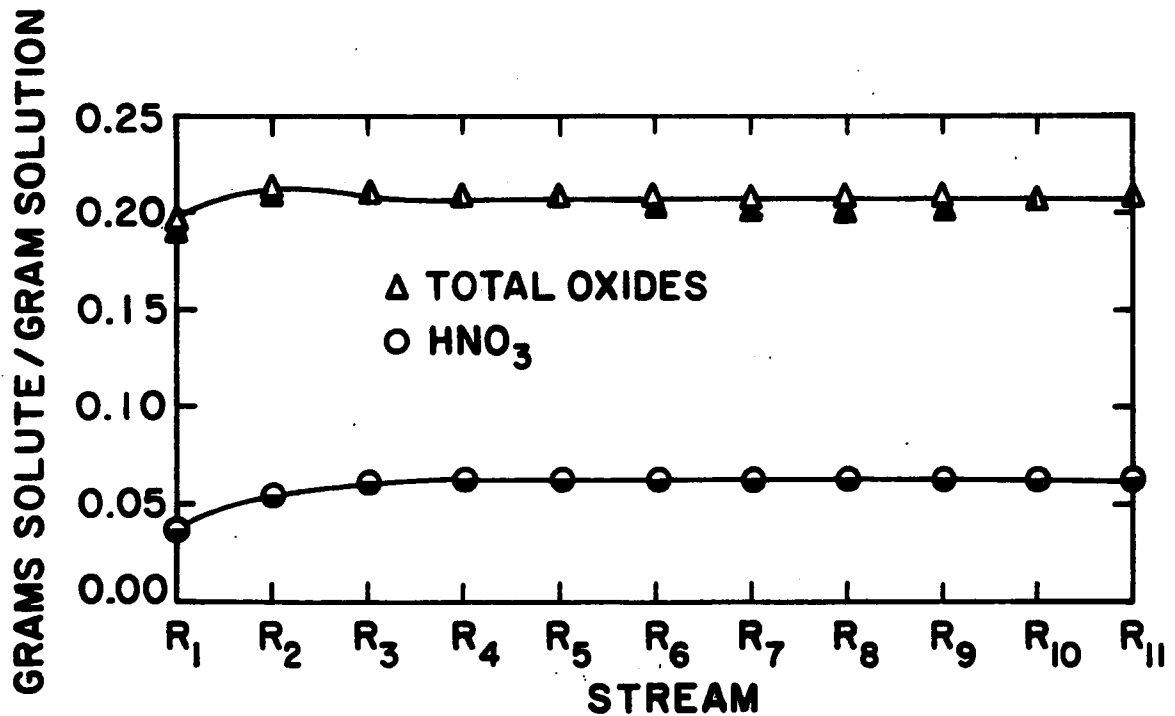


Figure 16. Stagewise aqueous rare earth oxide and nitric acid concentrations for Simulated Column Experiment I

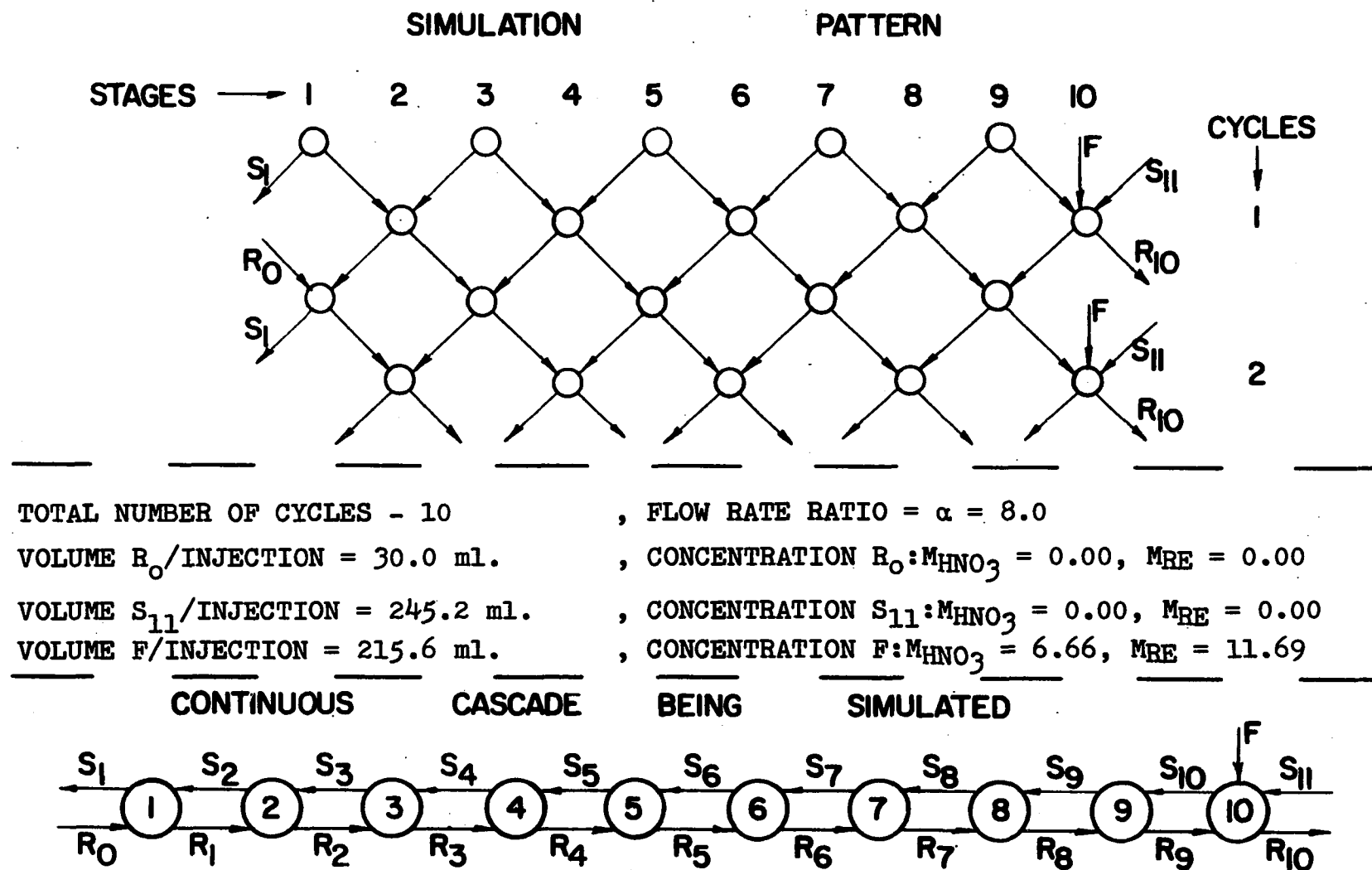


Figure 17. General information pertaining to Simulated Column Experiment II

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

	Weight % La 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.
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

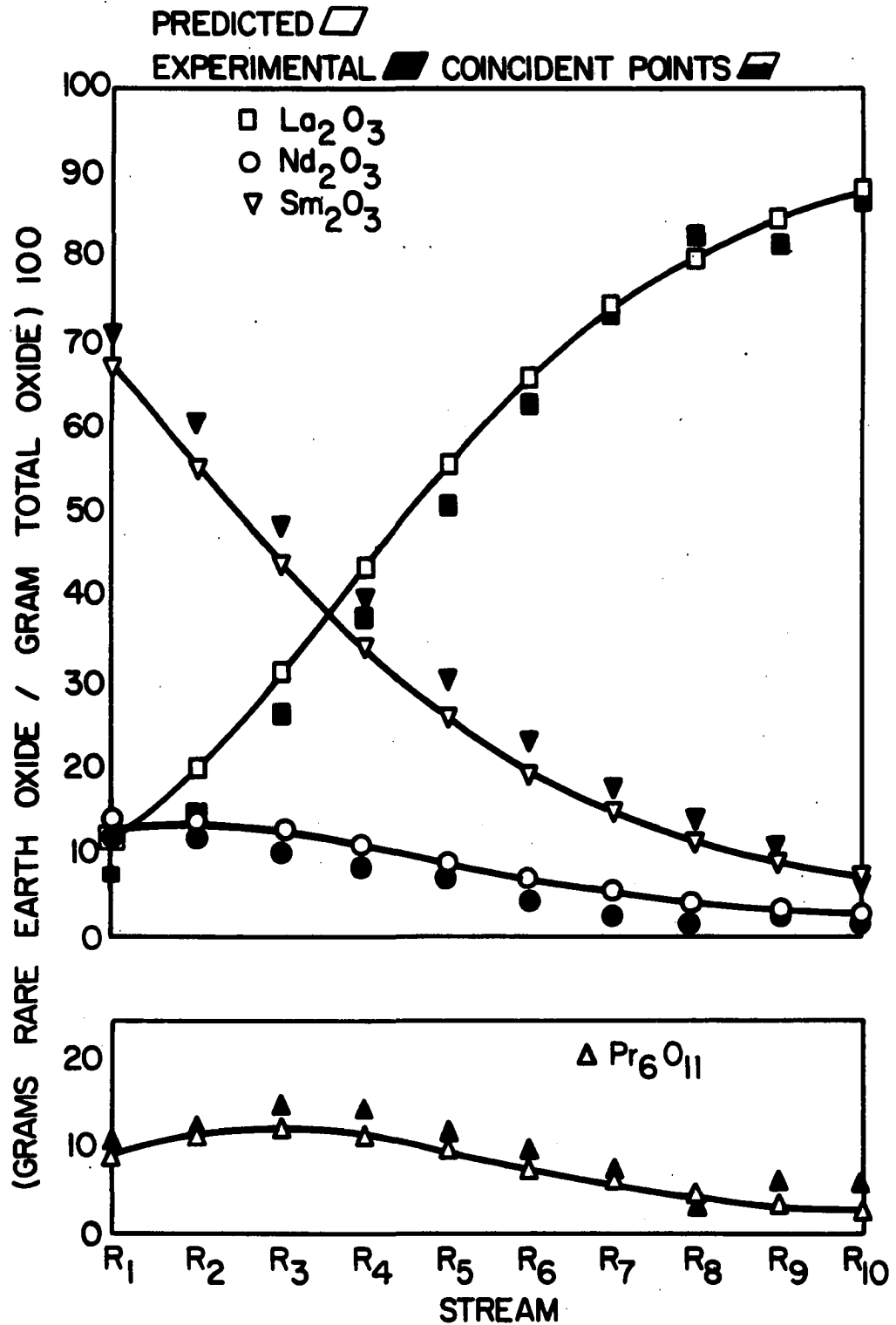


Figure 18. Stagewise aqueous rare earth oxide composition for Simulated Column Experiment II

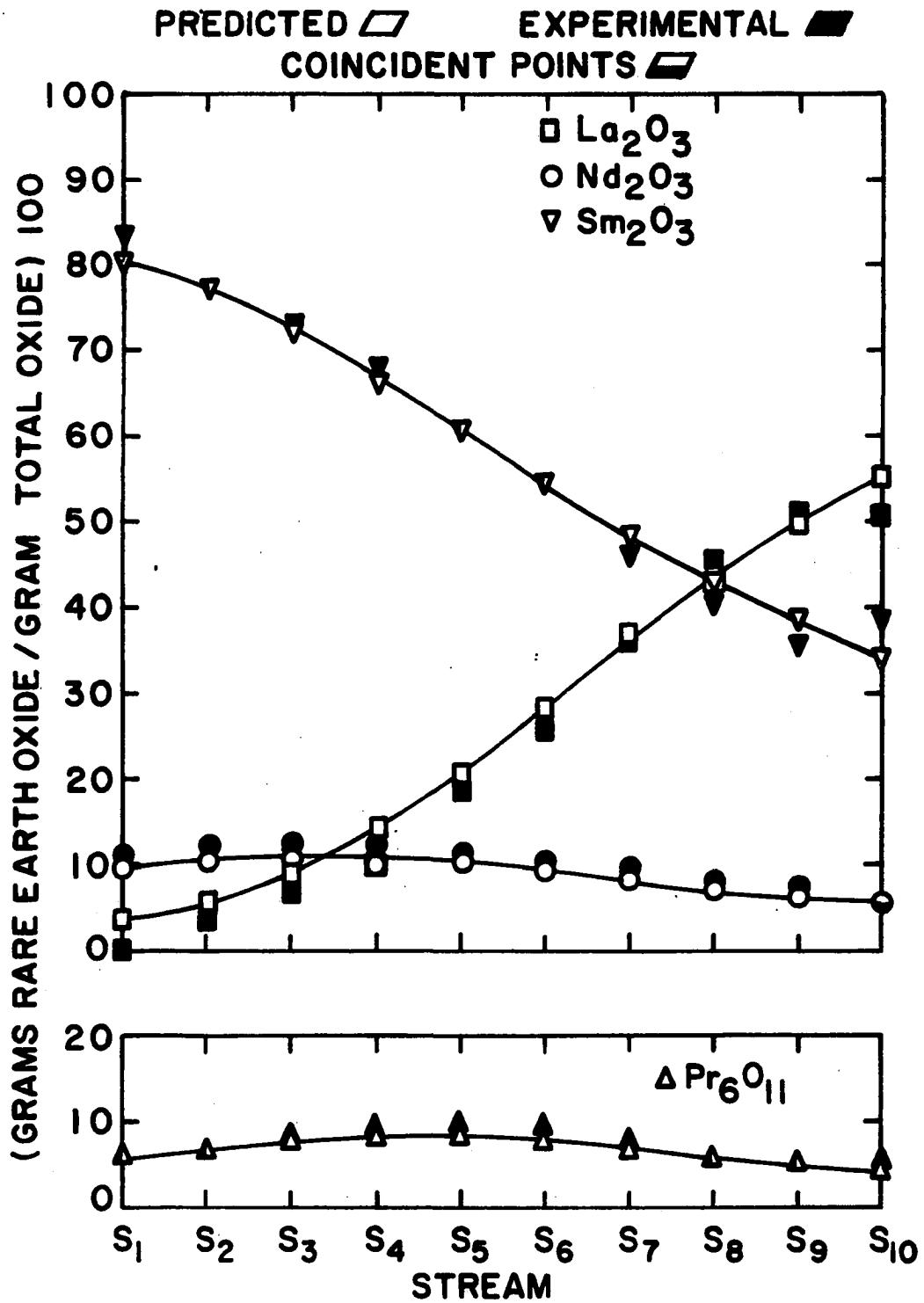


Figure 19. Stagewise organic rare earth oxide composition for Simulated Column Experiment II

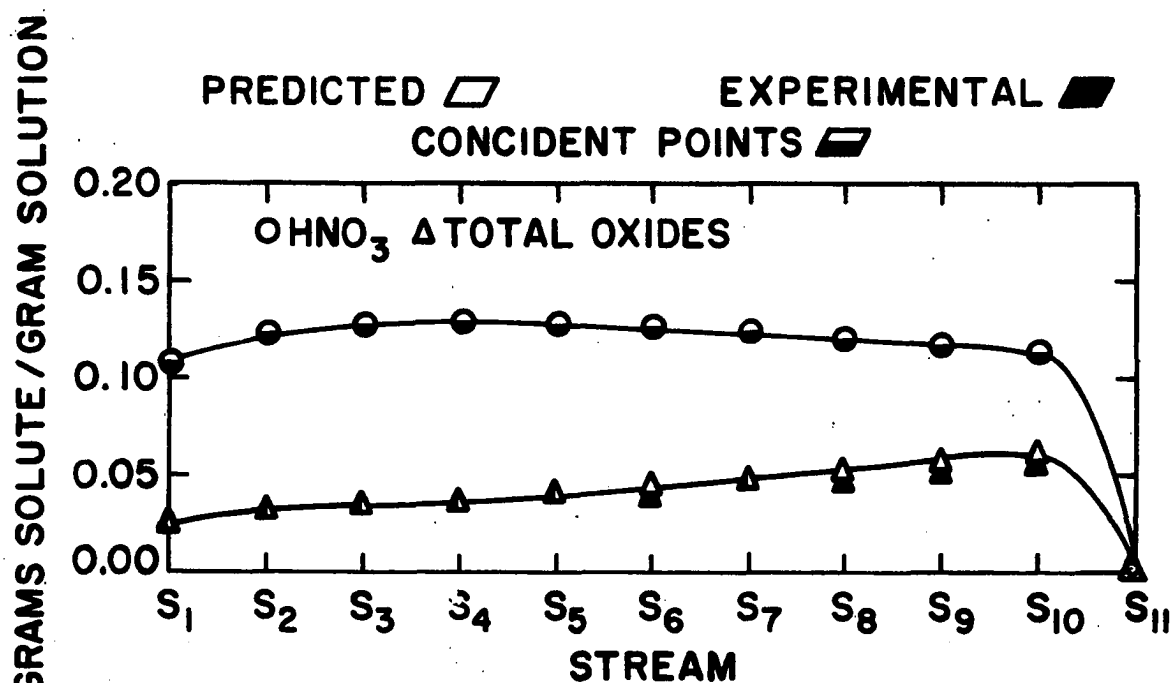


Figure 20. Stagewise organic rare earth oxide and nitric acid concentrations for Simulated Column Experiment II

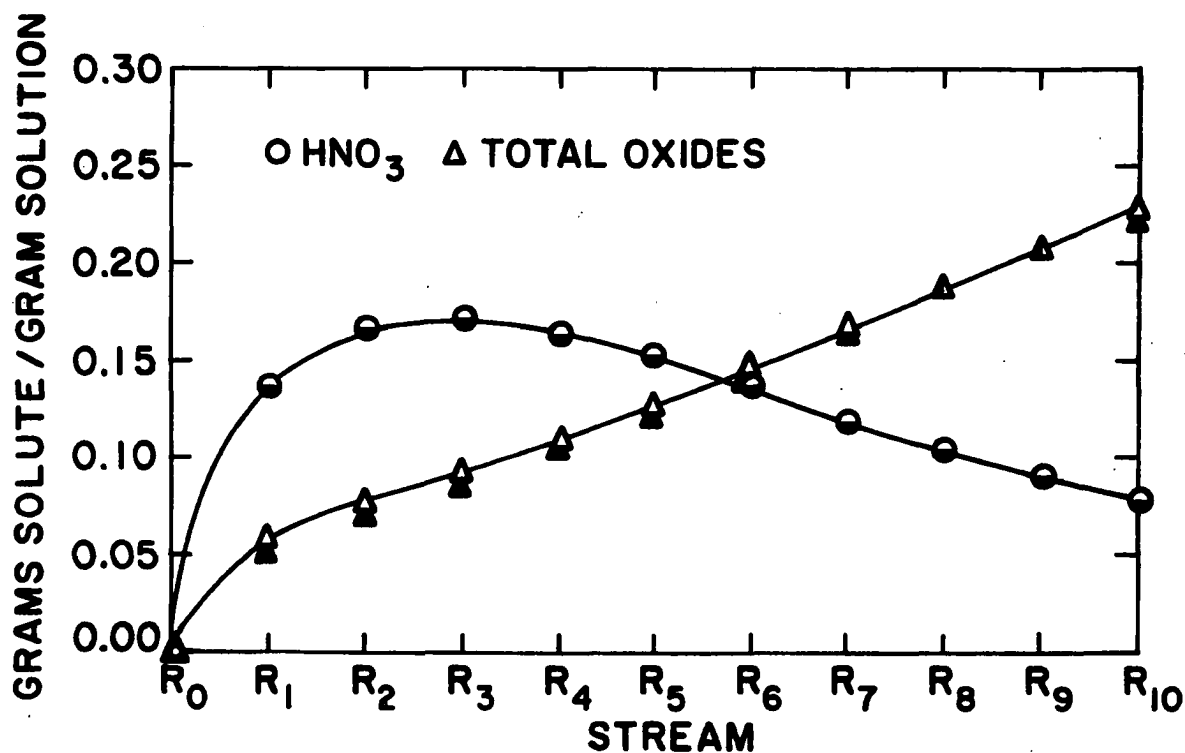


Figure 21. Stagewise aqueous rare earth oxide and nitric acid concentrations for Simulated Column Experiment II

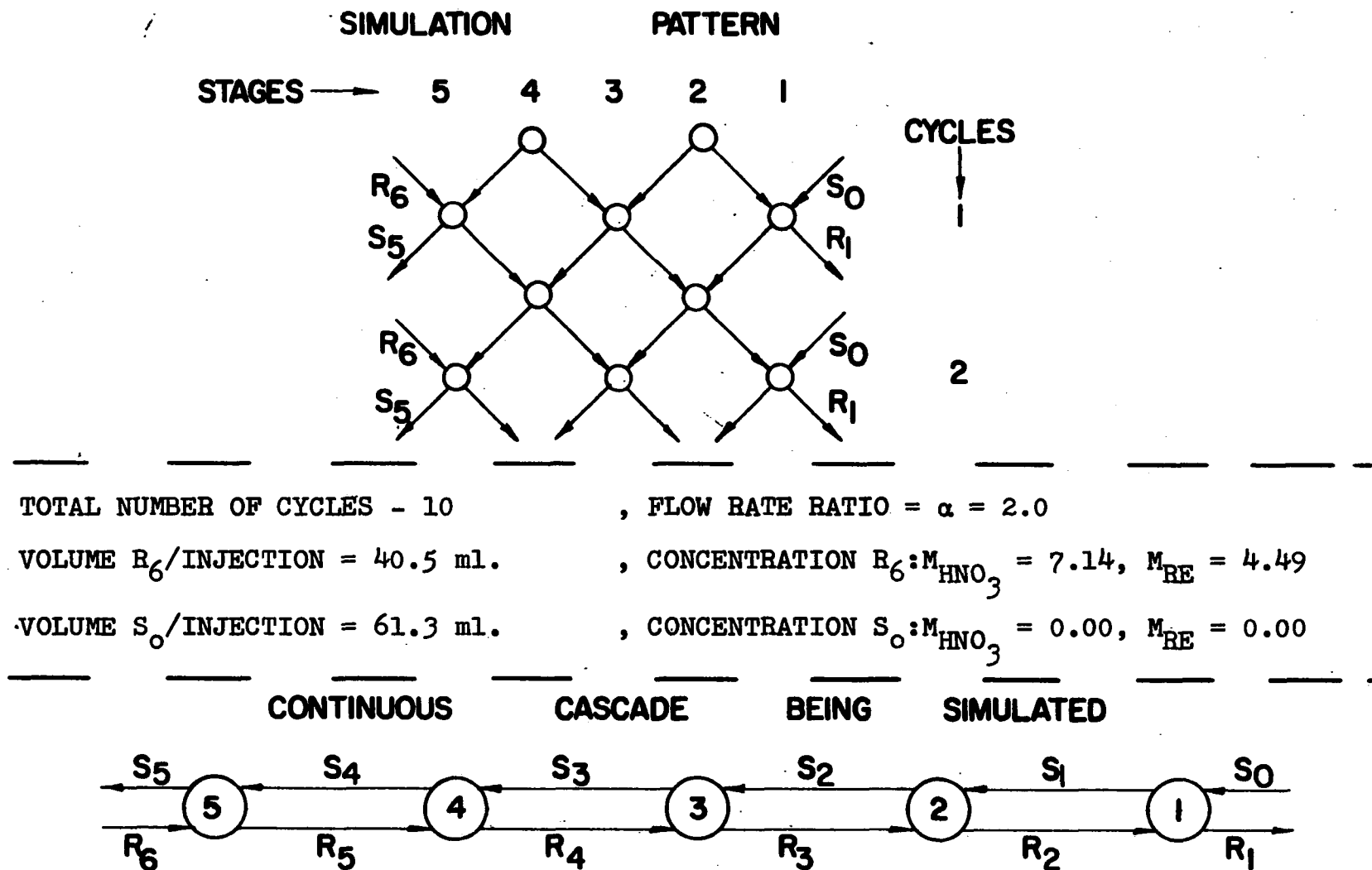


Figure 22. General information pertaining to Simulated Column Experiment III

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

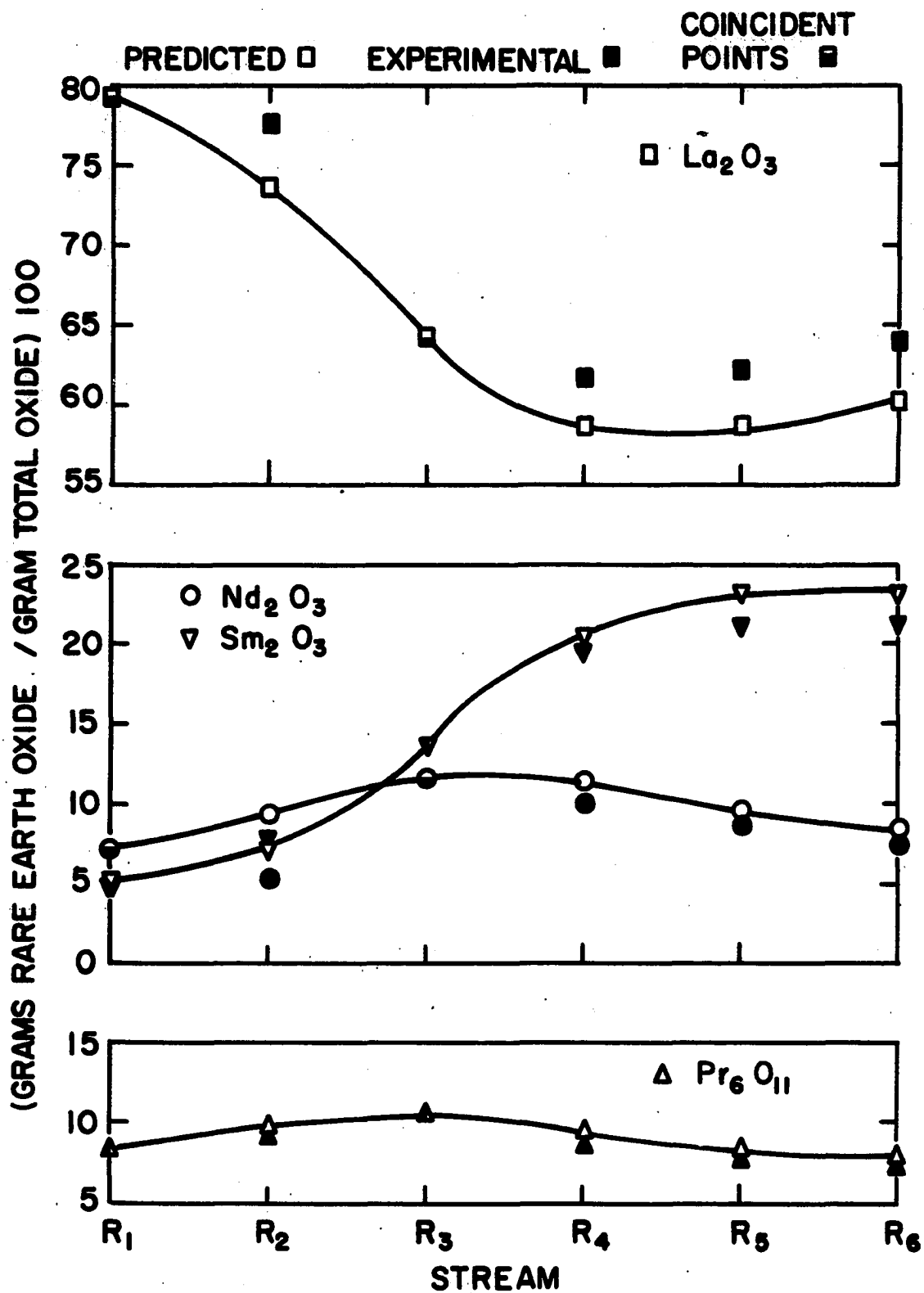


Figure 23. Stagewise aqueous rare earth oxide composition for Simulated Column Experiment III

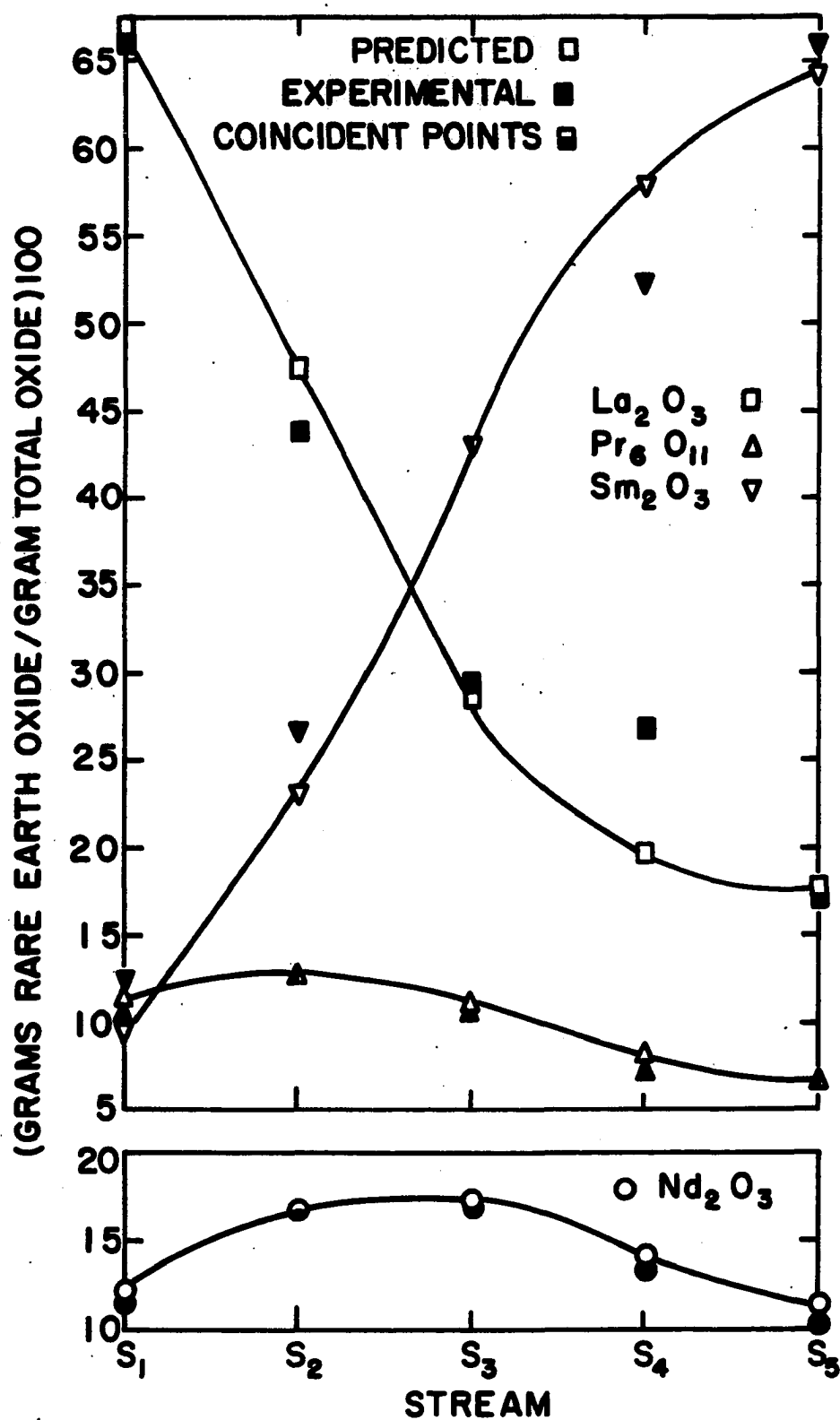


Figure 24. Stagewise organic rare earth oxide composition for Simulated Column Experiment III

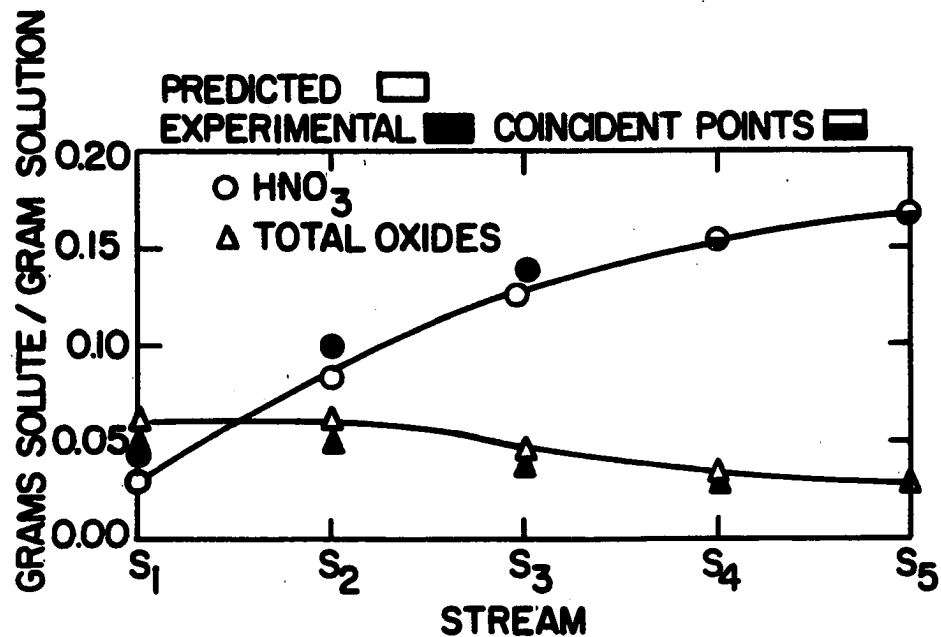


Figure 25. Stagewise organic rare earth oxide and nitric acid concentrations for Simulated Column Experiment III

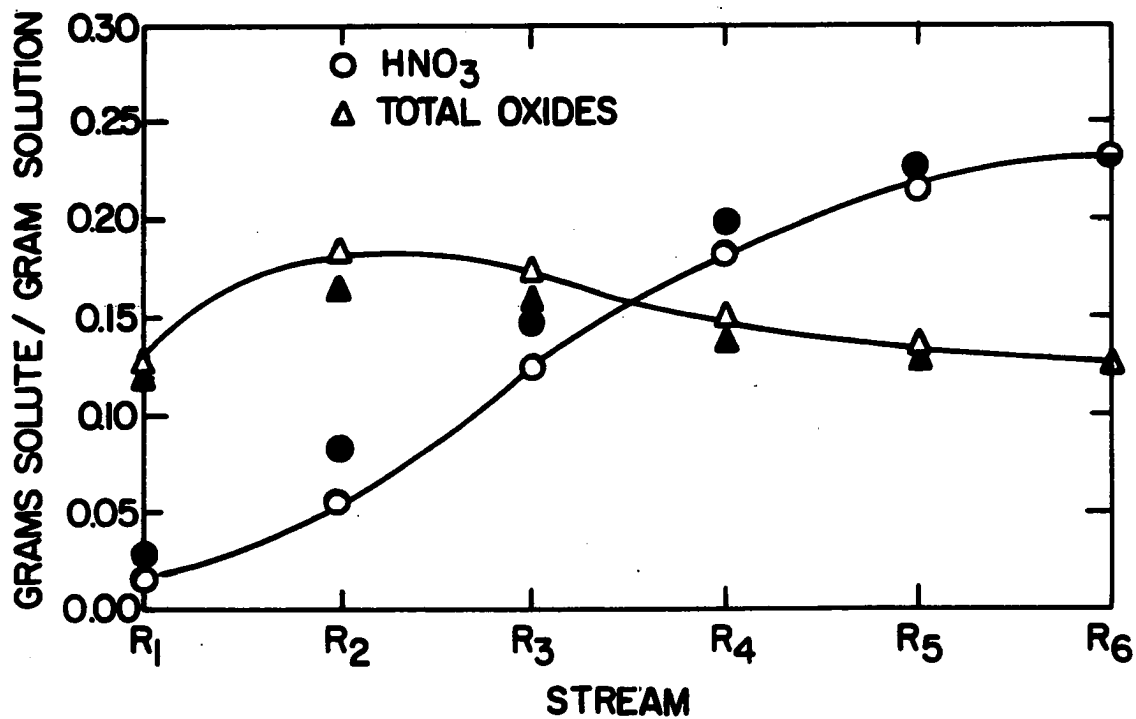
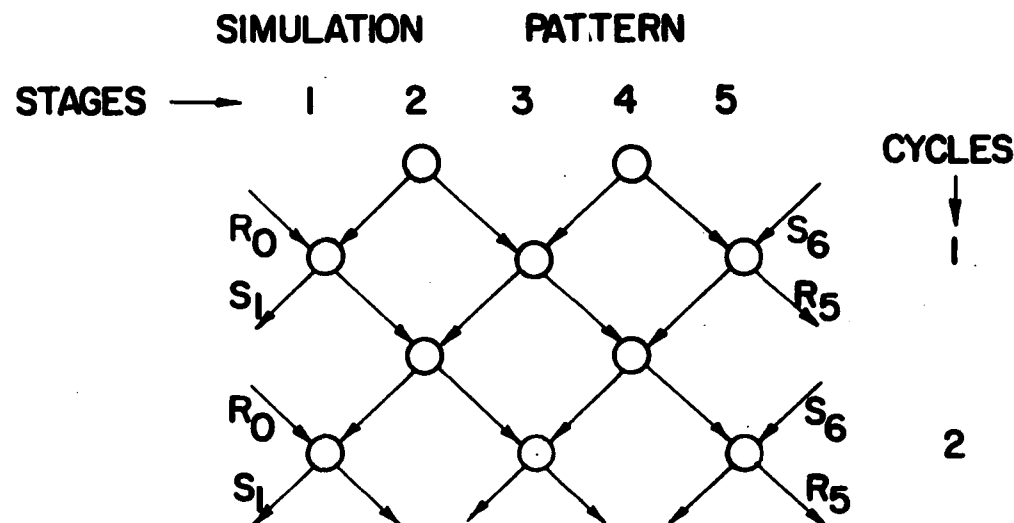


Figure 26. Stagewise aqueous rare earth oxide and nitric acid concentrations for Simulated Column Experiment III



TOTAL NUMBER OF CYCLES - 10 , FLOW RATE RATIO = $\alpha = 1.0$

VOLUME R_0 /INJECTION = 54.2 ml. , CONCENTRATION $R_0:M_{HNO_3} = 4.97$, $M_{RE} = 7.15$

VOLUME S_6 /INJECTION = 40.9 ml. , CONCENTRATION $S_6:M_{HNO_3} = 0.00$, $M_{RE} = 0.00$

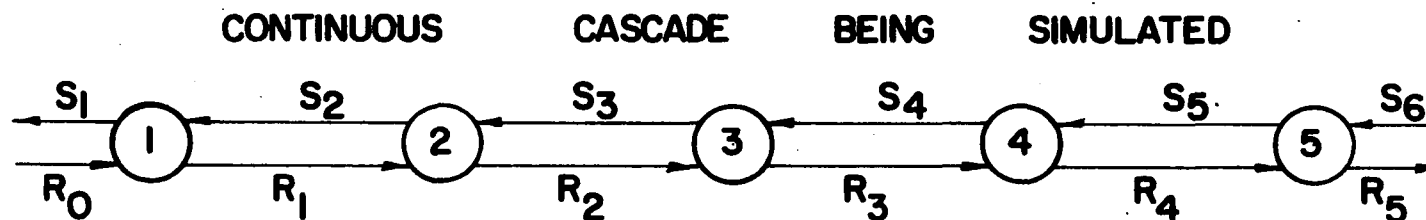


Figure 27. General information pertaining to Simulated Column Experiment IV

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

	Weight % La 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	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

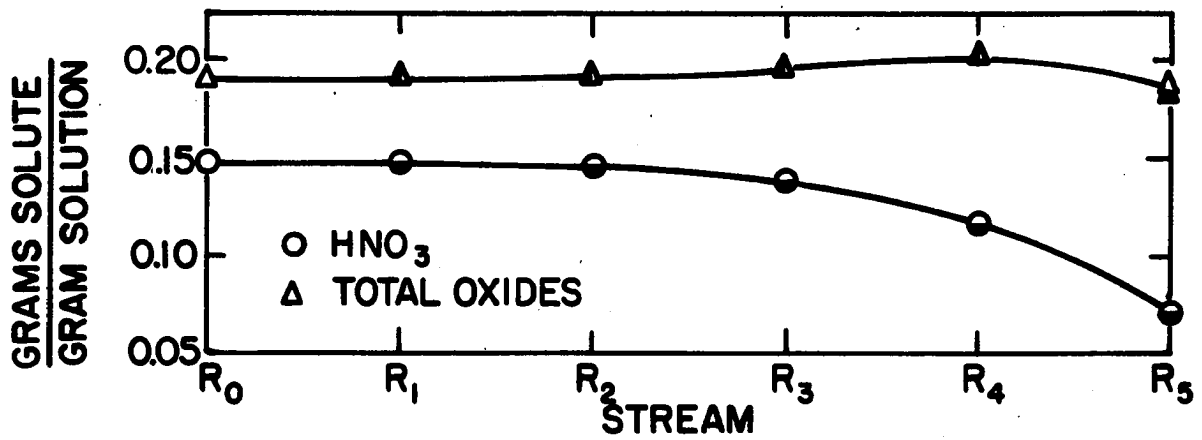


Figure 28. Stagewise aqueous rare earth oxide and nitric acid concentrations for Simulated Column Experiment IV

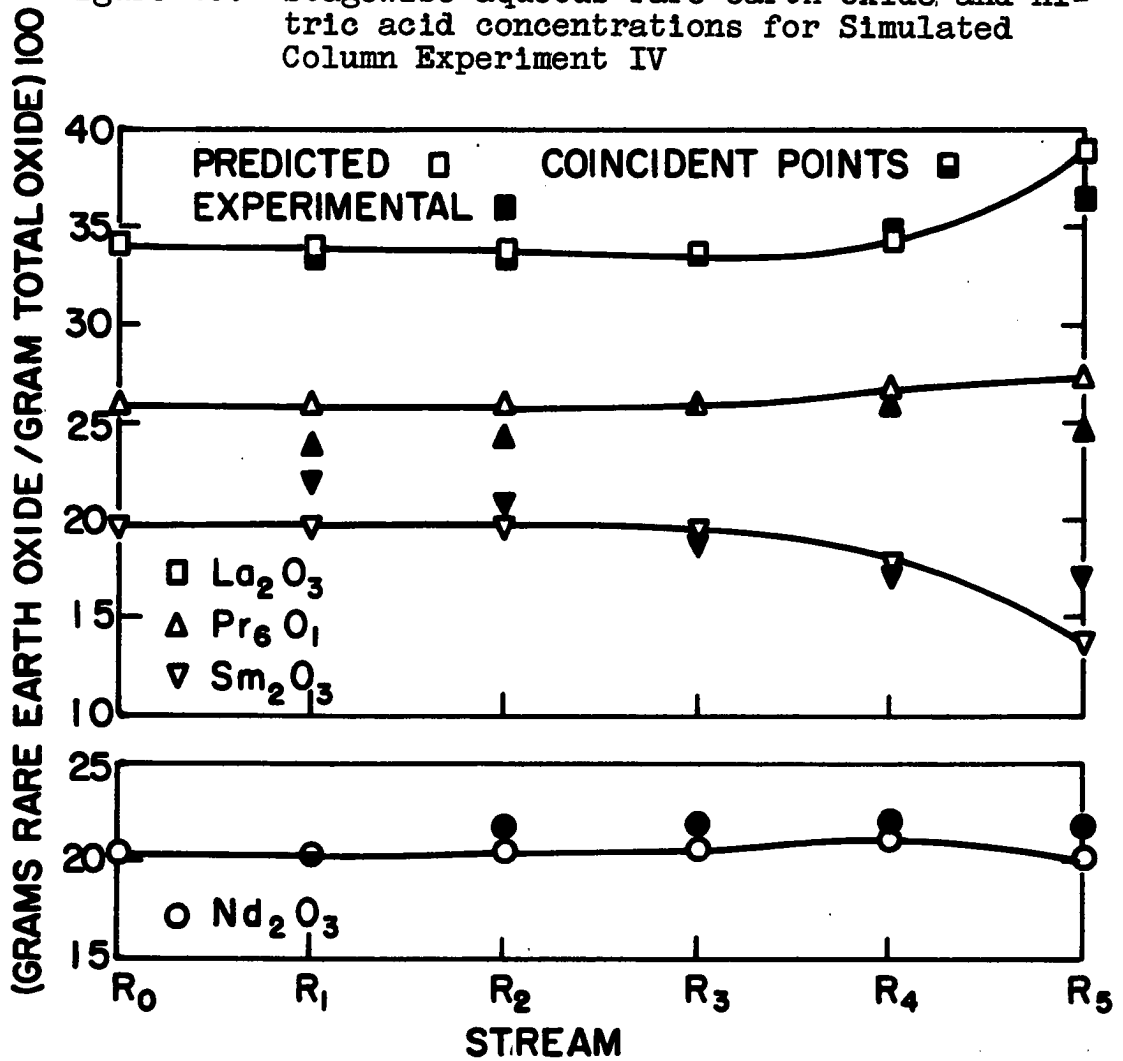


Figure 29. Stagewise aqueous rare earth oxide composition for Simulated Column Experiment IV

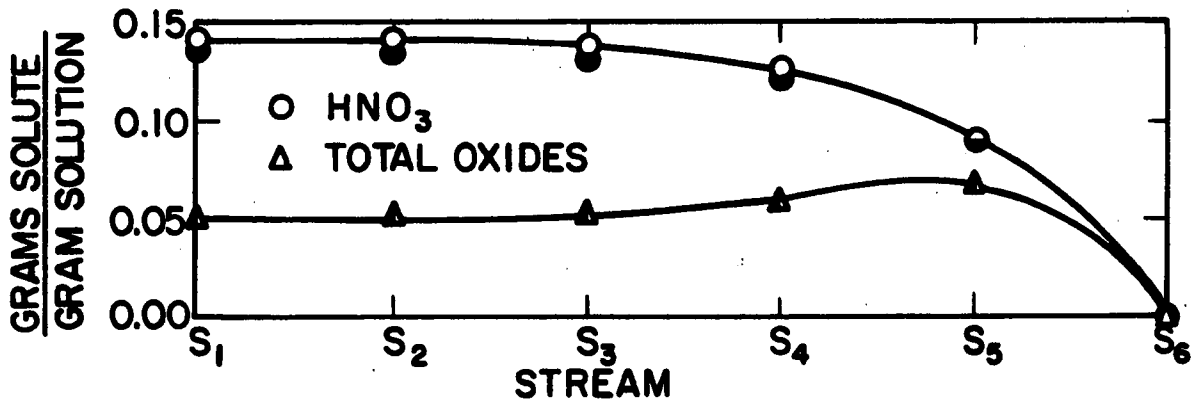


Figure 30. Stagewise organic rare earth oxide and nitric acid concentrations for Simulated Column Experiment IV

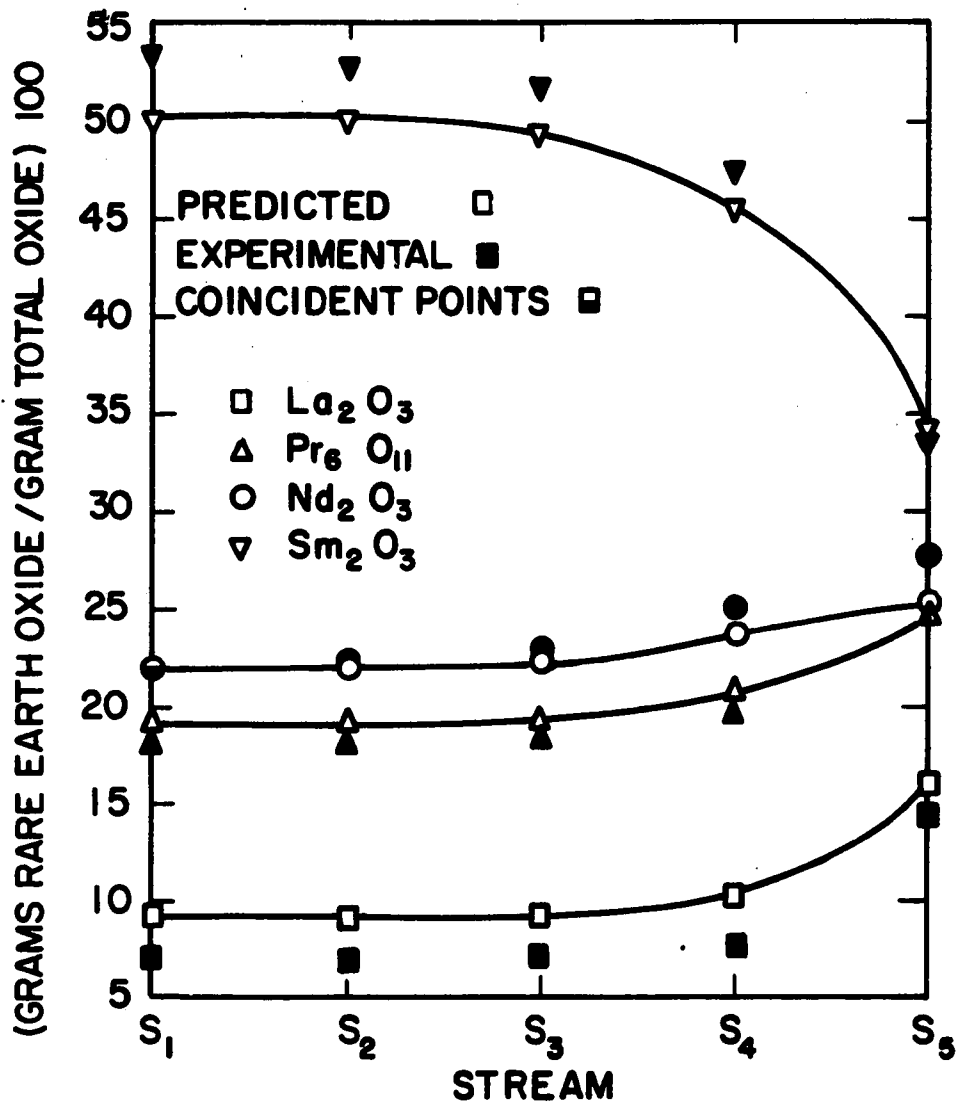


Figure 31. Stagewise organic rare earth oxide composition for Simulated Column Experiment IV

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	0.072	0.888
32	0.172	0.039	0.789	0.069	0.054	0.877
33	0.208	0.014	0.778	0.113	0.026	0.860
34	0.224	0.007	0.770	0.139	0.014	0.847
35	0.201	0.424	0.375	0.068	0.226	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	0.025	0.790
2	0.352	0.021	0.627	0.201	0.029	0.770
3	0.377	0.023	0.600	0.207	0.032	0.762
4	0.355	0.019	0.626	0.205	0.028	0.767
5	0.458	0.023	0.519	0.222	0.037	0.742
6	0.483	0.026	0.491	0.218	0.043	0.739
7	0.454	0.093	0.454	0.142	0.110	0.748
8	0.427	0.076	0.498	0.151	0.091	0.757
9	0.397	0.081	0.522	0.144	0.091	0.764
10	0.370	0.074	0.556	0.146	0.081	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 $\text{Nd}(\text{NO}_3)_3 - \text{Pr}(\text{NO}_3)_3 - \text{HNO}_3 - \text{TBP} - \text{H}_2\text{O}$

	Aqueous phase				Organic phase			
	Grams of $\text{Pr}(\text{NO}_3)_3$ per gram of solution	Grams of $\text{Nd}(\text{NO}_3)_3$ 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

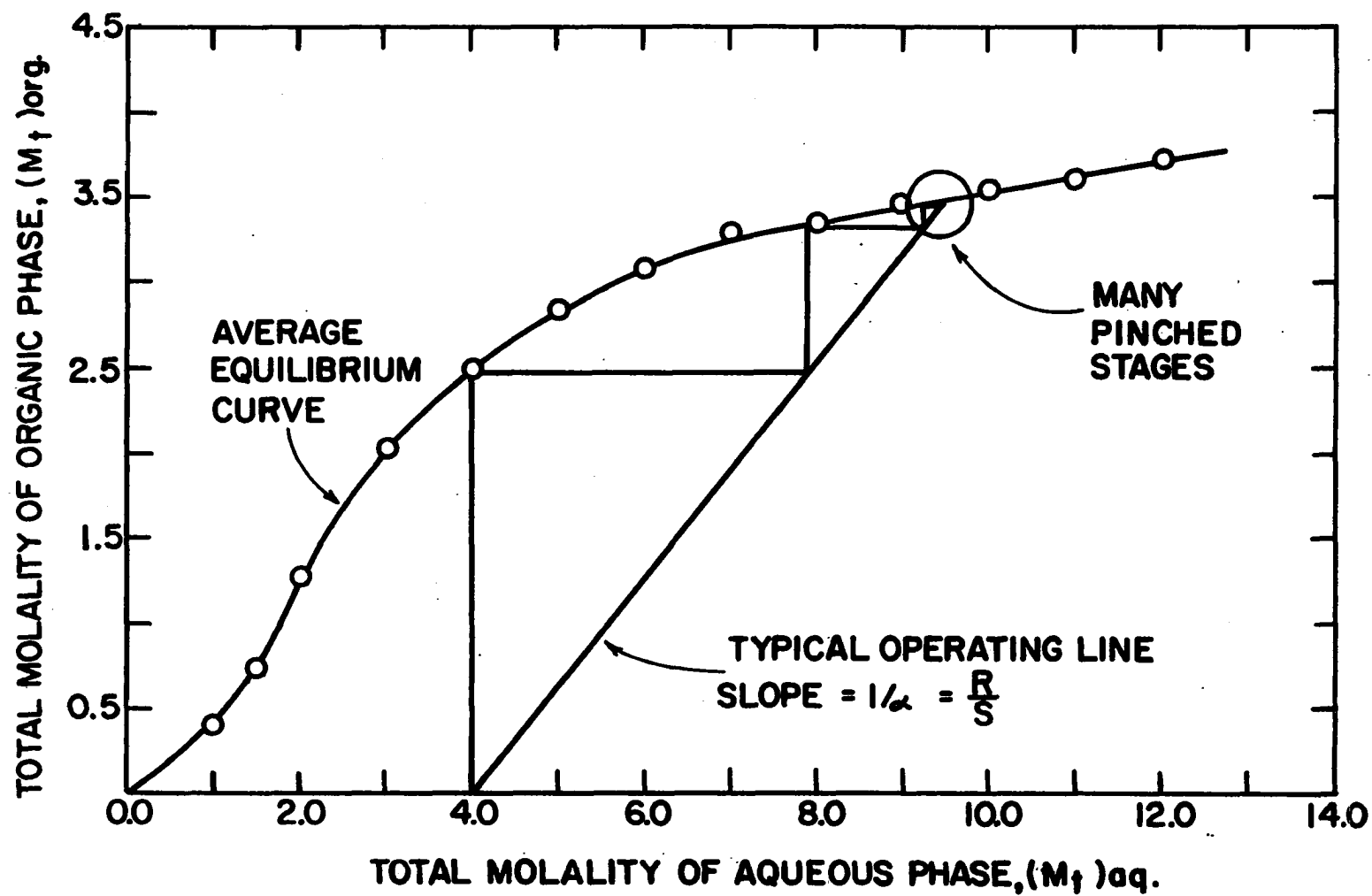


Figure 32. McCabe-Thiele representation of "pinched" total molality

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 $(M_1)_n$ will be inserted for $(M_1)_{S_n}$ 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

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

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

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

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:

$$\begin{aligned}\alpha &= 1.0 & , \\ M_t &= 3.50 & , \\ \beta_{1-Pr} &= 0.43 & , \\ \beta_{2-Pr} &= 1.00 & , \\ (M_t)_{R_1} &= 8.00 & , \\ (M_1)_{R_1} &= 4.00 & , \\ (M_2)_{R_2} &= 4.00 & .\end{aligned}$$

Using these values

$$\begin{aligned}G_{1+} &= -3.472 & , \\ G_{1-} &= -15.344 & , \\ \alpha_1 &= -16.175 & , \\ G_{2+} &= 15.344 & , \\ G_{2-} &= 3.472 & , \\ \alpha_2 &= 12.675 & ,\end{aligned}$$

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

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

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

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 preceding 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 preceding 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.

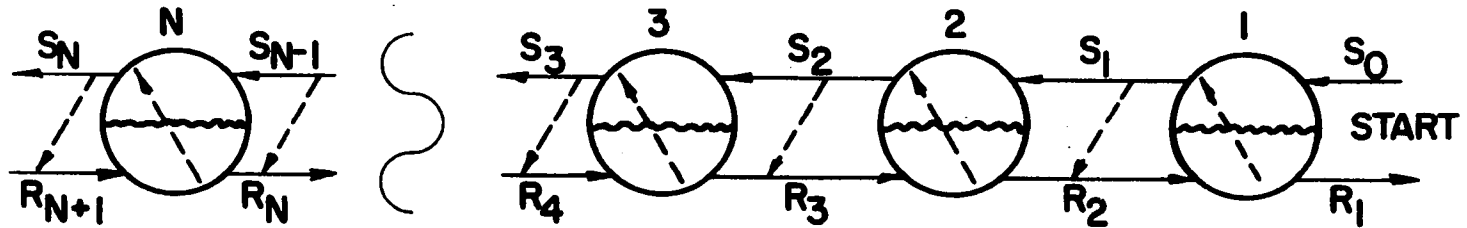


Figure 33. Cascade I

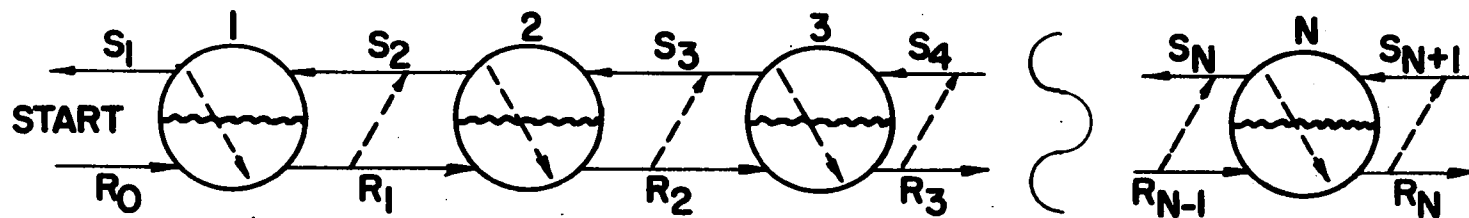


Figure 34. Cascade II

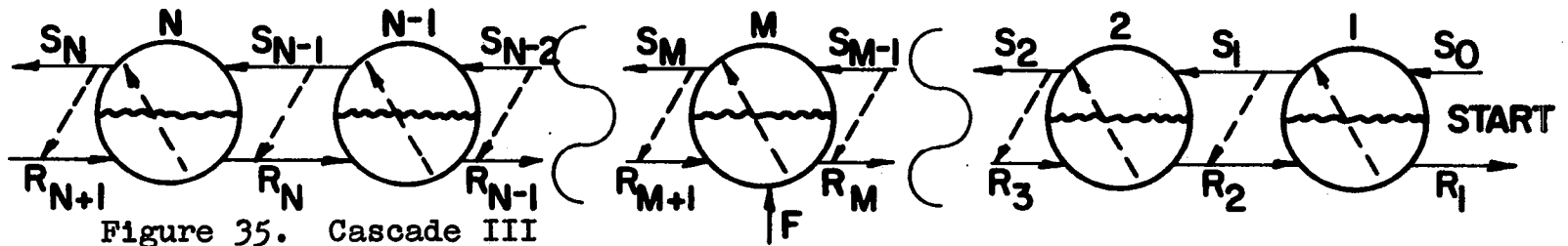


Figure 35. Cascade III

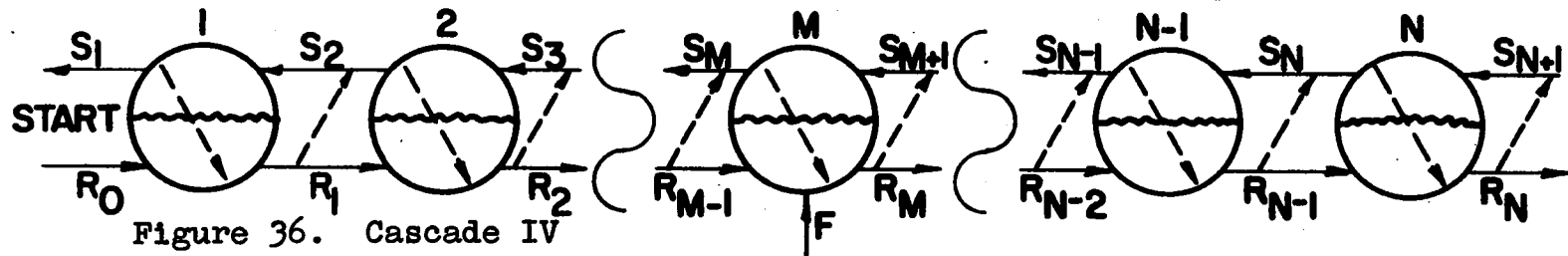


Figure 36. Cascade IV

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 $\text{Pr}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O 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 $\text{Nd}(\text{NO}_3)_3$ - HNO_3 - TBP - H_2O 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

Table 17. 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 $(M_t)_{\text{aq.}}$ and X_{La}

[illegible]

Table 18. Array of values of K_{HNO_3} 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}

[illegible]

Table 19. 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 $(M_t)_{\text{aq.}}$ and X_{Nd}

[illegible]

Table 20. 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 $(M_t)_{\text{aq.}}$ and X_{Sm}

[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 - $(M_{Nd})_{S_0}$

SOSMM - $(M_{Sm})_{S_0}$

For Programs 2 and 4:

ROTM - $(M_t)_{R_0}$

ROAM - $(M_{HNO_3})_{R_0}$

ROLAM - $(M_{La})_{R_0}$

ROPRM - $(M_{Pr})_{R_0}$

RONDM - $(M_{Nd})_{R_0}$

ROSMM - $(M_{Sm})_{R_0}$

SLTM - $(M_t)_{S_1}$

SLAM - $(M_{HNO_3})_{S_1}$

SLLAM - $(M_{La})_{S_1}$

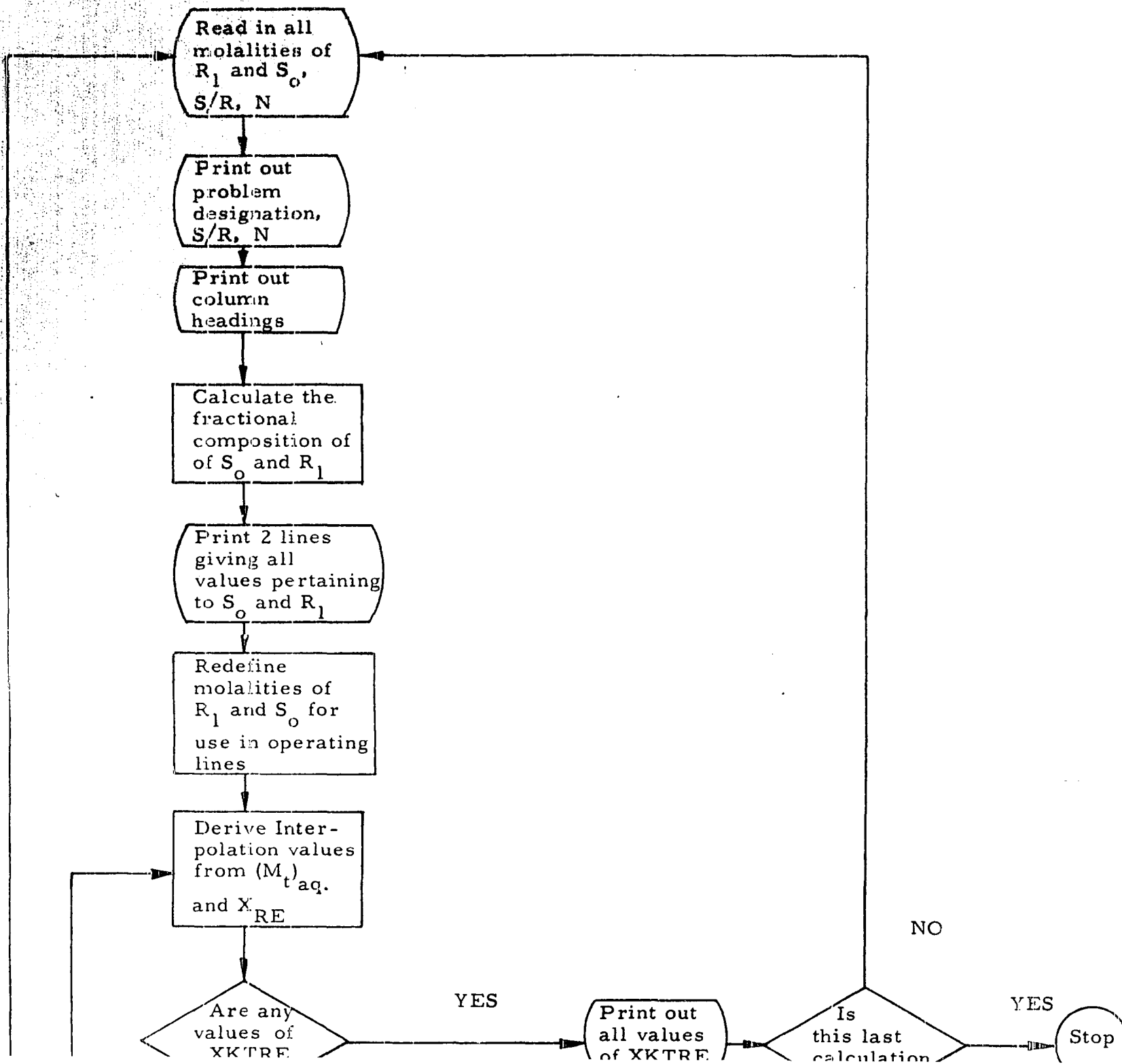
SLPRM - $(M_{Pr})_{S_1}$

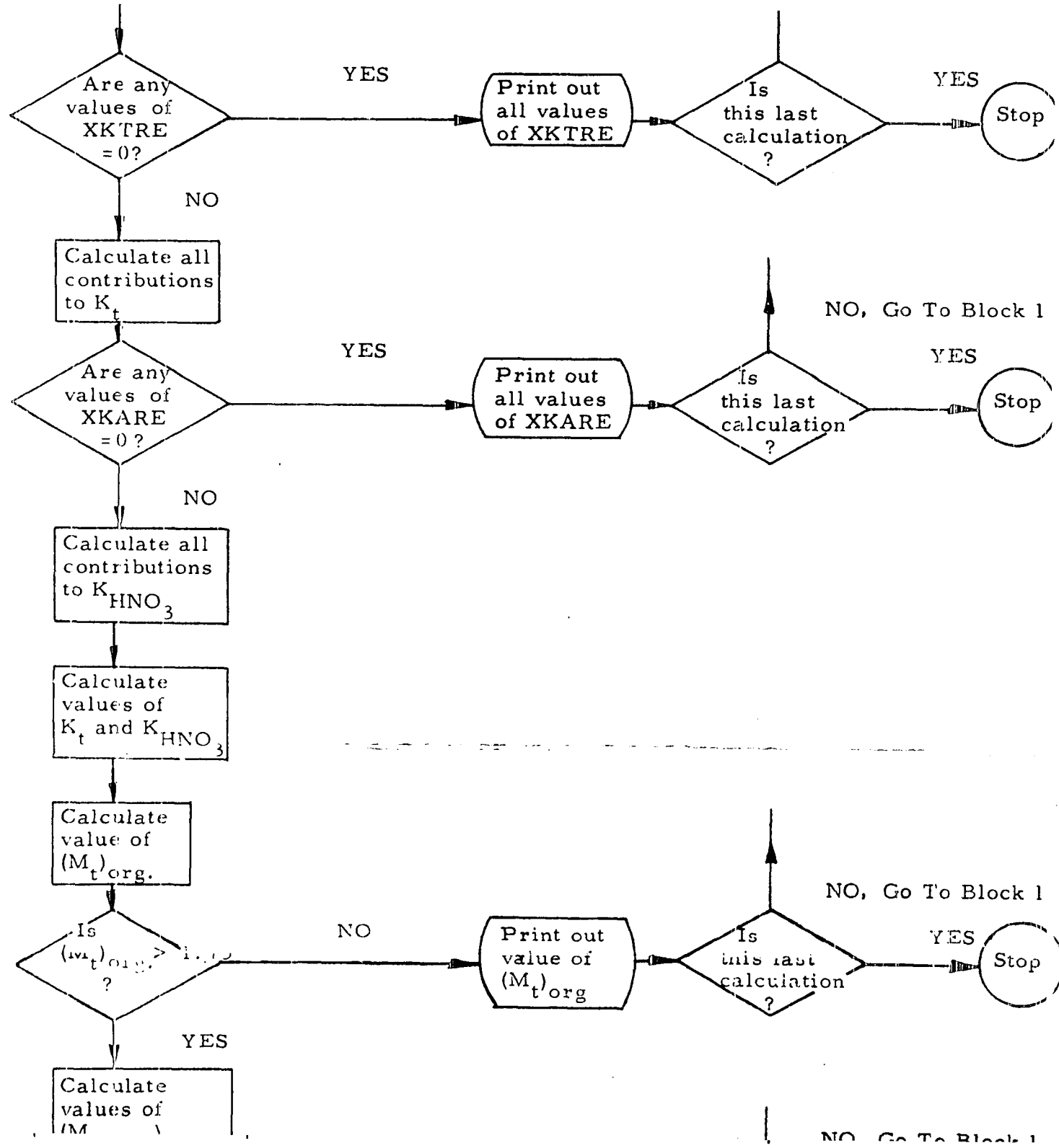
SLNDM - $(M_{Nd})_{S_1}$

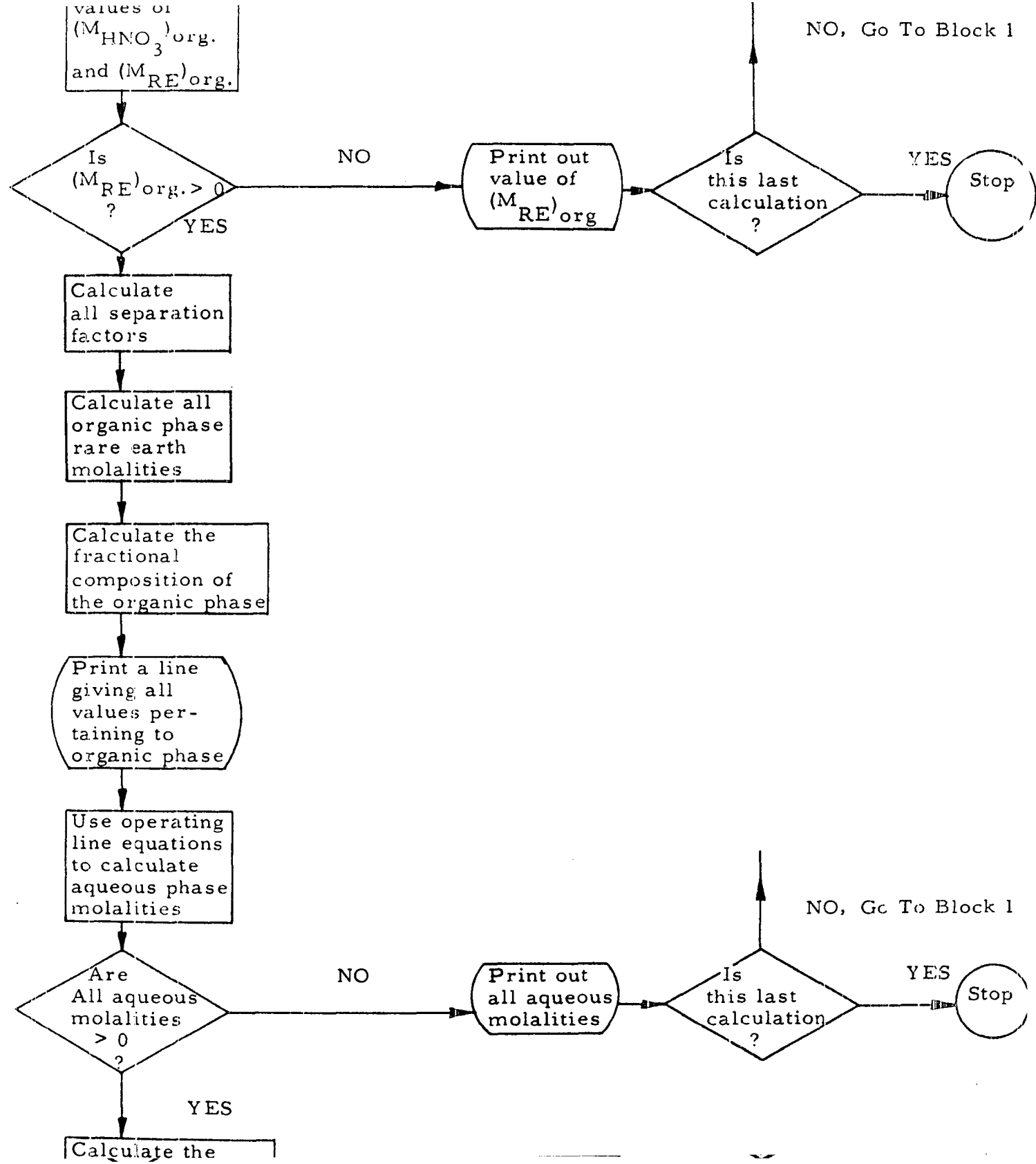
SLSMM - $(M_{Sm})_{S_1}$

Figure 37. (Continued)

Block 1







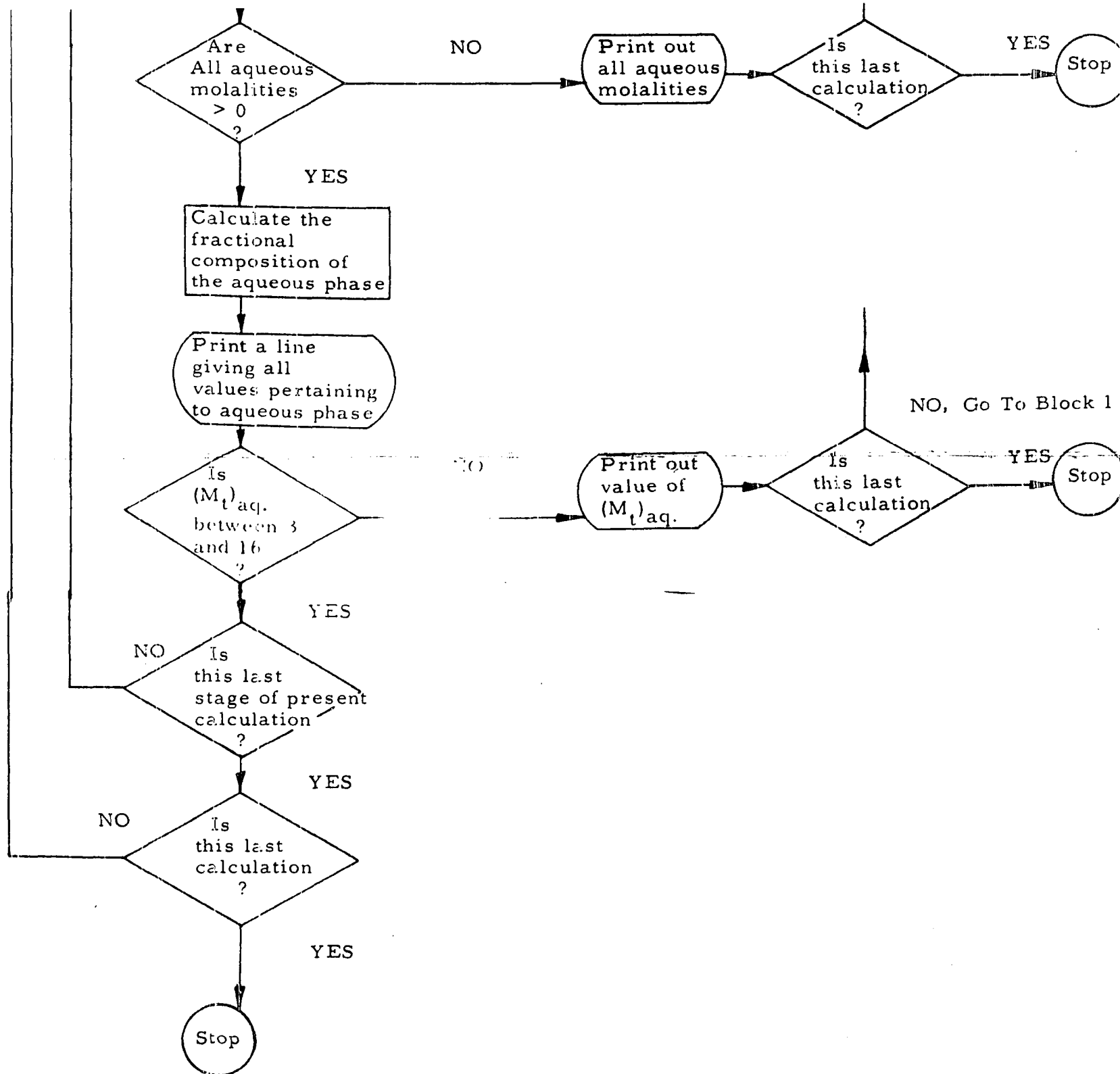


Figure 38. Flow diagram, Program I

```

      DIMENSION XKTLA(21,7),XKTPR(21,7),XKTND(21,7),XKTSH(21,7),XKALA(21,7)
      1,7),XKAPR(21,7),XKAND(21,7),XKASM(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,SMAAQ,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 = SMAAQ/TMAQ
      XRE = REMAQ/TMAQ
      SXA = XHNO3 + XLA + XPR + XND + XSM
      XLASF = XLAMAQ/REMAQ
      XPRSF = PRMAQ/REMAQ
      XNDSF = XNDMAQ/REMAQ
      XSMSF = SMAAQ/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,SMAAQ,REMAQ,XHNO3,XLA,XPR
      1,XND,XSM,XRE,XLASF,XPRSF,XNDSF,XSMSF,SXA,SXREA
      RITH = TMAQ
      RIAM = AMAQ
      RILAM = XLAMAQ
      RIPRM = PRMAQ
      RINDM = XNDMAQ
      RISMM = SMAAQ
      SOTH = TMOR
      SOAM = AMOR
      SOLAM = XLAMOR
      SOPRM = PRMOR
      SONDM = XNDMOR

```

Figure 39. Fortran statements, Program I

```

50      SOSMH = SMHOR                                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),
2XKTN(IX,KZ),XKTN(IX+1,KZ),XKTN(IX,KZ+1),XKTN(IX+1,KZ+1),XKTS(IX,KZ),
3IX,KZ),XKTS(IX+1,KZ),XKTS(IX,KZ+1),XKTS(IX+1,KZ+1))
      IF(SKT) 85,85,90                                BMS1 099
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),
2KTN(IX,KZ),XKTN(IX+1,KZ),XKTN(IX,KZ+1),XKTN(IX+1,KZ+1),XKTS(IX,KZ),
3X,KZ),XKTS(IX+1,KZ),XKTS(IX,KZ+1),XKTS(IX+1,KZ+1),TMAQ,XRE
      IF(K) 495,495,45                                BMS1 104
90      XKTLA1 = XKTLA(IX,KZ)*(1.0 - FRX) + XKTLA(IX+1,KZ)*FRX
      XKTLA2 = XKTLA(IX,KZ+1)*(1.0 - FRX) + XKTLA(IX+1,KZ+1)*FRX
      XKTLA3 = XKTLA1*(1.0 - FRZ) + XKTLA2*FRZ
      CKTLA = XKTLA3 * XLASF
      XKTPR1 = XKTPR(IX,KZ)*(1.0 - FRX) + XKTPR(IX+1,KZ)*FRX
      XKTPR2 = XKTPR(IX,KZ+1)*(1.0 - FRX) + XKTPR(IX+1,KZ+1)*FRX
      XKTPR3 = XKTPR1*(1.0 - FRZ) + XKTPR2*FRZ
      CKTPR = XKTPR3 * XPRSF
      XKTN1 = XKTN(IX,KZ)*(1.0 - FRX) + XKTN(IX+1,KZ)*FRX
      XKTN2 = XKTN(IX,KZ+1)*(1.0 - FRX) + XKTN(IX+1,KZ+1)*FRX
      XKTN3 = XKTN1*(1.0 - FRZ) + XKTN2*FRZ
      CKTN = XKTN3 * XNDSF
      XKTS1 = XKTS(IX,KZ)*(1.0 - FRX) + XKTS(IX+1,KZ)*FRX
      XKTS2 = XKTS(IX,KZ+1)*(1.0 - FRX) + XKTS(IX+1,KZ+1)*FRX
      XKTS3 = XKTS1*(1.0 - FRZ) + XKTS2*FRZ
      CKTS = XKTS3 * XSMSF
      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),
2XKAND(IX,KZ),XKAND(IX+1,KZ),XKAND(IX,KZ+1),XKAND(IX+1,KZ+1),XKAS(IX,KZ),
3IX,KZ),XKAS(IX+1,KZ),XKAS(IX,KZ+1),XKAS(IX+1,KZ+1))
      IF(SKA) 95,95,100                                BMS1 125
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),
2KAND(IX,KZ),XKAND(IX+1,KZ),XKAND(IX,KZ+1),XKAND(IX+1,KZ+1),XKAS(IX,KZ),
3X,KZ),XKAS(IX+1,KZ),XKAS(IX,KZ+1),XKAS(IX+1,KZ+1),TMAQ,XRE
      IF(K) 495,495,45                                BMS1 130
100     XKALA1 = XKALA(IX,KZ)*(1.0 - FRX) + XKALA(IX+1,KZ)*FRX
      XKALA2 = XKALA(IX,KZ+1)*(1.0 - FRX) + XKALA(IX+1,KZ+1)*FRX
      XKALA3 = XKALA1*(1.0 - FRZ) + XKALA2*FRZ
      CKALA = XKALA3 * XLASF
      XKAPR1 = XKAPR(IX,KZ)*(1.0 - FRX) + XKAPR(IX+1,KZ)*FRX
      XKAPR2 = XKAPR(IX,KZ+1)*(1.0 - FRX) + XKAPR(IX+1,KZ+1)*FRX
      XKAPR3 = XKAPR1*(1.0 - FRZ) + XKAPR2*FRZ
      CKAPR = XKAPR3 * XPRSF
      XKAND1 = XKAND(IX,KZ)*(1.0 - FRX) + XKAND(IX+1,KZ)*FRX
      XKAND2 = XKAND(IX,KZ+1)*(1.0 - FRX) + XKAND(IX+1,KZ+1)*FRX

```

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 = XLAMQ*BLAPR + PRMAQ*BPRPR + XNDMAQ*BNDPR + SMMAQ*BSMPR	BMS1 162
	XLAMOR = REMOR*BLAPR*XLAMQ/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
	YNDSE = XNDMOR/REMOR	BMS1 176
	YSMSF = SMMOR/REMOR	BMS1 177
	SYREQ = YLASF + YPRSF + YNDSE + YSMSF	BMS1 178
	PRINT 511,L, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,YHNO3,YLA,YPBMS1 179	
	IR,YND,YSM,YRE,YLASF,YPRSF,YNDSE,YSMSF,SYO,SYREQ	BMS1 180
	TMAQ = TMOR*SOVR - SOTM*SOVR + RITM	BMS1 181
	AMAQ = AMOR*SOVR - SOAM*SOVR + RIAM	BMS1 182
	XLAMQ = XLAMOR*SOVR - SOLAM*SOVR + RILAM	BMS1 183
	PRMAQ = PRMOR*SOVR - SOPRM*SOVR + RIPRM	BMS1 184
	XNDMAQ = XNDMOR*SOVR - SONDM*SOVR + RINDM	BMS1 185
	SMMAQ = SMMOR*SOVR - SOSMM*SOVR + RISMM	BMS1 186
	REMAQ = TMAQ - AMAQ	BMS1 187
	SAM = MIN1F(TMAQ,AMAQ,XLAMQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ)	BMS1 188
	IF(SAM) 125,125,130	BMS1 189
125	PRINT 512,TMAQ,AMAQ,XLAMQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ	BMS1 190
	IF(K) 495,495,45	BMS1 191
130	XHNO3 = AMAQ/TMAQ	BMS1 192
	XLA = XLAMQ/TMAQ	BMS1 193
	XPR = PRMAQ/TMAQ	BMS1 194
	XND = XNDMAQ/TMAQ	BMS1 195
	XSM = SMMAQ/TMAQ	BMS1 196
	XRE = REMAQ/TMAQ	BMS1 197
	XSA = XHNO3 + XLA + XPR + XND + XSM	BMS1 198
	XLASF = XLAMQ/REMAQ	BMS1 199
	XPRSF = PRMAQ/REMAQ	BMS1 200
	XNDSE = XNDMAQ/REMAQ	BMS1 201
	XSMSF = SMMAQ/REMAQ	BMS1 202

Figure 39. (Continued)

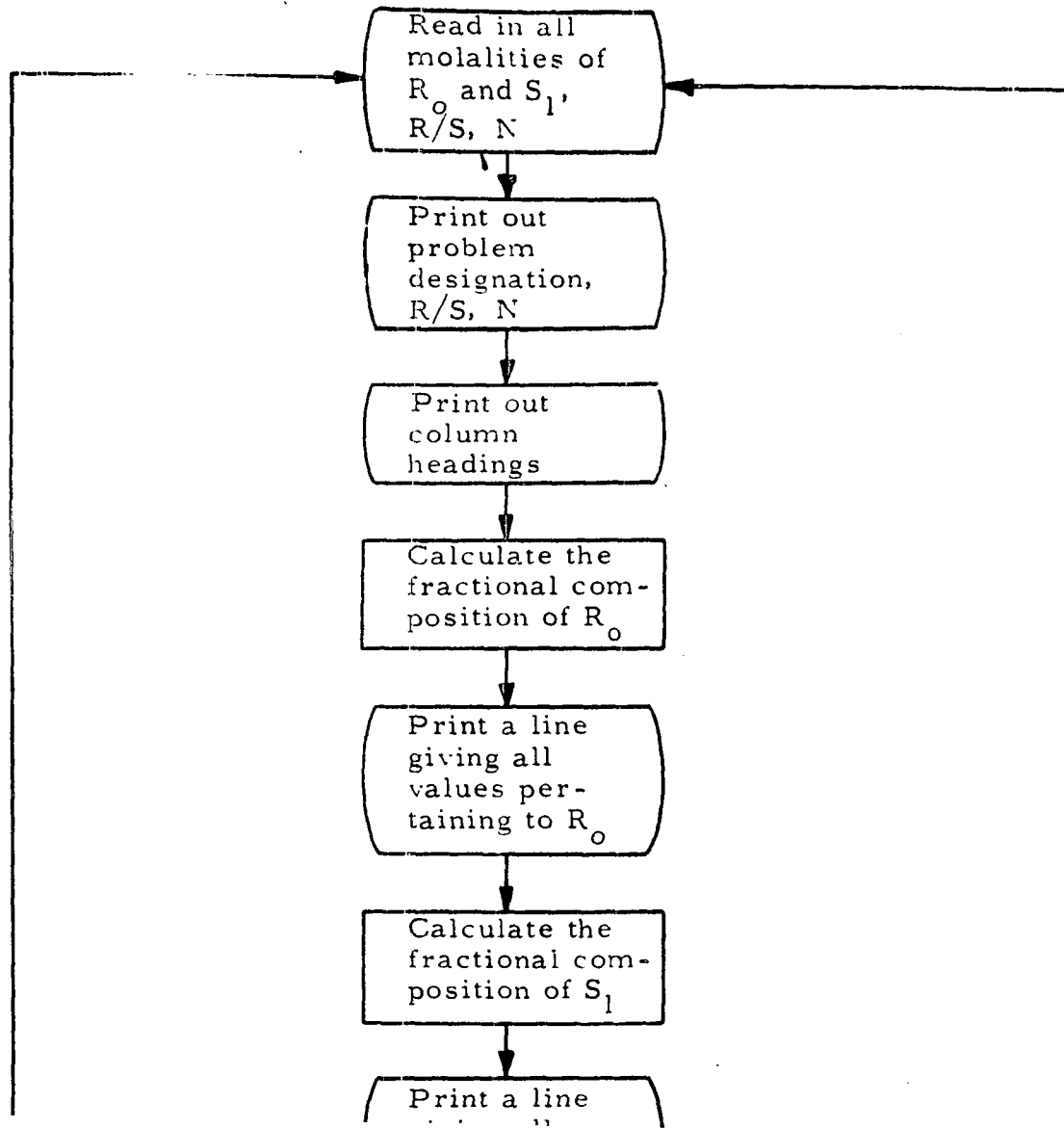
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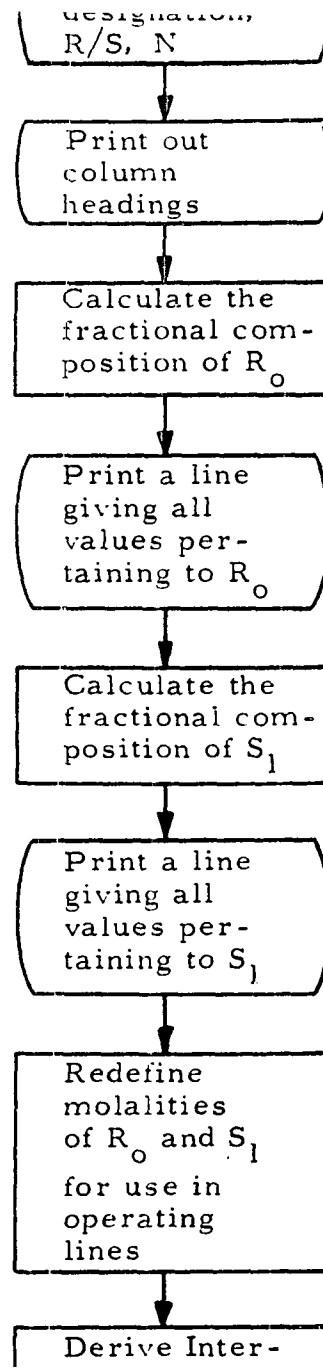
SXREA = XLASF + XPRSF + XNDSF + XSMSF
LL = L+1
PRINT 513,LL,TMAQ,AM AQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ,XHNO3,XLA,XBMS1 203
1 PR,XND,XSM,XRE,XLASF,XPRSF,XNDSF,XSMSF,SXA,SXREA
IF(TMAQ - 3.0) 135,140,140
135 PRINT 514, TMAQ
IF(K) 495,495,45
140 IF(TMAQ - 16.0) 150,145,145
145 PRINT 514,TMAQ
IF(K) 495,495,45
150 CONTINUE
IF(K)495,495,45
500 FORMAT (7F10.3)
501 FORMAT (7F9.4)
502 FORMAT (7F7.4,F8.4,I3,I3)
503 FORMAT (31H1EXTRACT SIDE CALCULATION SOVR= F8.4,4H N= I3)
504 FORMAT (120HJ TOTALMOLHNO3 MOL LA MOL PR MOL ND MOL SM MOL
1RE MOL ACFR LAFR PRFR NDFR SMFR REFRLA/REPR/REND/RESM/RE STFRSREFR
2)
505 FORMAT (4HJS 0 7F8.4,12F5.3)
506 FORMAT (4H R 1 7F8.4,12F5.3)
507 FORMAT (8HJXKTRE=0 16F6.3,F8.4,F6.3)
508 FORMAT (8HJXKARE=0 16F6.3,F8.4,F6.3)
509 FORMAT (6HJTMOR= F10.4,6H TMAQ= F8.4,6H TOTK= F8.4)
510 FORMAT (6HJTMOR= F10.4,6H AMOR= F10.8,7H REMOR= F10.8,7H HNO3K= F10.8)
511 FORMAT (2HJS I2,7F8.4,12F5.3)
512 FORMAT (6HJTMAQ= F10.4,6H AMAQ= F10.4,8H XLAMAQ= F10.4,7H PRMAQ= F10.4,8H XNDMAQ= F10.4,7H SMMAQ= F10.4,7H REMAQ= F10.4)
513 FORMAT (2H R I2,7F8.4,12F5.3)
514 FORMAT (6HJTMAQ= F10.4)
495 STOP 89
END

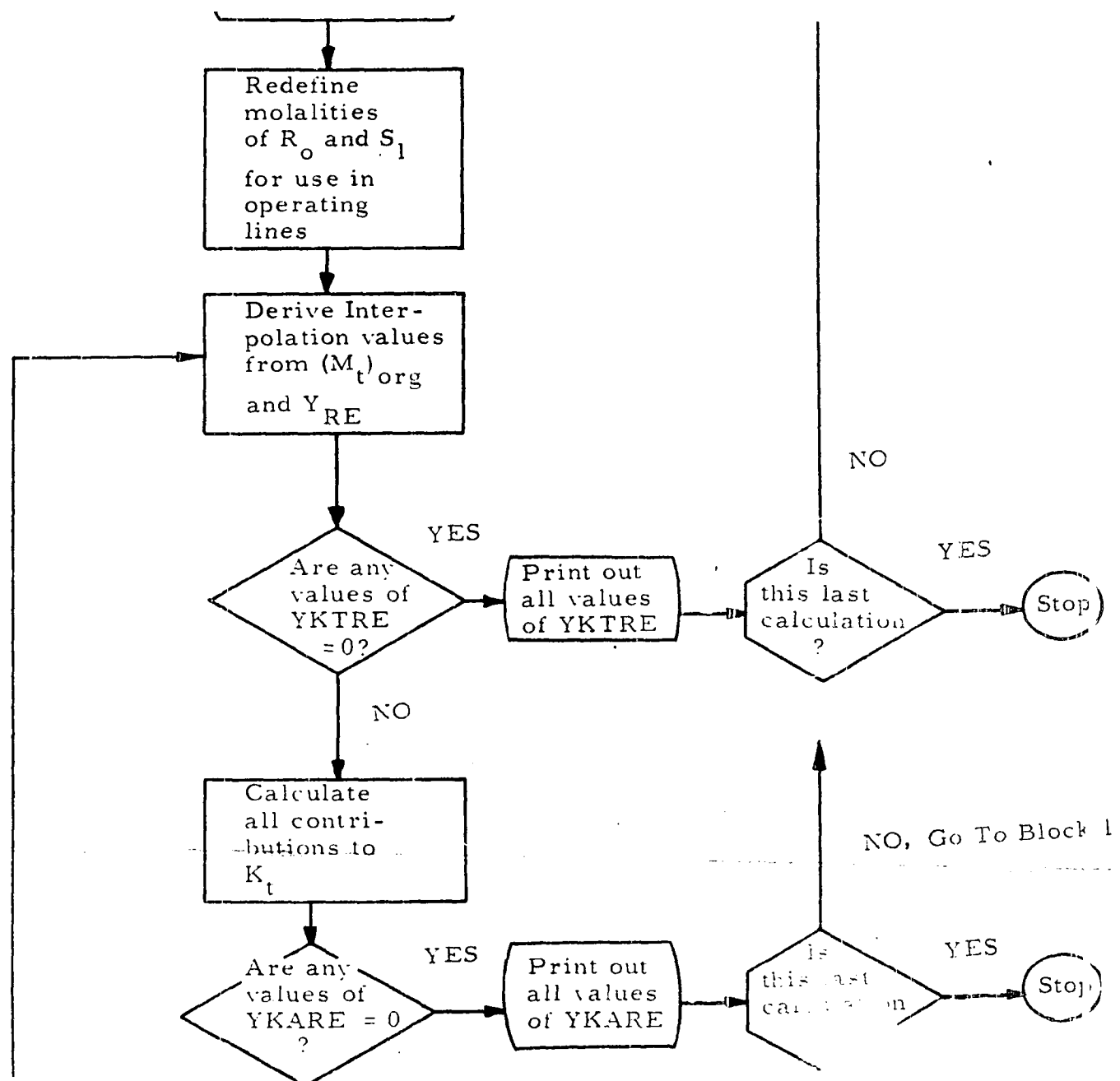
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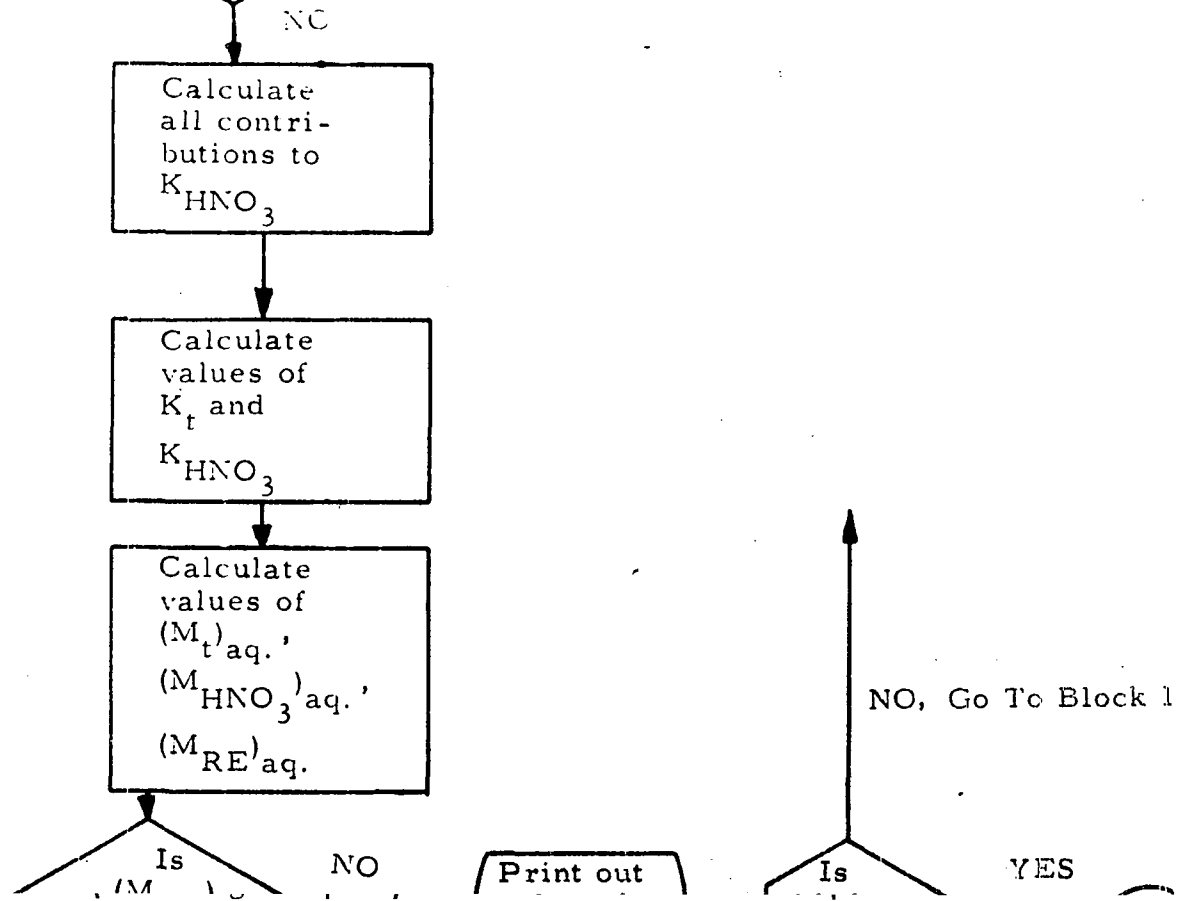
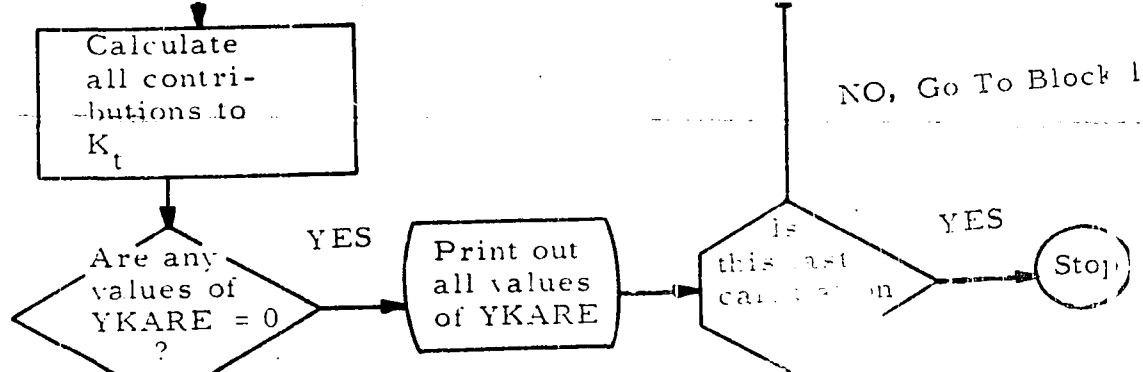
Figure 39. (Continued)

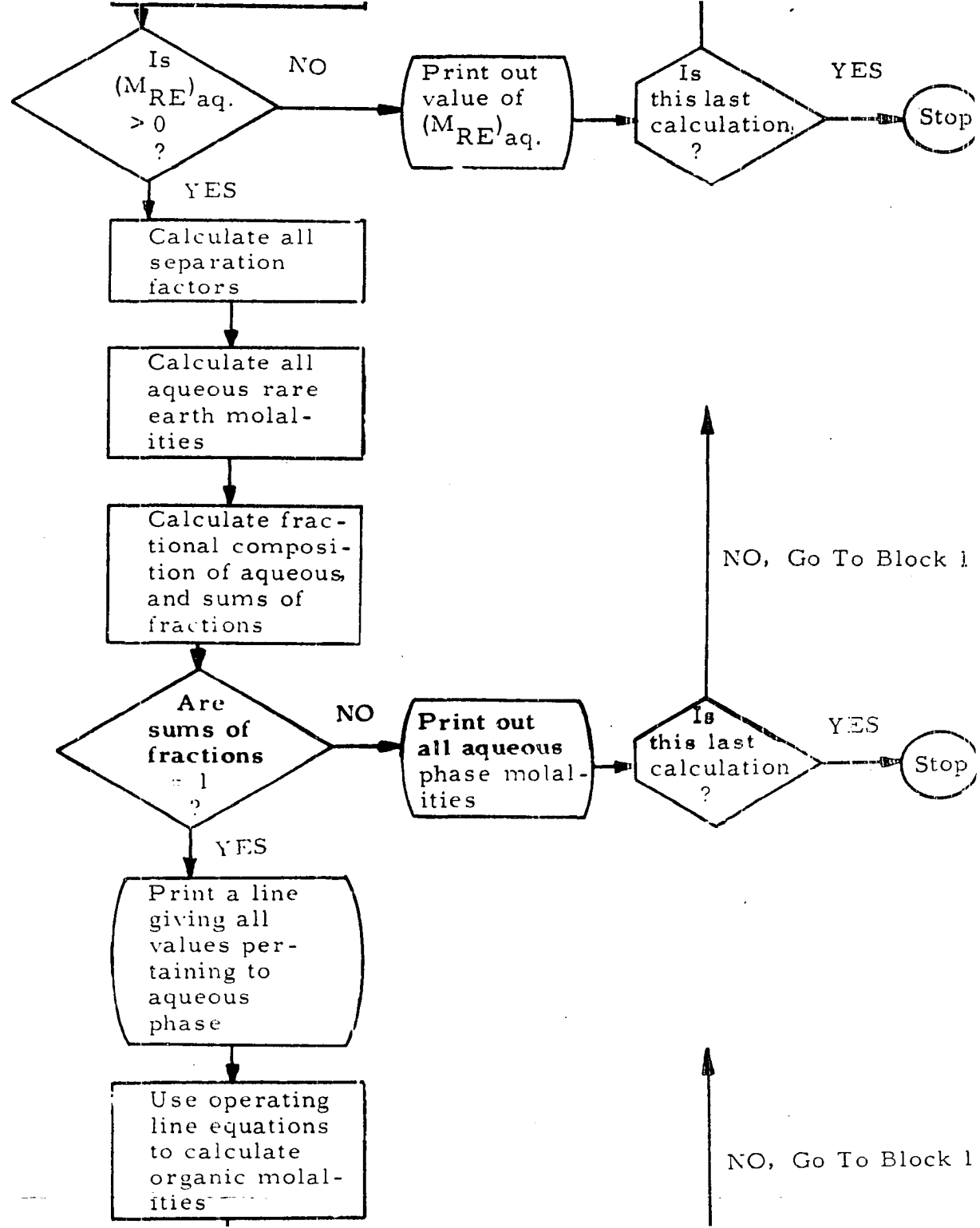
Block 1

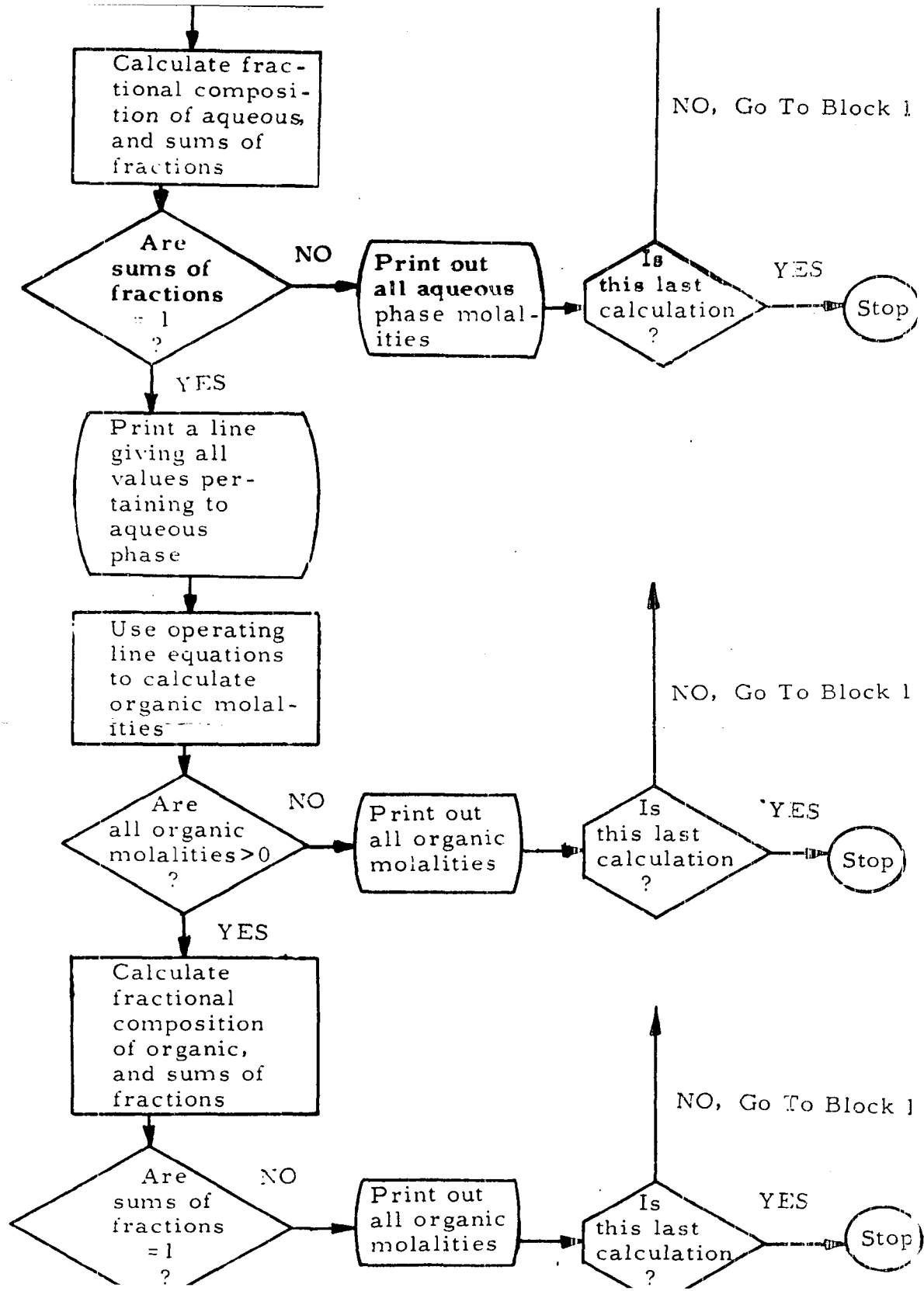


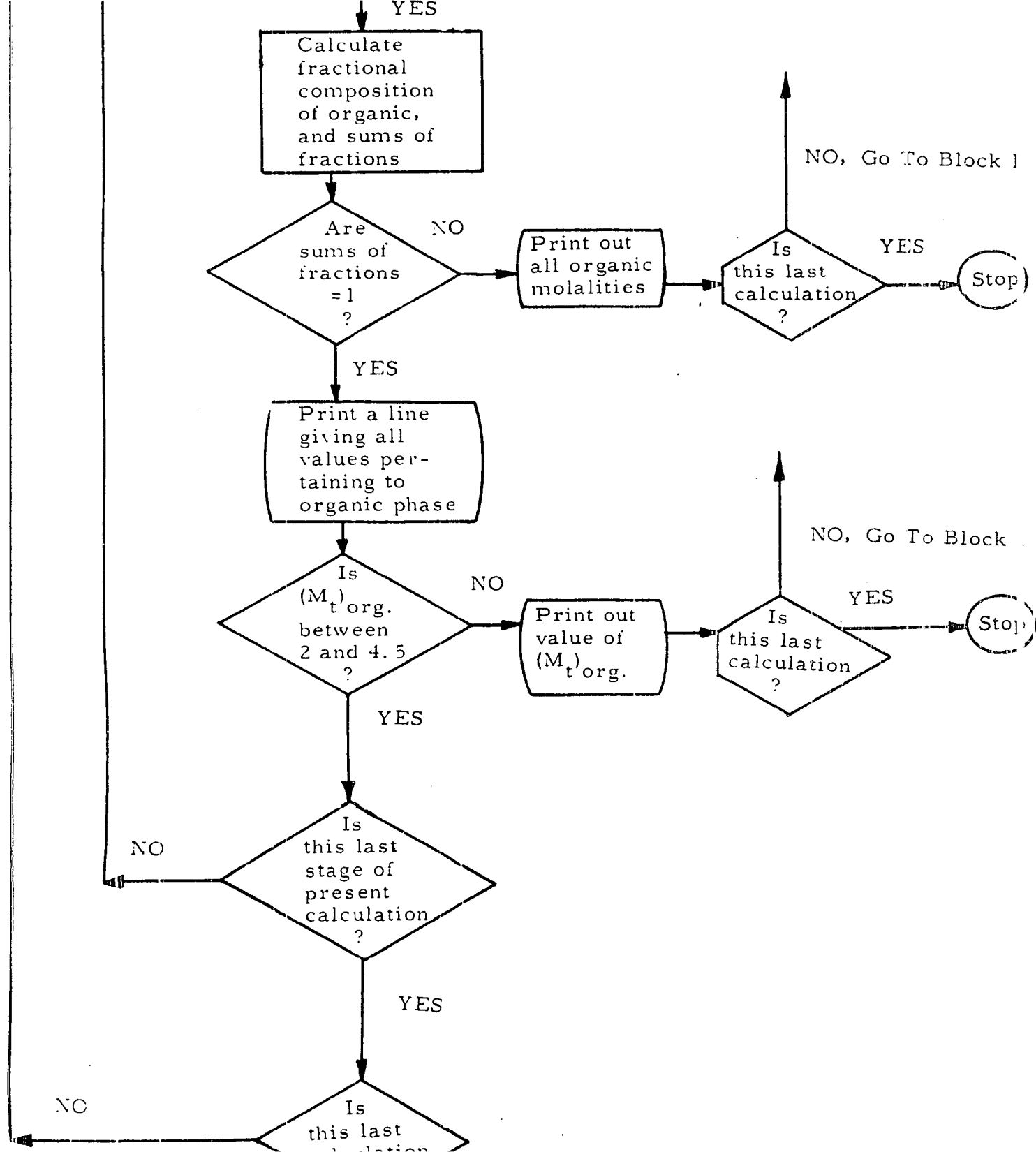












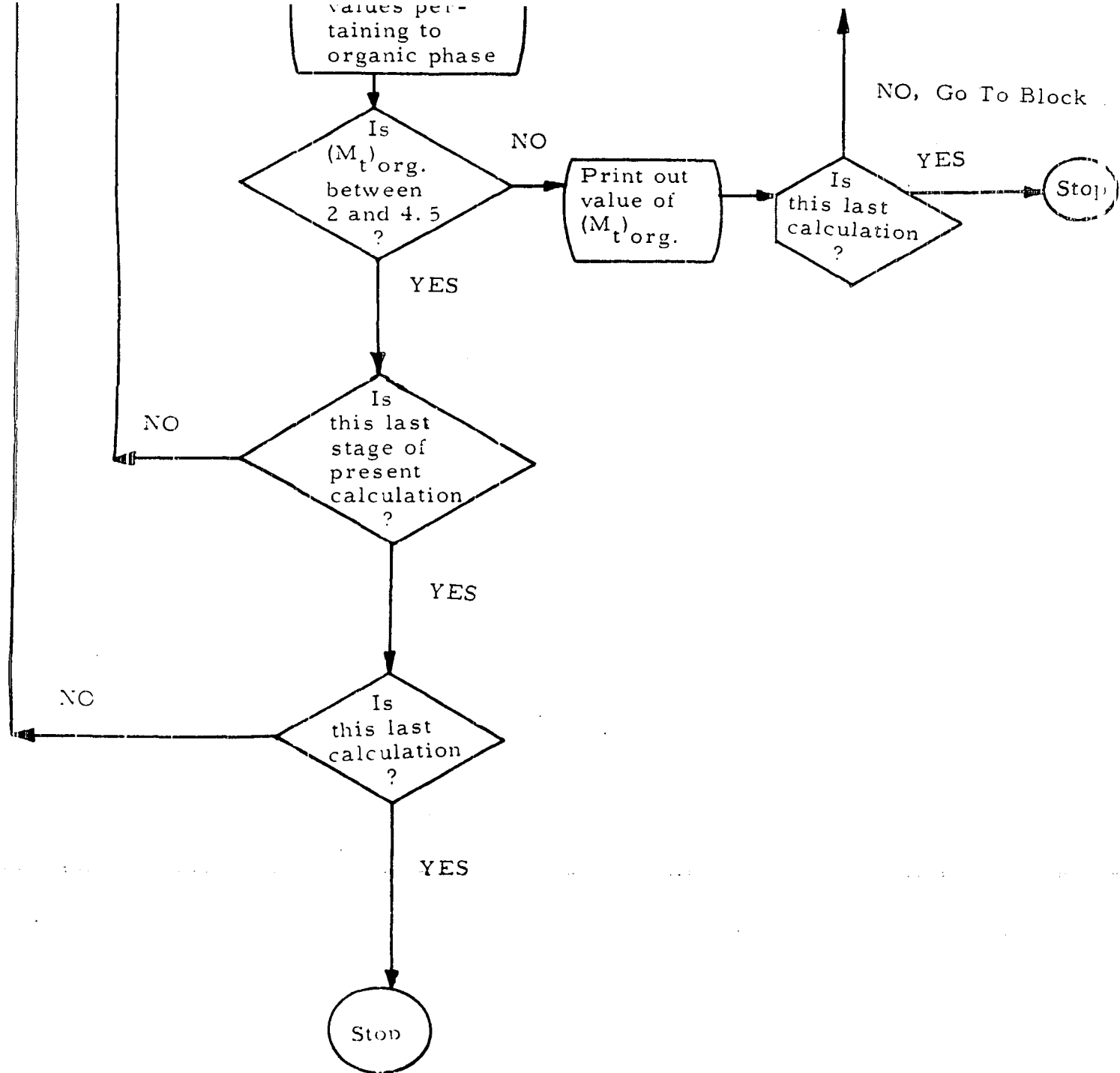


Figure 40. Flow diagram, Program II

```

      DIMENSION YKTLA(21,6),YKTPR(21,6),YKTND(21,6),YKTSM(21,6),YKALA(21,6)  BMS2 001
      1,6),YKAPR(21,6),YKAND(21,6),YKASM(21,6)  BMS2 002
      DO 5 I = 1,21  BMS2 003
5      READ INPUT TAPE 5, 500, (YKTLA(I,J),J = 1,6)  BMS2 004
      DO 10 I = 1,21  BMS2 005
10     READ INPUT TAPE 5, 500, (YKTPR(I,J),J = 1,6)  BMS2 006
      DO 15 I = 1,21  BMS2 007
15     READ INPUT TAPE 5, 500, (YKTND(I,J),J = 1,6)  BMS2 008
      DO 20 I = 1,21  BMS2 009
20     READ INPUT TAPE 5, 500, (YKTSM(I,J),J = 1,6)  BMS2 010
      DO 25 I = 1,21  BMS2 011
25     READ INPUT TAPE 5, 500, (YKALA(I,J),J = 1,6)  BMS2 012
      DO 30 I = 1,21  BMS2 013
30     READ INPUT TAPE 5, 500, (YKAPR(I,J),J = 1,6)  BMS2 014
      DO 35 I = 1,21  BMS2 015
35     READ INPUT TAPE 5, 500, (YKAND(I,J),J = 1,6)  BMS2 016
      DO 40 I = 1,21  BMS2 017
40     READ INPUT TAPE 5, 500, (YKASM(I,J),J = 1,6)  BMS2 018
45     READ INPUT TAPE 5, 501, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMMAQ,REMAQ  BMS2 019
      READ INPUT TAPE 5, 502, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,  BMS2 020
      IR(IVS,N,K)  BMS2 021
      PRINT 503, ROVS,N  BMS2 022
      PRINT 504  BMS2 023
      IF(TMAQ) 600,65,50  BMS2 024
50     XHNO3 = AMAQ/TMAQ  BMS2 025
      XLA = XLAMAQ/TMAQ  BMS2 026
      XPR = PRMAQ/TMAQ  BMS2 027
      XND = XNDMAQ/TMAQ  BMS2 028
      XSM = SMMMAQ/TMAQ  BMS2 029
      XRE = REMAQ/TMAQ  BMS2 030
      IF(REMAQ) 600,60,55  BMS2 031
55     XLASF = XLAMAQ/REMAQ  BMS2 032
      XPRSF = PRMAQ/REMAQ  BMS2 033
      XNDSF = XNDMAQ/REMAQ  BMS2 034
      XSMSF = SMMMAQ/REMAQ  BMS2 035
      PRINT 505, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMMAQ,REMAQ,XHNO3,XLA,XPR  BMS2 036
      1,XND,XSM,XRE,XLASF,XPRSF,XNDSF,XSMSF  BMS2 037
      GO TO 70  BMS2 038
60     PRINT 506, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMMAQ,REMAQ,XHNO3,XLA,XPR  BMS2 039
      1,XND,XSM,XRE  BMS2 040
      GO TO 70  BMS2 041
65     PRINT 507, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMMAQ,REMAQ  BMS2 042
70     YHNO3 = AMOR/TMOR  BMS2 043
      YLA = XLAMOR/TMOR  BMS2 044
      YPR = PRMOR/TMOR  BMS2 045
      YND = XNDMOR/TMOR  BMS2 046
      YSM = SMMOR/TMOR  BMS2 047
      YRE = REMOR/TMOR  BMS2 048
      YLASF = XLAMOR/REHOR  BMS2 049
      YPRSF = PRMOR/REMOR  BMS2 050
      YNDSF = XNDMOR/REMOR  BMS2 051
      YSMSF = SMMOR/REMOR  BMS2 052
      PRINT 508, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,YHNO3,YLA,YPR  BMS2 053
      1,YND,YSM,YRE,YLASF,YPRSF,YNDSF,YSMSF  BMS2 054
      ROTM = TMAQ  BMS2 055
      ROAM = AMAQ  BMS2 056
      RCLAM = XLAMAQ  BMS2 057
      ROPRM = PRMAQ  BMS2 058
      RNDM = XNDMAQ  BMS2 059
      ROSMM = SMMMAQ  BMS2 060
      S1TM = TMOR  BMS2 061
      S1AM = AMOR  BMS2 062

```

Figure 41. Fortran statements, Program II

```

SILAM = XLAMOR                                BMS2 063
SIPRM = PRMOR                                  BMS2 064
SINDM = XNDMOR                                BMS2 065
SISMM = SMMOR                                  BMS2 066
DO 165 I = 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 = (TMOR*10.0 - 15.0)/5.0                    BMS2 072
KZ = Z                                          BMS2 073
ZK = KZ                                         BMS2 074
FRZ = Z - ZK                                   BMS2 075
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)) BMS2 076
1KZ+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 077
2YKTND(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 078
3IY,KZ),YKTSM(IY+1,KZ),YKTSM(IY,KZ+1),YKTSM(IY+1,KZ+1)) BMS2 079
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
1Z+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 082
2KTND(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 083
3Y,KZ),YKTSM(IY+1,KZ),YKTSM(IY,KZ+1),YKTSM(IY+1,KZ+1),TMOR,YRE BMS2 084
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 = 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)) BMS2 102
1KZ+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 103
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)) BMS2 104
3IY,KZ),YKASM(IY+1,KZ),YKASM(IY,KZ+1),YKASM(IY+1,KZ+1)) BMS2 105
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
1Z+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 108
2KAND(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 109
3Y,KZ),YKASM(IY+1,KZ),YKASM(IY,KZ+1),YKASM(IY+1,KZ+1),TMOR,YRE BMS2 110
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

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Figure 41. (Continued)

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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 + CKTSH                             BMS2 128
HNO3K = CKALA + CKAPR + CKAND + CKASM                             BMS2 129
TMAQ = TMOR/TOTK                                                  BMS2 130
AMAQ = AMOR/HNO3K                                                 BMS2 131
REMAQ = TMAQ - AMAQ                                               BMS2 132
IF (REMAQ) 95,95,100                                             BMS2 133
95  PRINT 511, TMAQ,AMAQ,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
    XLAMAQ = 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 = XLAMAQ/TMAQ                                             BMS2 146
    XPR = PRMAQ/TMAQ                                             BMS2 147
    XND = XNDMAQ/TMAQ                                             BMS2 148
    XSM = SMMAQ/TMAQ                                             BMS2 149
    XRE = REMAQ/TMAQ                                             BMS2 150
    XLASF = XLAMAQ/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,AMAQ,XLAMAQ,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,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ      BMS2 163
    IF (K) 600,600,45                                             BMS2 164
130  PRINT 514, L, TMAQ,AMAQ,XLAMAQ,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 = XLAMAQ*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 = MIN1F(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)

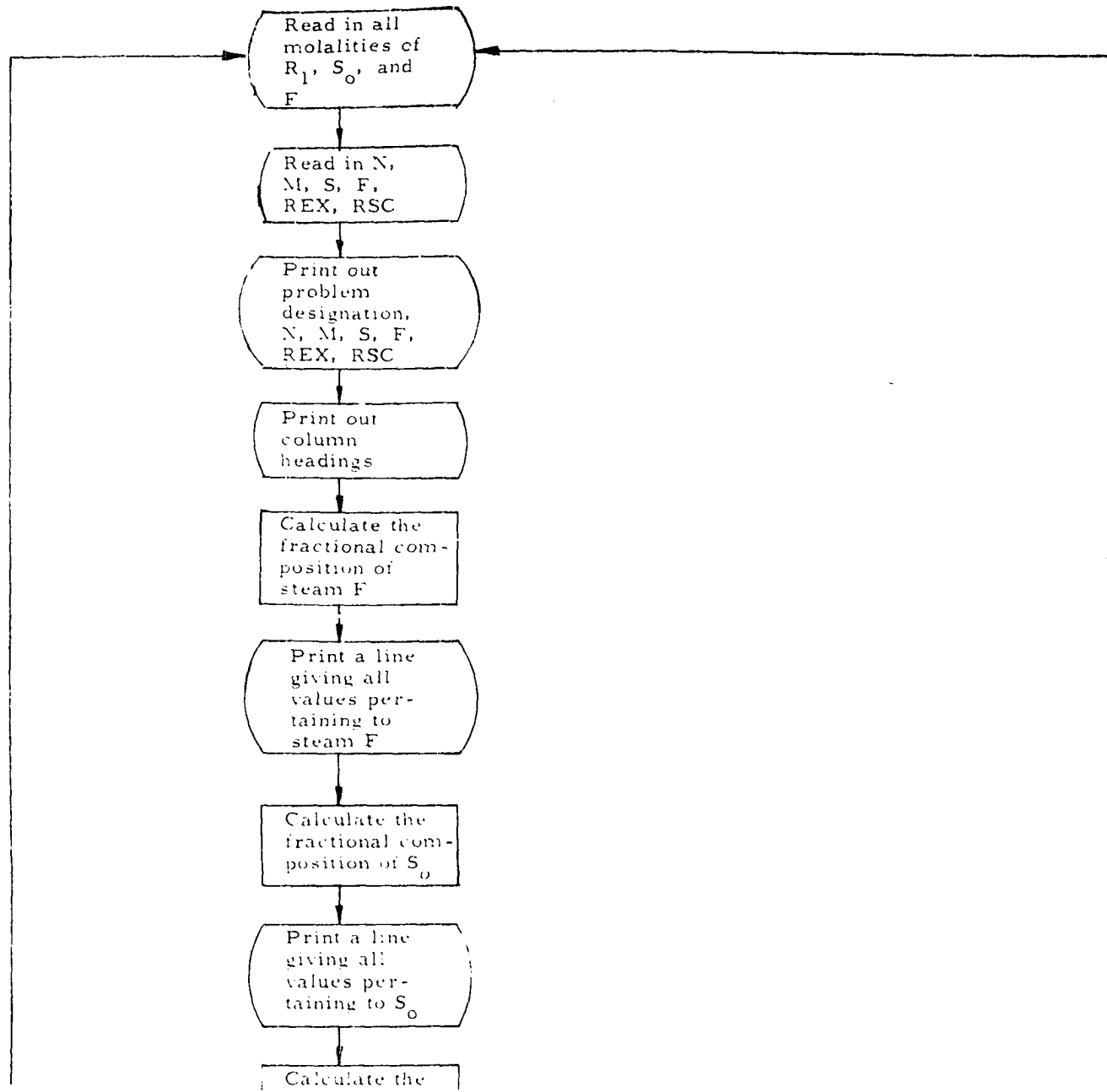
```

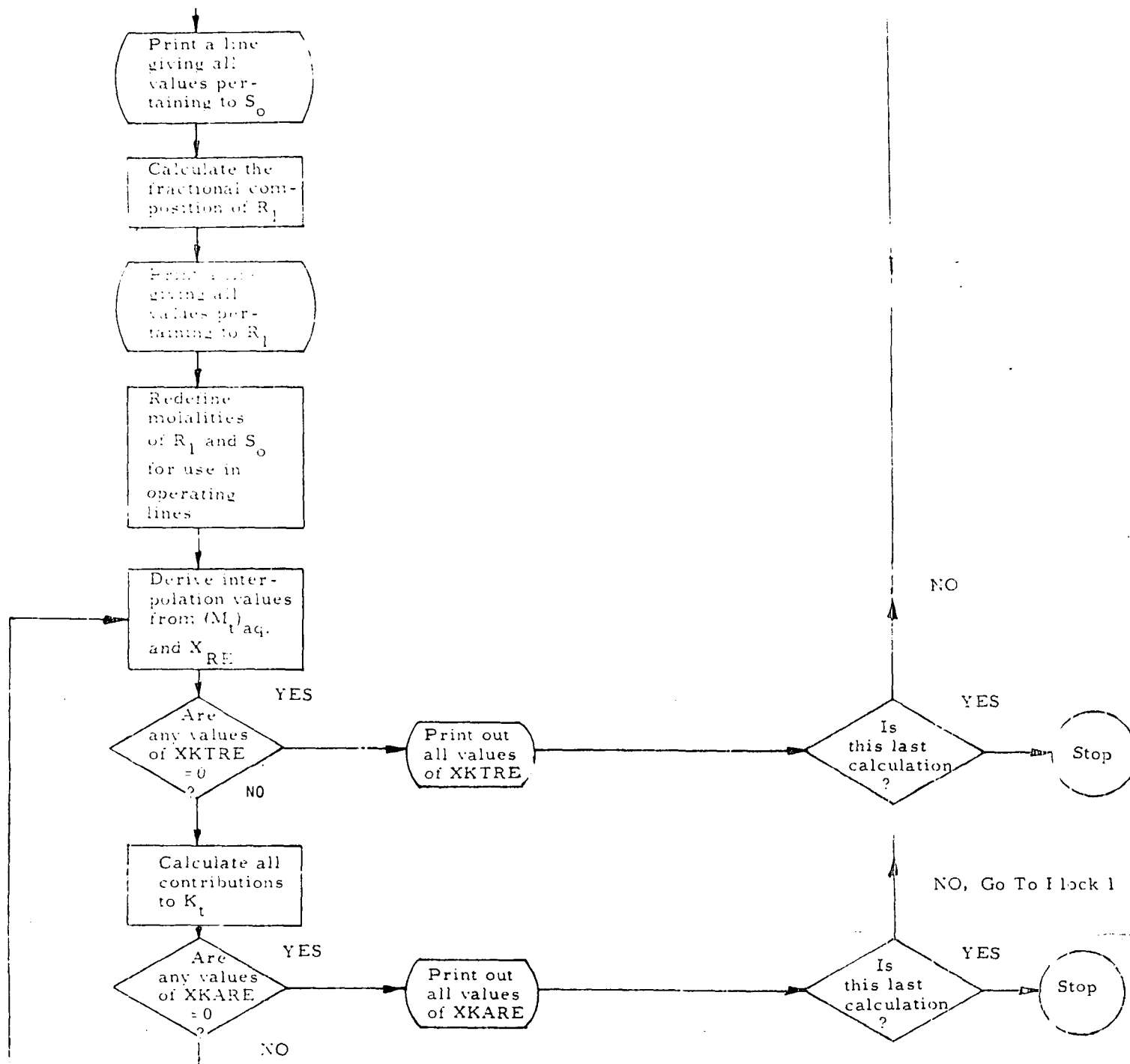
      YSMSF = SMMOR/REMOR
      SYO = YHNO3 + YLA + YPR + YND + YSM
      IF (0.9999 - SYO) 145,155,150
      IF (1.0001 - SYO) 150,155,155
145  PRINT 516, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR
150  IF (K) 600,600,45
      SYREO = YLASF + YPRSF + YNDSF + YSMSF
      IF (0.9999 - SYREO) 160,170,165
      IF (1.0001 - SYREO) 165,170,170
160  PRINT 517, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR
165  IF (K) 600,600,45
      LL = L + 1
170  PRINT 518, LL, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR, YHNO3, YLA,
      LYPR, YND, YSM, YRE, YLASF, YPRSF, YNDSF, YSMSF
      IF (TMOR - 2.0) 175,180,180
175  PRINT 519, TMOR
      IF (K) 600,600,45
180  IF (TMOR - 4.5) 185,175,175
185  CONTINUE
      IF (K) 600,600,45
500  FORMAT (6F10.3)
501  FORMAT (7F9.4)
502  FORMAT (7F7.4,F8.4,I3,I3)
503  FORMAT (29H1SCRUB SIDE CALCULATION ROVS=F8.4,4H N=I3)
504  FORMAT (120HJ TOTALMOLHNO3 MOL LA MOL PR MOL ND MOL SM MOL
1RE MOL ACFR LAFR PRFR NDFR SMFR REFR LA/RE PR/RE ND/RE SM/RE
2)
505  FORMAT (4HJR 07F8.4,10F6.3)
506  FORMAT (4HJR 07F8.4,6F6.3)
507  FORMAT (4HJR 07F8.4)
508  FORMAT (4H S 17F8.4,10F6.3)
509  FORMAT (8HJYKTRE=016F6.3,F8.4,F6.3)
510  FORMAT (8HJYKARE=016F6.3,F8.4,F6.3)
511  FORMAT (18HJREMAQ LESS THAN 04F10.4)
512  FORMAT (16HJSXA NOT EQUAL 17F10.4)
513  FORMAT (18HJSXREA NOT EQUAL 17F10.4)
514  FORMAT (2HJR12,7F8.4,10F6.3)
515  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)
516  FORMAT (16HJSYO NOT EQUAL 17F10.4)
517  FORMAT (18HJSYREO NOT EQUAL 17F10.4)
518  FORMAT (2H S12,7F8.4,10F6.3)
519  FORMAT (6HJTMOR=F10.4)
600  STOP 89
      END

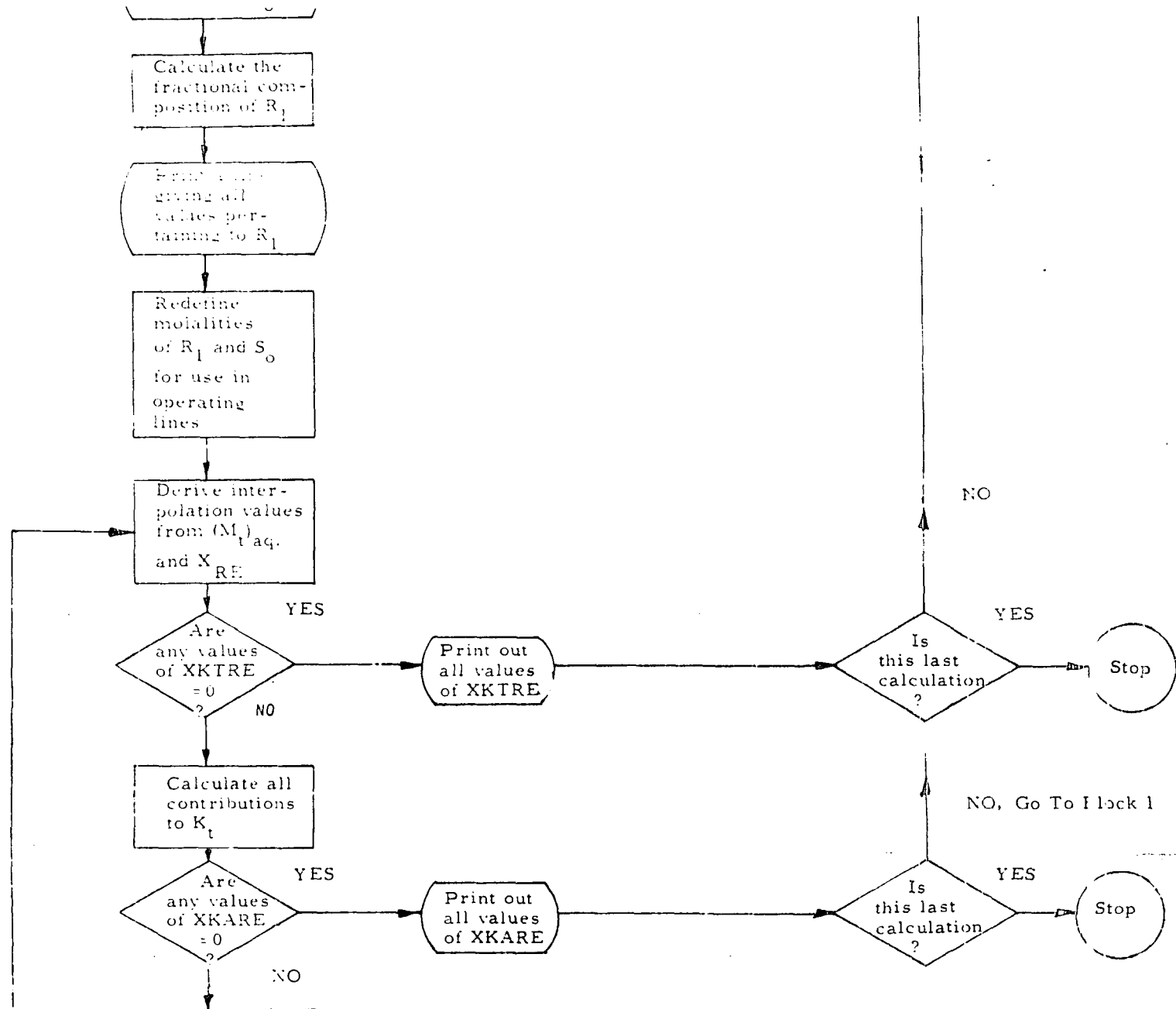
```

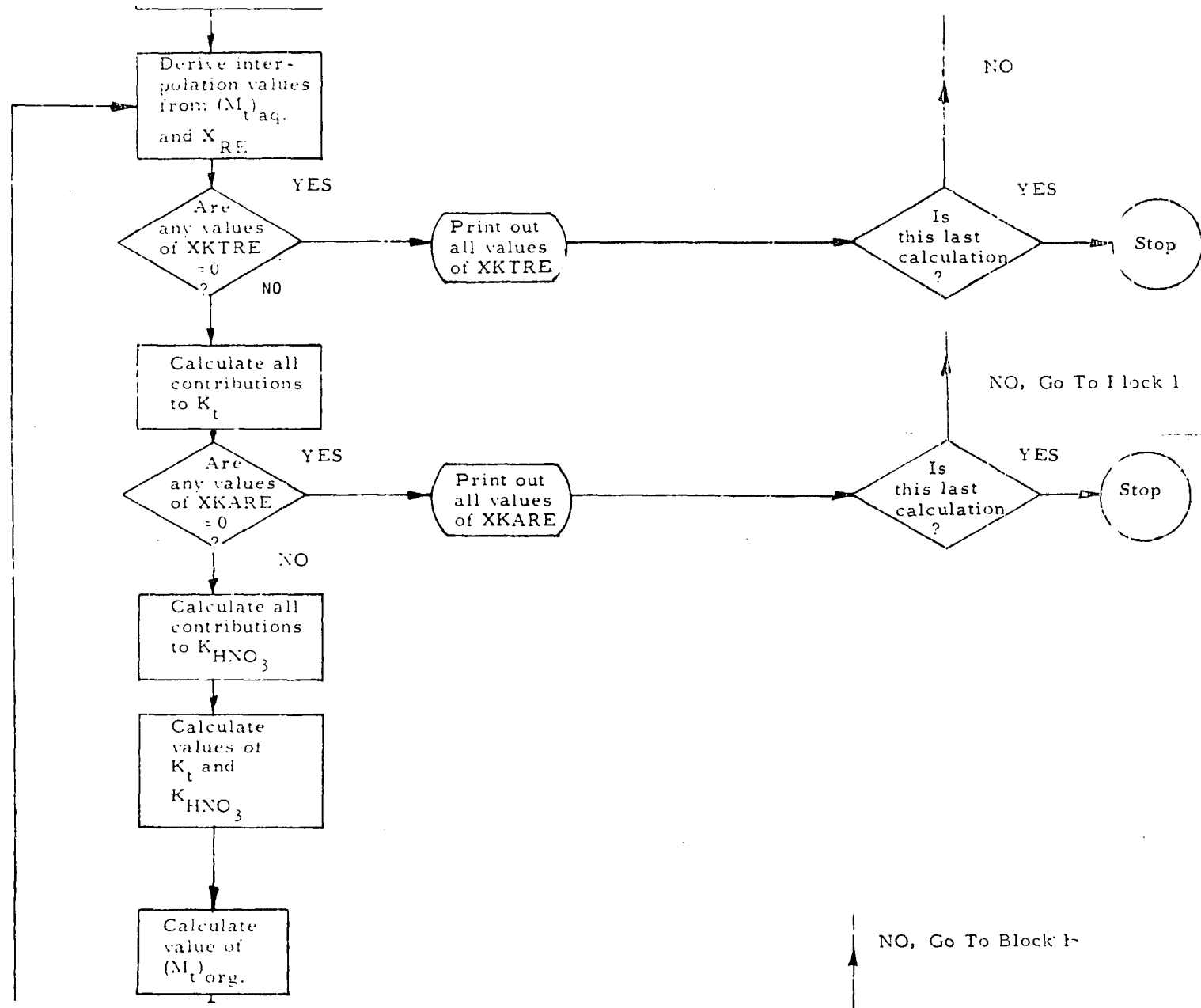
Figure 41. (Continued)

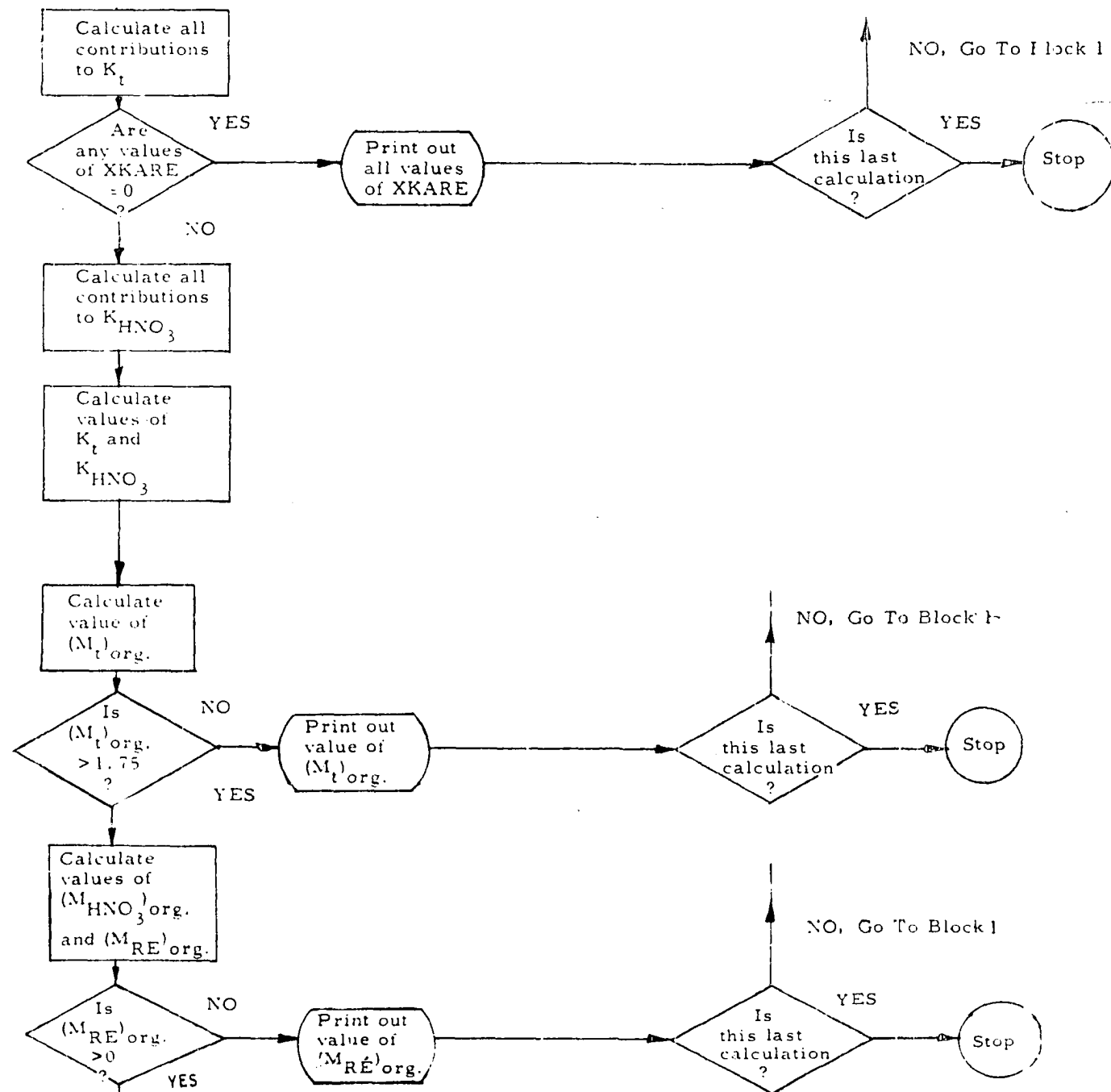
Block 1

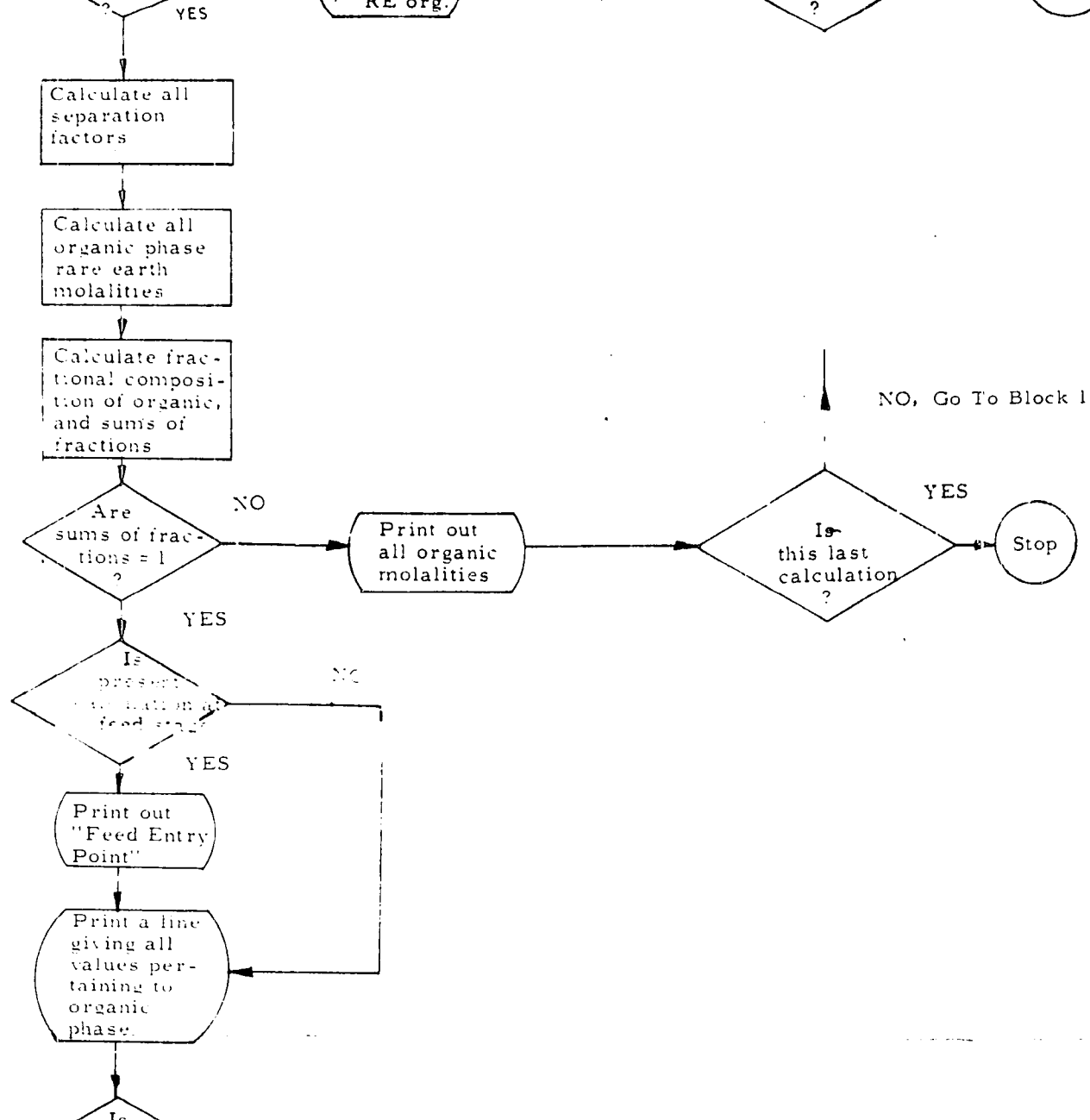


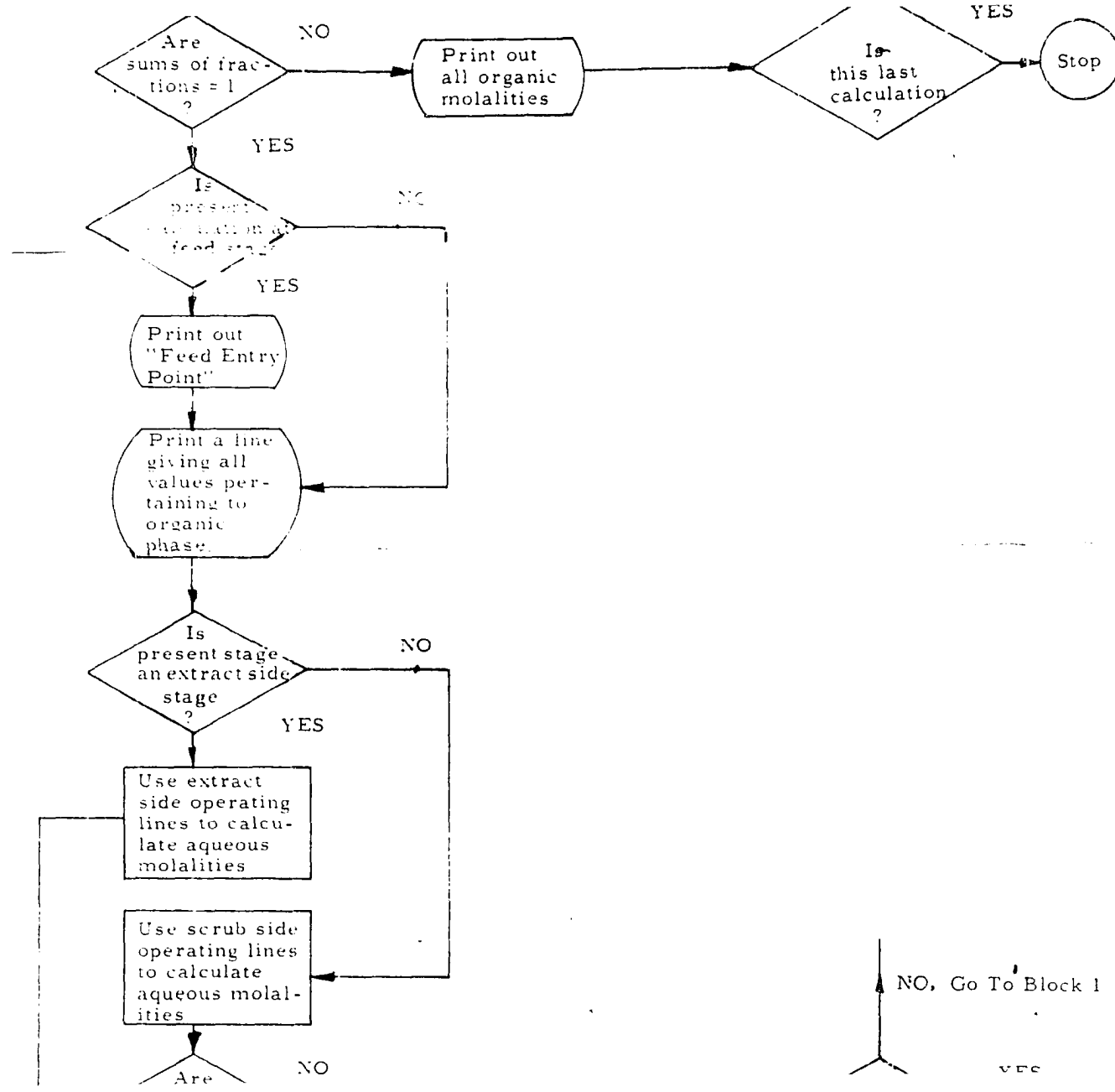


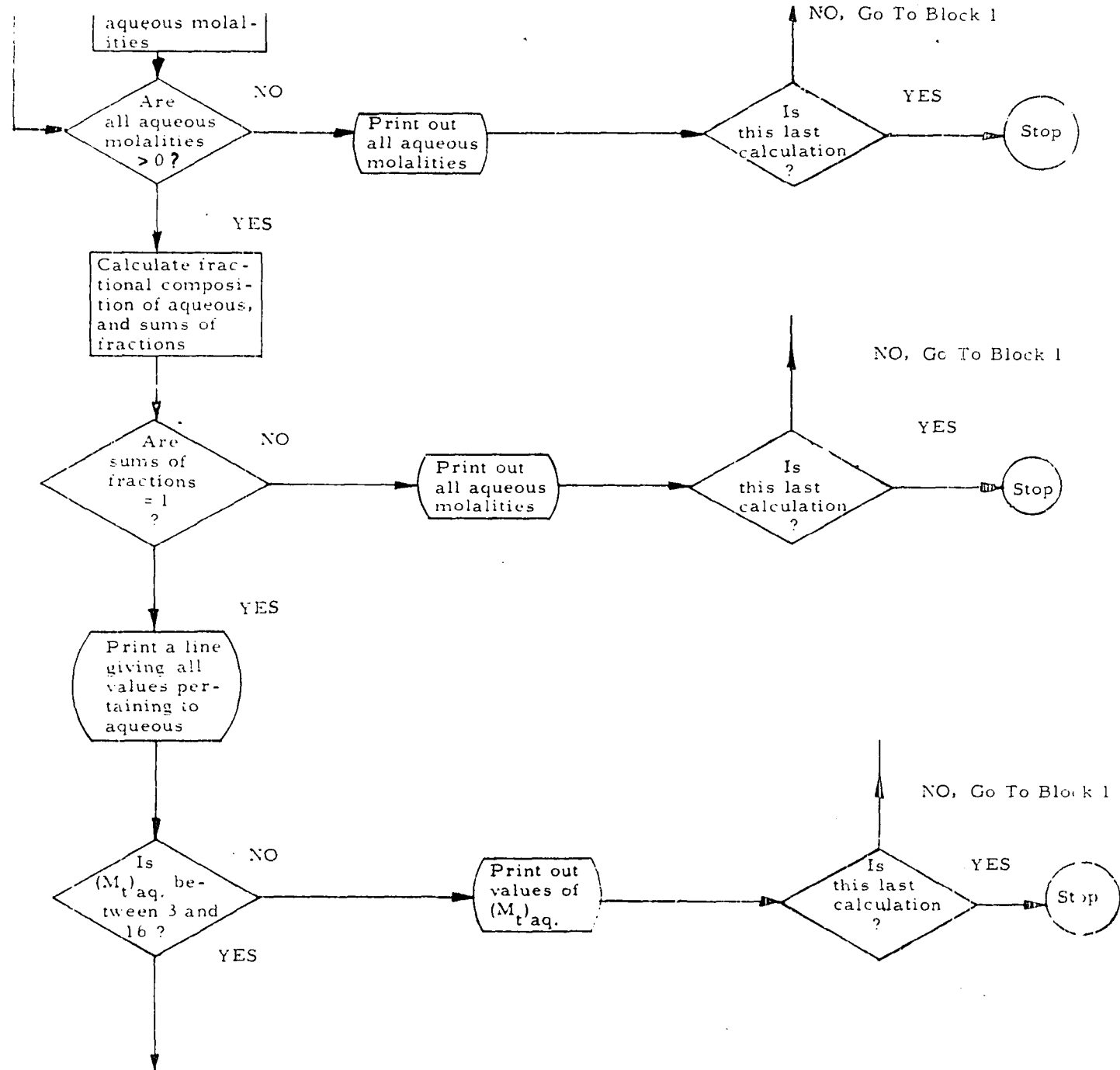












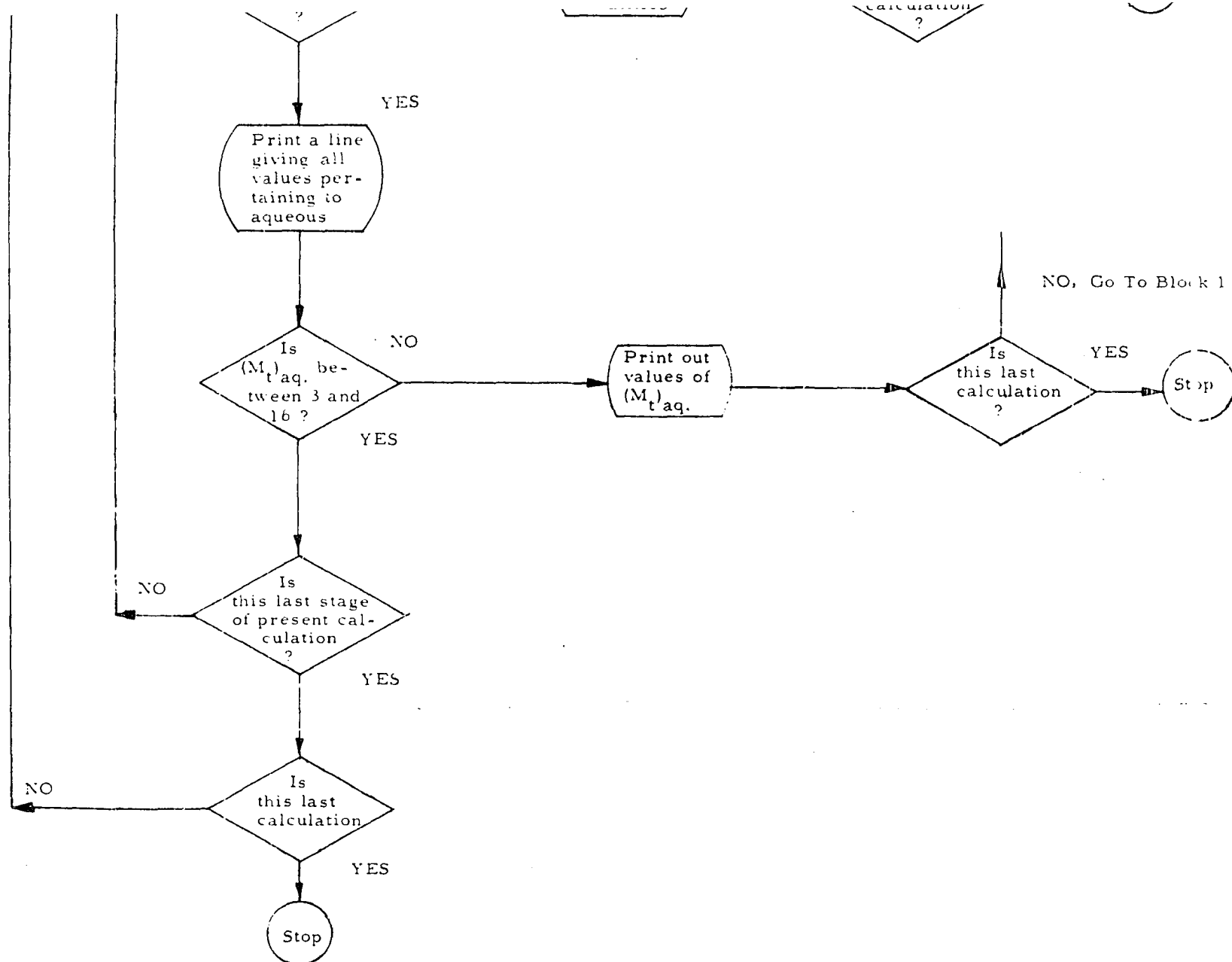


Figure 42. Flow diagram, Program III

```

        DIMENSION XKTLA(21,7),XKTPR(21,7),XKTND(21,7),XKTSM(21,7),XKALA(21,7)
        1,7),XKAPR(21,7),XKAND(21,7),XKASM(21,7)
        DO 5 I = 1,21
5          READ INPUT TAPE 5, 500, (XKTLA(I,J),J = 1,7)
          DO 10 J = 1,21
10           READ INPUT TAPE 5, 500, (XKTPR(I,J),J = 1,7)
           DO 15 J = 1,21
15            READ INPUT TAPE 5, 500, (XKTND(I,J),J = 1,7)
            DO 20 J = 1,21
20             READ INPUT TAPE 5, 500, (XKTSM(I,J),J = 1,7)
             DO 25 J = 1,21
25              READ INPUT TAPE 5, 500, (XKALA(I,J),J = 1,7)
              DO 30 J = 1,21
30               READ INPUT TAPE 5, 500, (XKAPR(I,J),J = 1,7)
               DO 35 J = 1,21
35                READ INPUT TAPE 5, 500, (XKAND(I,J),J = 1,7)
                DO 40 J = 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,SMMMAQ,REMAQ
          READ INPUT TAPE 5, 501, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR
          READ INPUT TAPE 5, 502, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM,S,F,REX,RBMS3 001
          1SC,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,XSMBMS3 002
          1F,XREF,XLASFF,XPRSFF,XNDSFF,XSMSFF
          GO TO 70
60          PRINT 506, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM,XAF,XLAF,XPRF,XNDF,XSMBMS3 003
          1F,XREF
          GO TO 70
65          PRINT 507, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM
70          IF(TMOR) 600,90,75
75          YHNO3 = AMOR/TMOR
          YLA = XLAMOR/TMOR
          YPR = PRMOR/TMOR
          YND = XNDMOR/TMOR
          YSM = SMMOR/TMOR
          YRE = REMOR/TMOR
          IF (REMOR) 600,85,80
80          YLASF = XLAMOR/REMOR
          YPRSF = PRMOR/REMOR
          YNDSF = XNDMOR/REMOR
          YSMF = SMMOR/REMOR
          PRINT 508, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,YHNO3,YLA,YPRBMS3 004
          1,YND,YSM,YRE,YLASF,YPRSF,YNDSF,YSMSF
          GO TO 95
85          PRINT 509, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR,YHNO3,YLA,YPRBMS3 005
          1,YND,YSM,YRE
          GO TO 95
90          PRINT 510, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR
          BMS3 006

```

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
        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
        SDAM = 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
        IF (7.0 - TMAQ) 115,115,110                      BMS3 092
100      Z = TMAQ - 2.0                                  BMS3 093
105      GO TO 120                                         BMS3 094
        Z = (TMAQ + 1.0)/2.0                             BMS3 095
110      GO TO 120                                         BMS3 096
        Z = (TMAQ + 5.0)/3.0                             BMS3 097
115      KZ = Z                                           BMS3 098
120      ZK = KZ                                           BMS3 099
        FRZ = Z - ZK                                      BMS3 100
        SKT = MIN1F(XKTLA(IX,KZ),XKTLA(IX+1,KZ),XKTLA(IX,KZ+1),XKTLA(IX+1,KZ+1),XKTPR(IX,KZ),XKTPR(IX+1,KZ),XKTPR(IX,KZ+1),XKTPR(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),XKTPR(IX,KZ),XKTPR(IX+1,KZ),XKTPR(IX,KZ+1),XKTPR(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
        XKTPR1 = XKTPR(IX,KZ)*(1.0-FRX) + XKTPR(IX+1,KZ)*FRX BMS3 109
        XKTPR2 = XKTPR(IX,KZ+1)*(1.0-FRX) + XKTPR(IX+1,KZ+1)*FRX BMS3 110
        XKTPR3 = XKTPR1*(1.0-FRZ) + XKTPR2 *FRZ        BMS3 111
        CKTPR = XKTPR3*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

```

Figure 43. (Continued)

```

      XKTSM2 = XKTSM(IX,KZ+1)*(1.0 -FRX) + XKISM(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,BMS3 128
1KZ+1),XKAPR(IX,KZ),XKAPR(IX+1,KZ),XKAPR(IX,KZ+1),XKAPR(IX+1,KZ+1),BMS3 129
2XKAND(IX,KZ),XKAND(IX+1,KZ),XKAND(IX,KZ+1),XKAND(IX+1,KZ+1),XKASM(BMS3 130
3IX,KZ),XKASM(IX+1,KZ),XKASM(IX,KZ+1),XKASM(IX+1,KZ+1))             BMS3 131
      IF (SKA) 135,135,140                                             BMS3 132
135 PRINT 513, XKALA(IX,KZ),XKALA(IX+1,KZ),XKALA(IX,KZ+1),XKALA(IX+1,KBMS3 133
1Z+1),XKAPR(IX,KZ),XKAPR(IX+1,KZ),XKAPR(IX,KZ+1),XKAPR(IX+1,KZ+1),XBMS3 134
2KAND(IX,KZ),XKAND(IX+1,KZ),XKAND(IX,KZ+1),XKAND(IX+1,KZ+1),XKASM(1BMS3 135
3X,KZ),XKASM(IX+1,KZ),XKASM(IX,KZ+1),XKASM(IX+1,KZ+1),TMAQ,XRE      BMS3 136
      IF (K) 600,600,45                                              BMS3 137
140 XKALA1 = XKALA(IX,KZ)*(1.0 - FRX) + XKALA(IX+1,KZ)*FRX          BMS3 138
      XKALA2 = XKALA(IX,KZ+1)*(1.0 -FRX) + XKALA(IX+1,KZ+1)*FRX      BMS3 139
      XKALA3 = XKALA1*(1.0 -FRZ) + XKALA2*FRZ                         BMS3 140
      CKALA = XKALA3 * XLASF                                           BMS3 141
      XKAPR1 = XKAPR(IX,KZ)*(1.0 -FRX) + XKAPR(IX+1,KZ)* FRX        BMS3 142
      XKAPR2 = XKAPR(IX,KZ+1)*(1.0 -FRX) + XKAPR(IX+1,KZ+1)*FRX     BMS3 143
      XKAPR3 = XKAPR1*(1.0 -FRZ) + XKAPR2 * FRZ                     BMS3 144
      CKAPR = XKAPR3 * XPRSF                                           BMS3 145
      XKAND1 = XKAND(IX,KZ)*(1.0 -FRX) + XKAND(IX+1,KZ)*FRX          BMS3 146
      XKAND2 = XKAND(IX,KZ+1)* (1.0 -FRX) +XKAND(IX+1,KZ+1)*FRX     BMS3 147
      XKAND3 = XKAND1*(1.0 -FRZ) + XKAND2 * FRZ                     BMS3 148
      CKAND = XKAND3 * XNDSF                                           BMS3 149
      XKASM1 = XKASM(IX,KZ)*(1.0 - FRX) + XKASM(IX+1,KZ)*FRX          BMS3 150
      XKASM2 = XKASM(IX,KZ+1)*(1.0 -FRX) + XKASM(IX+1,KZ+1)*FRX     BMS3 151
      XKASM3 = XKASM1*(1.0 -FRZ) + XKASM2 *FRZ                       BMS3 152
      CKASM = XKASM3 * XSMSF                                           BMS3 153
      TOTK = CKTLA + CKTPR + CKTND + CKTSM                             BMS3 154
      HNO3K = CKALA + CKAPR + CKAND + CKASM                             BMS3 155
      TMOR = TMAQ * TOTK                                              BMS3 156
      IF(TMOR - 1.75) 145,150,150                                     BMS3 157
145 PRINT 514, TMOR,TMAQ,TOTK                                         BMS3 158
      IF (K) 600,600,45                                              BMS3 159
150 AMOR = AMAQ * HNO3K                                              BMS3 160
      REMOR = TMOR - AMOR                                             BMS3 161
      IF(REMOR) 155,155,160                                           BMS3 162
155 PRINT 515, TMOR,AMOR,REMOR,HNO3K                                  BMS3 163
      IF (K) 600,600,45                                              BMS3 164
160 BLAPR = 0.8187 - 0.1106*TMOR                                     BMS3 165
      BPRPR = 1.0                                                    BMS3 166
      BNDPR = 1.0448 + 0.09874*TMOR                                   BMS3 167
      BSMPR = -0.3795 + 0.9214*TMOR                                   BMS3 168
      DEMS = XLAMAQ*BLAPR + PRMAQ* BPRPR + XNDMAQ*BNDPR + SMMAQ*BSMPR BMS3 169
      XLAMOR = REMOR*BLAPR*XLAMAQ/DEMS                               BMS3 170
      PRMOR = REMOR*BPRPR*PRMAQ/DEMS                                 BMS3 171
      XNDMOR= REMOR*BNDPR*XNDMAQ/DEMS                                BMS3 172
      SMMOR = REMOR*BSMPR*SMMAQ/DEMS                                 BMS3 173
      YHNO3 = AMOR/TMOR                                              BMS3 174
      YLA = XLAMOR/TMOR                                              BMS3 175
      YPR = PRMOR/TMOR                                              BMS3 176
      YND = XNDMOR/TMOR                                              BMS3 177
      YSM = SMMOR/TMOR                                              BMS3 178
      YRE = REMOR/TMOR                                              BMS3 179
      SYD = YHNO3 + YLA + YPR + YND + YSM                             BMS3 180
      IF (0.9999 - SYD) 165,175,170                                   BMS3 181
165 IF (1.0001 - SYD) 170,175,175                                   BMS3 182
170 PRINT 516, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMOR           BMS3 183
      IF (K) 600,600,45                                              BMS3 184
175 YLASF = XLAMOR/REMOR                                             BMS3 185
      YPRSF = PRMOR/REMOR                                             BMS3 186

```

Figure 43. (Continued)

```

YNSDF = XNDMOR/REMOR
YSMSF = SHMOR/REMOR
SYRED = YLASF + YPRSF + YNSDF + YSMSF
IF (0.9999 - SYRED) 180,190,185
IF (1.0001 - SYRED) 185,190,190
180 PRINT 517, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SHMOR, REMOR
185 IF (K) 600,600,45
190 IF (L - M) 200,195,200
195 PRINT 518
200 PRINT 519, L, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SHMOR, REMOR, YHNO3, YLA, YPBMS3
1R, YND, YSM, YRE, YLASF, YPRSF, YNSDF, YSMSF
IF (L-M) 205,210,210
205 TMAQ = TMOR*S/REX - SOTM*S/REX + R1TM
AMAQ = AMOR*S/REX - SOAM*S/REX + R1AM
XLAMAQ = XLAMOR*S/REX - SOLAM*S/REX + R1LAM
PRMAQ = PRMOR*S/REX - SOPRM*S/REX + R1PRM
XNDMAQ = XNDMOR*S/REX - SONDM*S/REX + R1NDM
SHMAQ = SHMOR*S/REX - SOSMM*S/REX + R1SMM
GO TO 215
210 TMAQ = TMOR*S/RSC - SOTM*S/RSC - FTM*F/RSC + R1TM*REX/RSC
AMAQ = AMOR*S/RSC - SOAM*S/RSC - FAM*F/RSC + R1AM*REX/RSC
XLAMAQ = XLAMOR*S/RSC - SOLAM*S/RSC - FLAM*F/RSC + R1LAM*REX/RSC
PRMAQ = PRMOR*S/RSC - SOPRM*S/RSC - FPRM*F/RSC + R1PRM*REX/RSC
XNDMAQ = XNDMOR*S/RSC - SONDM*S/RSC - FNDM*F/RSC + R1NDM*REX/RSC
SHMAQ = SHMOR*S/RSC - SOSMM*S/RSC - FSMM*F/RSC + R1SMM*REX/RSC
215 REMAQ = TMAQ - AMAQ
SAM = MIN1F(TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SHMAQ, REMAQ)
IF (SAM) 220,220,225
220 PRINT 520, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SHMAQ, REMAQ
IF (K) 600,600,45
225 XHNO3 = AMAQ/TMAQ
XLA = XLAMAQ/TMAQ
XPR = PRMAQ/TMAQ
XND = XNDMAQ/TMAQ
XSM = SHMAQ/TMAQ
XRE = REMAQ/TMAQ
SXA = XHNO3 + XLA + XPR + XND + XSM
IF (0.9999 - SXA) 230,240,235
230 IF (1.0001 - SXA) 235,240,240
235 PRINT 521, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SHMAQ, REMAQ
IF (K) 600,600,45
240 XLASF = XLAMAQ/REMAQ
XPRSF = PRMAQ/REMAQ
XNSDF = XNDMAQ/REMAQ
XSMSF = SHMAQ/REMAQ
SXREA = XLASF + XPRSF + XNSDF + XSMSF
IF (0.9999 - SXREA) 245,255,250
245 IF (1.0001 - SXREA) 250,255,255
250 PRINT 522, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SHMAQ, REMAQ
IF (K) 600,600,45
255 LL = L+1
PRINT 523, LL, TMAQ, AMAQ, XLAMAQ, PRMAQ, XNDMAQ, SHMAQ, REMAQ, XHNO3, XLA, XSM
1PR, XND, XSM, XRE, XLASF, XPRSF, XNSDF, XSMSF
IF (TMAQ - 3.0) 260,265,265
260 PRINT 524, TMAQ
IF (K) 600,600,45
265 IF (TMAQ - 16.0) 270,260,260
270 CONTINUE
IF (K) 600,600,45
500 FORMAT (7F10.3)
501 FORMAT (7F10.4)
502 FORMAT (7F7.4,4F5.2,3I3)

```

Figure 43. (Continued)

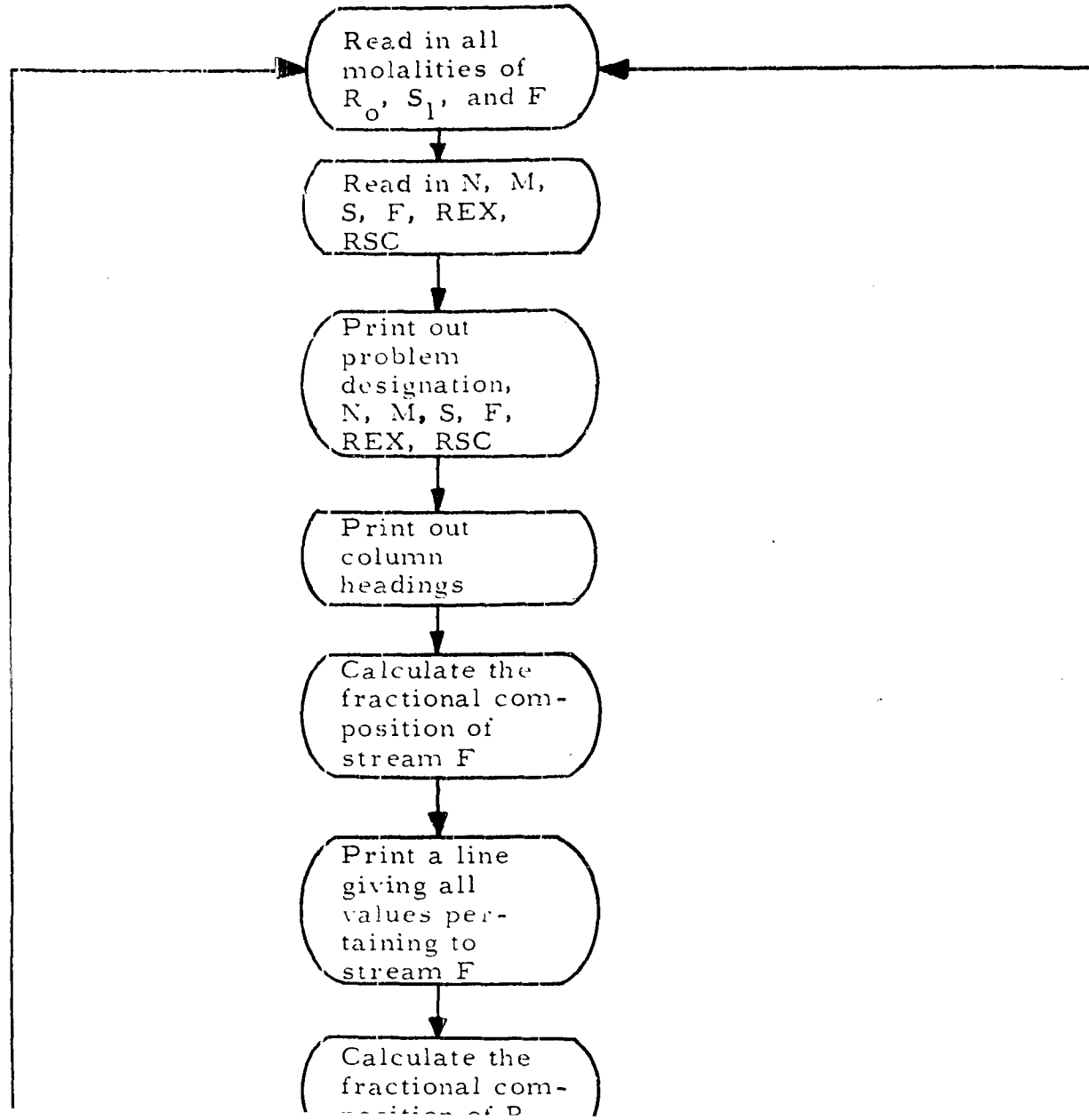
```

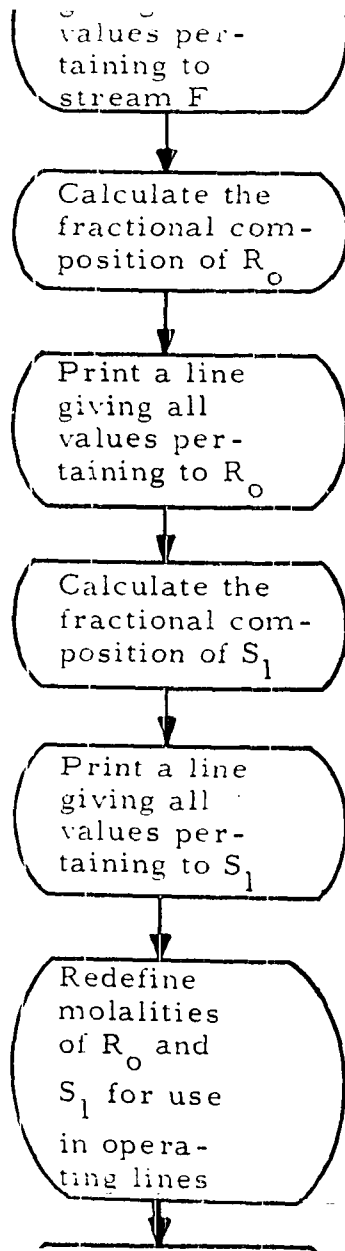
503  FORMAT (36HIINTERNAL FEED,EXTRACT SIDE START S=F5.2,3H F=F5.2,5H RBMS3 249
      1EX=F5.2,5H RSC=F5.2,3H N=13,3H M=13) BMS3 250
504  FORMAT (120HJ TOTALMOLHNO3 MOL LA MOL PR MOL ND MOL SM MOL BMS3 251
      1RE MOL ACFR LAFR PRFR NDFR SMFR REFR LA/RE PR/RE ND/RE SM/RE BMS3 252
      2) BMS3 253
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 (6HJTMQAQ=F10.4,6H AMAQ=F10.4,8H XLAMAQ=F10.4,7H PRMAQ=F10.4) BMS3 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 (6HJTMQAQ=F10.4) BMS3 274
600  STOP 89 BMS3 275
      END BMS3 276

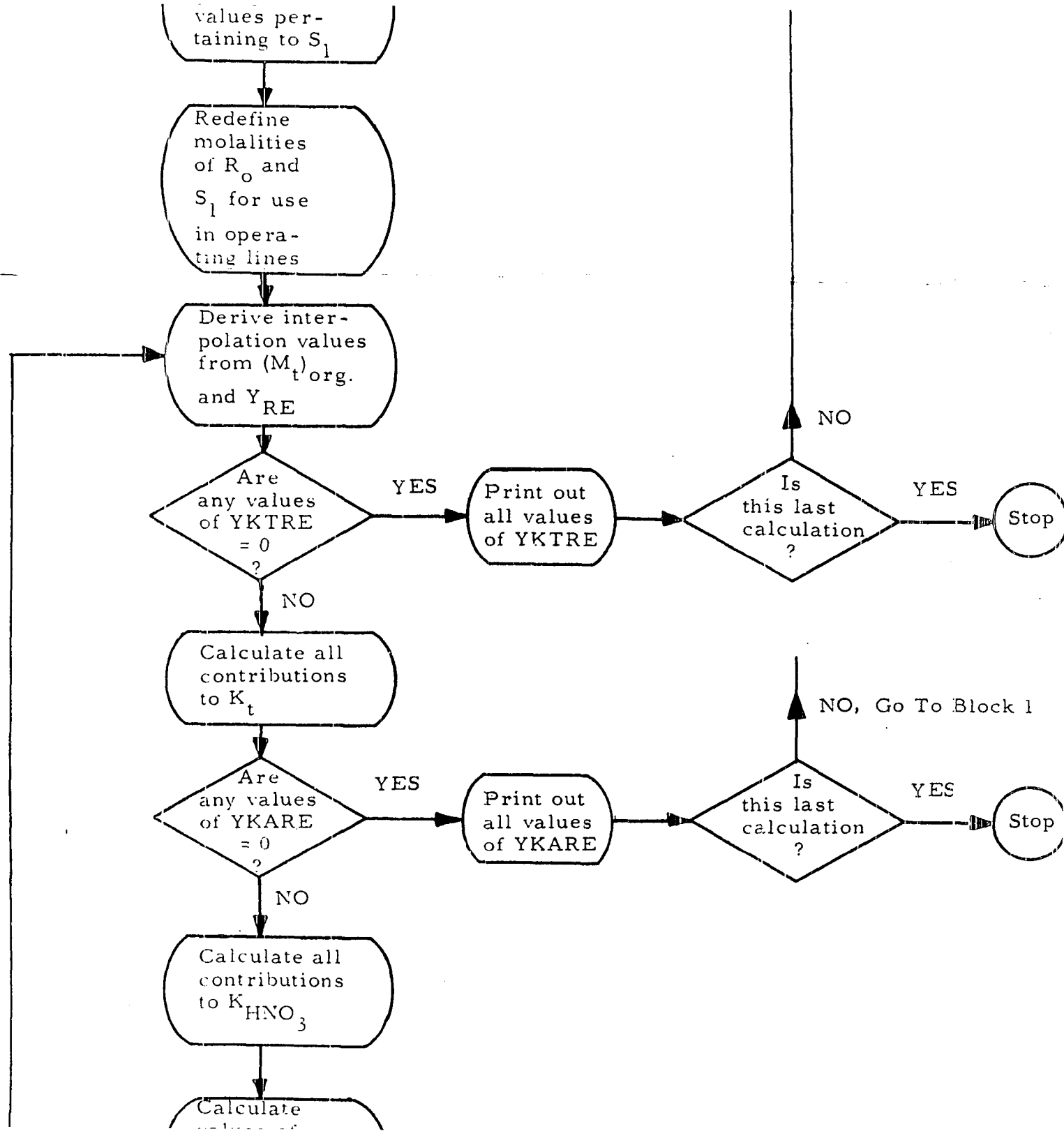
```

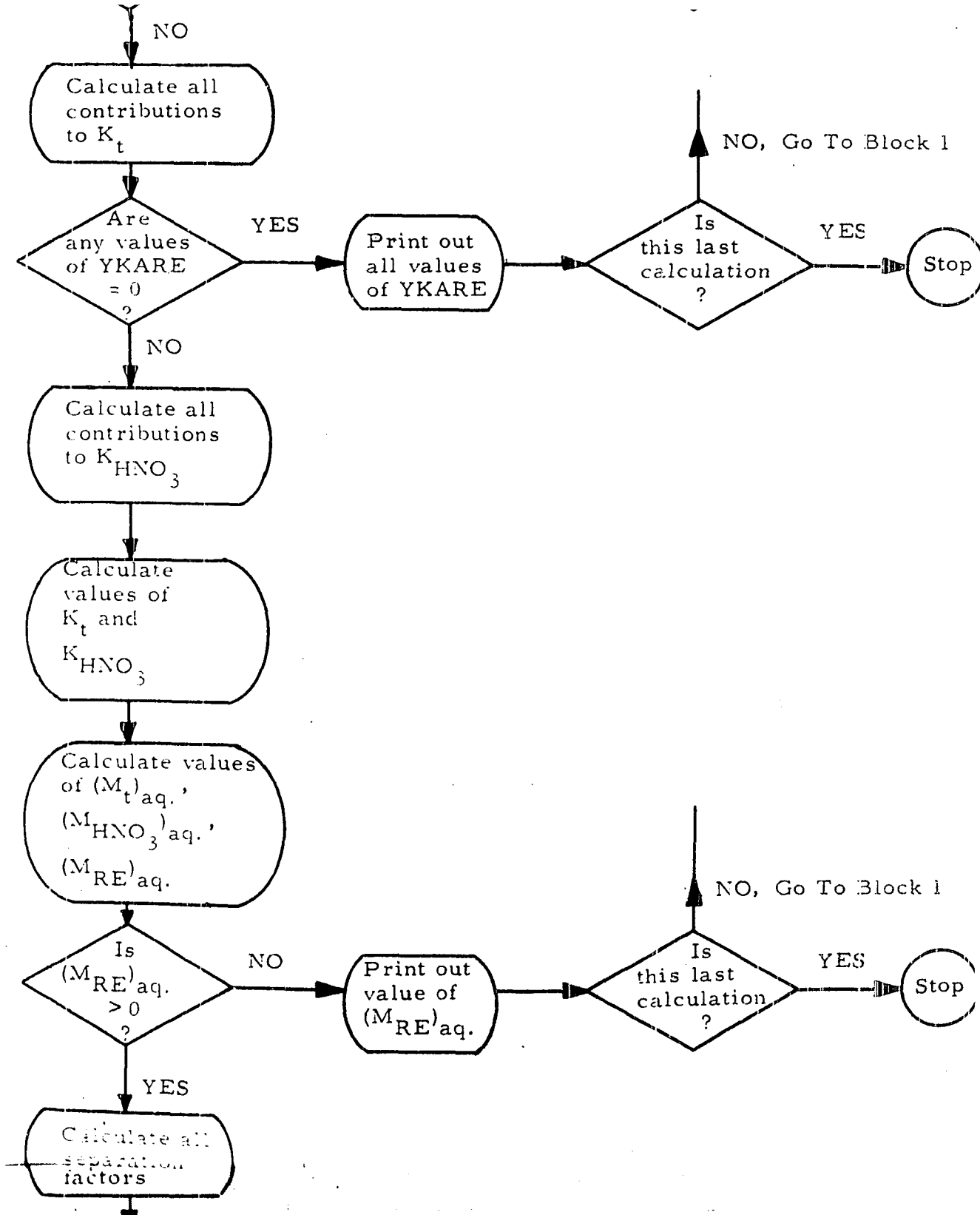
Figure 43. (Continued)

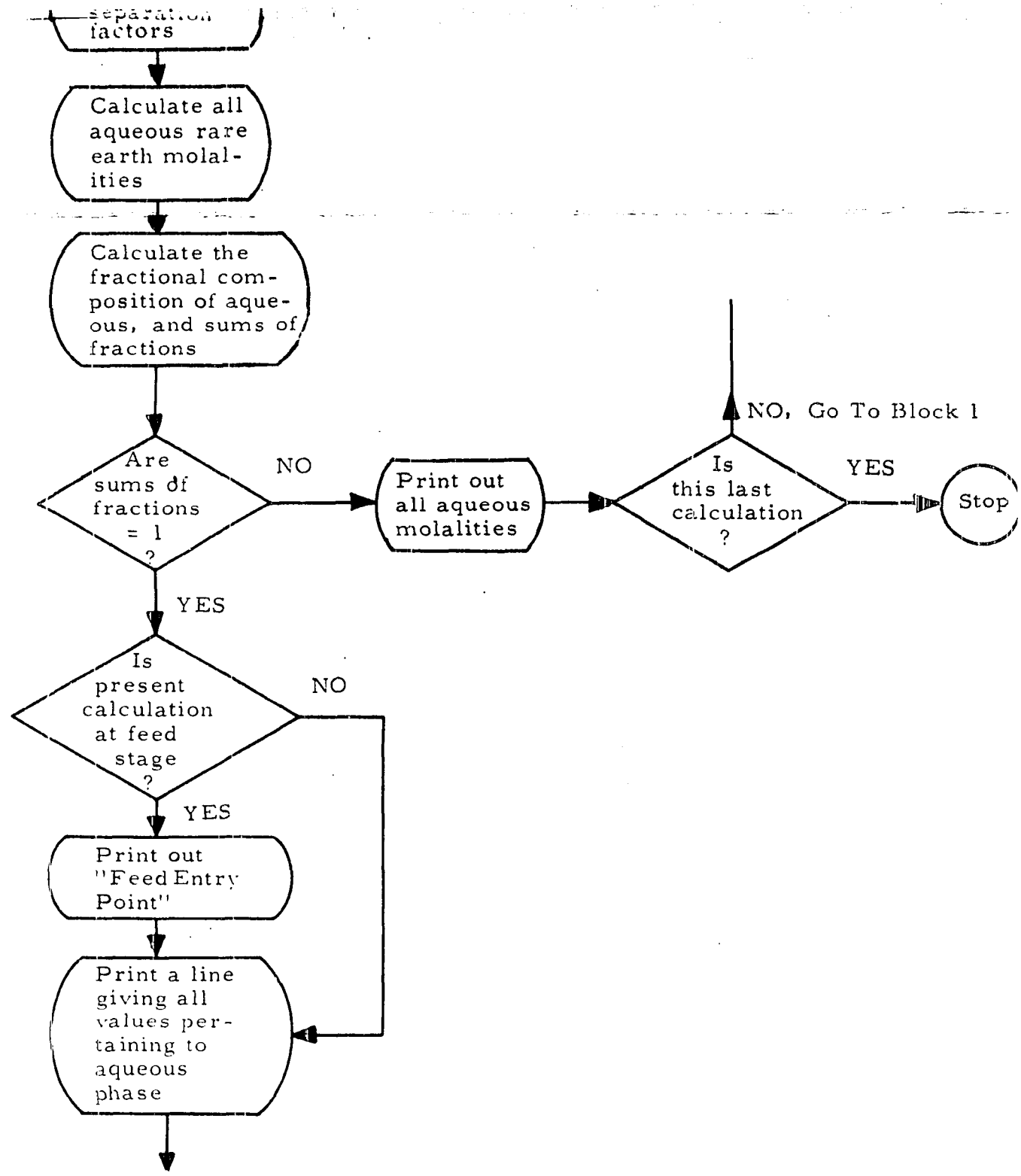
Block 1

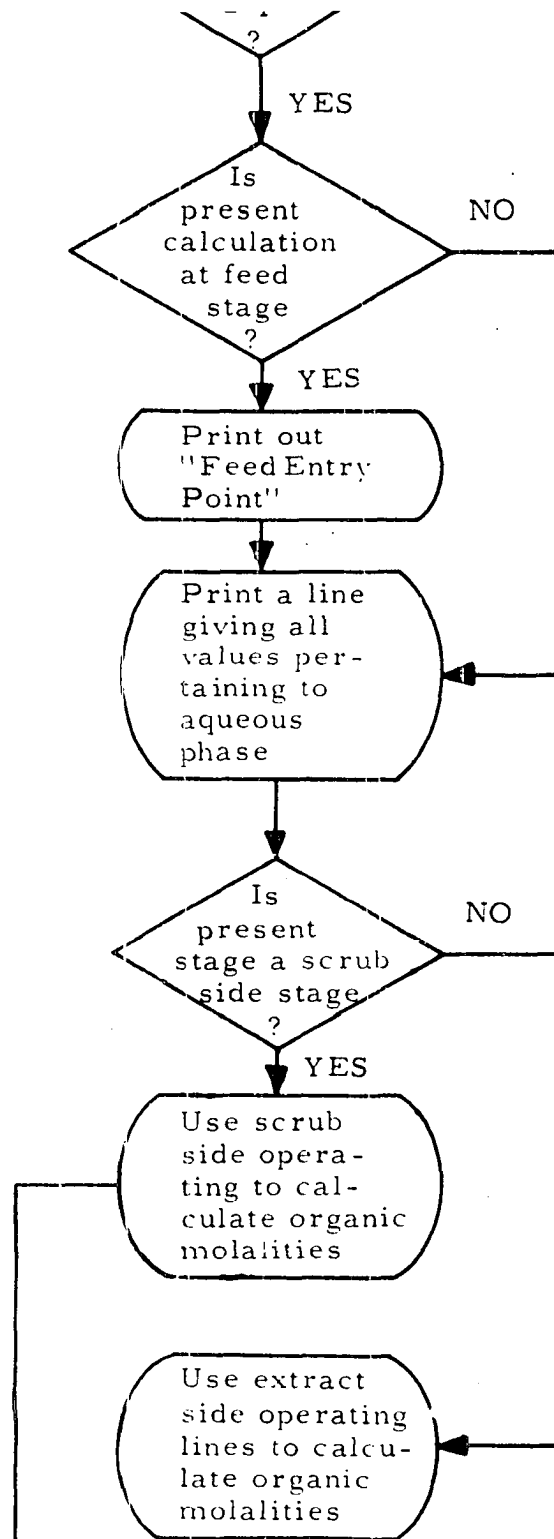


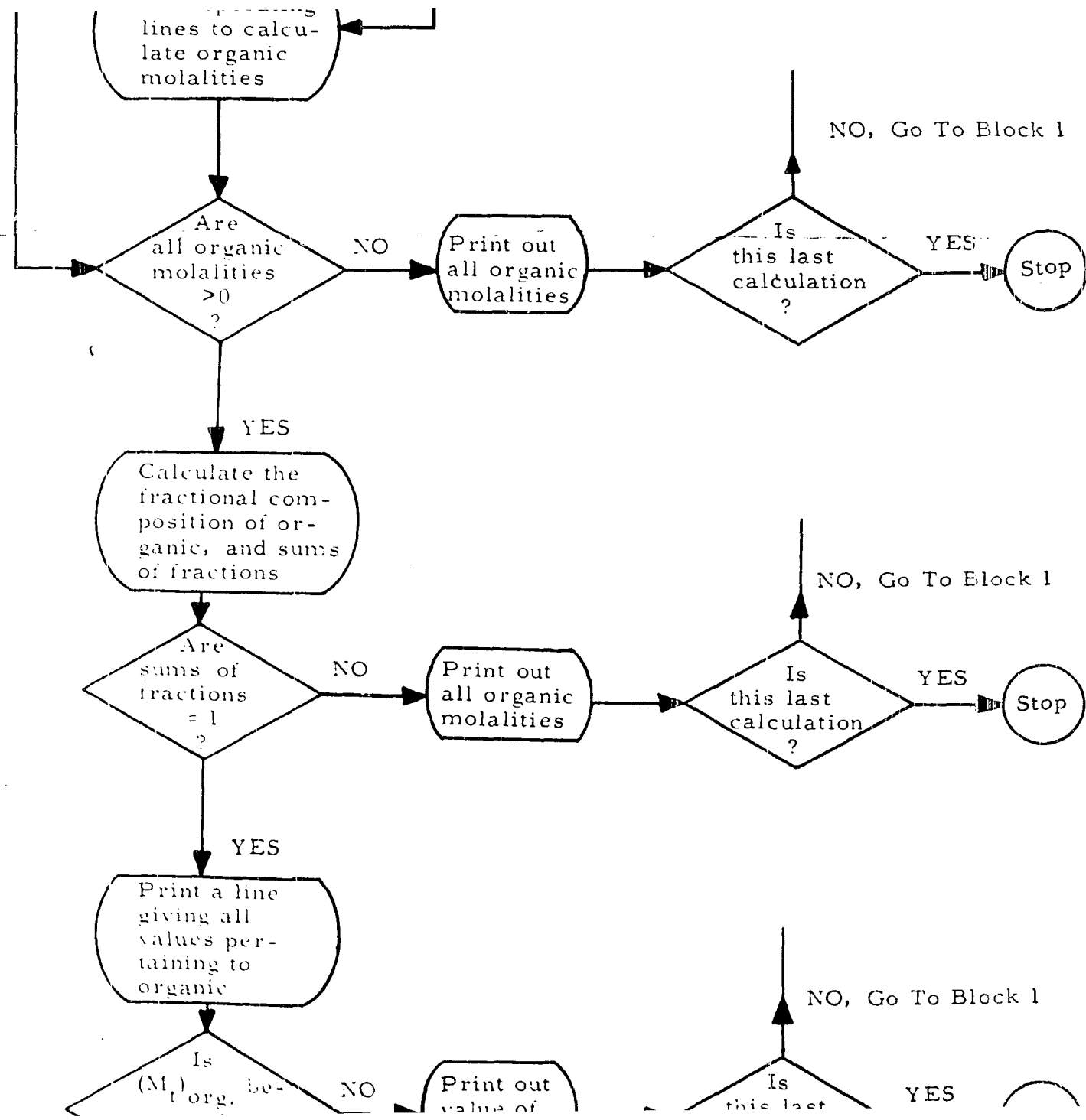












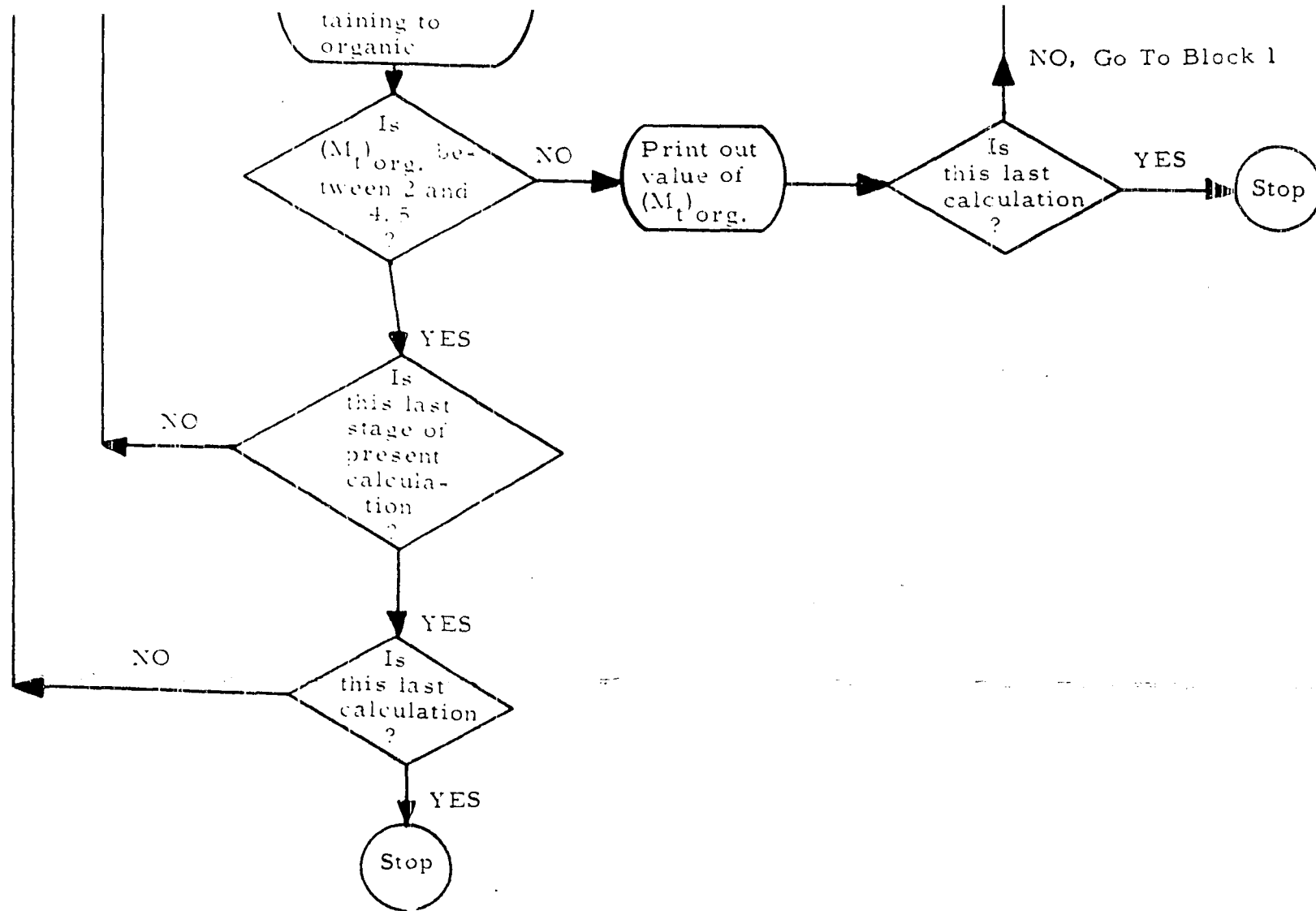


Figure 44. Flow diagram, Program IV.

```

      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,SMROR,REMOR
      READ INPUT TAPE 5, 502, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM,S,F,REX,RBMS4
1SC,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
1F,XREF,XLASFF,XPRSFF,XNDSFF,XSMSFF
      GO TO 70
60     PRINT 506, FTM,FAM,FLAM,FPRM,FNDM,FSMM,FREM,XAF,XLAF,XPRF,XNDF,XSMBMS4
1F,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
    YSMSF = SMMOR/REMOR                              BMS4 072
    PRINT 511, TMOR, AMOR, XLAMOR, PRMOR, XNDMOR, SMMOR, REMOR, YHNO3, YLA, YPR, BMS4 073
1   YND, YSM, YRE, YLASF, YPRSF, YNDSF, YSMSF        BMS4 074
    ROTM = TMAQ                                        BMS4 075
    ROAM = AMAQ                                        BMS4 076
    ROLAM = 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
    YREI = (YRE*100.0 + 5.0)/5.0                     BMS4 088
    IY = YREI                                         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, BMS4 096
1KZ+1),YKTPR(IY,KZ),YKTPR(IY+1,KZ),YKTPR(IY,KZ+1),YKTPR(IY+1,KZ+1), BMS4 097
2YKTND(IY,KZ),YKTND(IY+1,KZ),YKTND(IY,KZ+1),YKTND(IY+1,KZ+1),YKTSM( BMS4 098
3IY,KZ),YKTSM(IY+1,KZ),YKTSM(IY,KZ+1),YKTSM(IY+1,KZ+1)) BMS4 099
    IF (SKT) 100,100,105                             BMS4 100
100 PRINT 512, YKTLA(IY,KZ),YKTLA(IY+1,KZ),YKTLA(IY,KZ+1),YKTLA(IY+1, BMS4 101
1Z+1),YKTPR(IY,KZ),YKTPR(IY+1,KZ),YKTPR(IY,KZ+1),YKTPR(IY+1,KZ+1),Y BMS4 102
2KTND(IY,KZ),YKTND(IY+1,KZ),YKTND(IY,KZ+1),YKTND(IY+1,KZ+1),YKTSM( BMS4 103
3Y,KZ),YKTSM(IY+1,KZ),YKTSM(IY,KZ+1),YKTSM(IY+1,KZ+1),TMOR,YRE BMS4 104
    IF (K) 500,600,45                                 BMS4 105
105 YKTLA1 = YKTLA(IY,KZ)*(1.0 - FRY) + YKTLA(IY+1,KZ)*FRY BMS4 106
    YKTLA2 = YKTLA(IY,KZ+1)*(1.0 - FRY) + YKTLA(IY+1,KZ+1)*FRY BMS4 107
    YKTLA3 = YKTLA1*(1.0 - FRZ) + YKTLA2*FRZ          BMS4 108
    CKTLA = YKTLA3 * YLASF                             BMS4 109
    YKTPR1 = YKTPR(IY,KZ)*(1.0 - FRY) + YKTPR(IY+1,KZ)*FRY BMS4 110
    YKTPR2 = YKTPR(IY,KZ+1)*(1.0 - FRY) + YKTPR(IY+1,KZ+1)*FRY BMS4 111
    YKTPR3 = YKTPR1*(1.0 - FRZ) + YKTPR2*FRZ          BMS4 112
    CKTPR = YKTPR3 * YPRSF                             BMS4 113
    YKTND1 = YKTND(IY,KZ)*(1.0 - FRY) + YKTND(IY+1,KZ)*FRY BMS4 114
    YKTND2 = YKTND(IY,KZ+1)*(1.0 - FRY) + YKTND(IY+1,KZ+1)*FRY BMS4 115
    YKTND3 = YKTND1*(1.0 - FRZ) + YKTND2*FRZ          BMS4 116
    CKTND = YKTND3 * YNDSF                             BMS4 117
    YKTSM1 = YKTSM(IY,KZ)*(1.0 - FRY) + YKTSM(IY+1,KZ)*FRY BMS4 118
    YKTSM2 = YKTSM(IY,KZ+1)*(1.0 - FRY) + YKTSM(IY+1,KZ+1)*FRY BMS4 119
    YKTSM3 = YKTSM1*(1.0 - FRZ) + YKTSM2*FRZ          BMS4 120
    CKTSM = YKTSM3 * YSMSF                             BMS4 121
    SKA = MIN1F(YKALA(IY,KZ),YKALA(IY+1,KZ),YKALA(IY,KZ+1),YKALA(IY+1, BMS4 122
1KZ+1),YKAPR(IY,KZ),YKAPR(IY+1,KZ),YKAPR(IY,KZ+1),YKAPR(IY+1,KZ+1), BMS4 123
2YKAND(IY,KZ),YKAND(IY+1,KZ),YKAND(IY,KZ+1),YKAND(IY+1,KZ+1),YKASM( BMS4 124

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Figure 45. (Continued)

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3IY,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),YBMS4 127
    1Z+1),YKAPR(IY,KZ),YKAPR(IY+1,KZ),YKAPR(IY,KZ+1),YKAPR(IY+1,KZ+1),YBMS4 128
    2KAND(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 129
    3Y,KZ),YKASM(IY+1,KZ),YKASM(IY,KZ+1),YKASM(IY+1,KZ+1),TMOR,YRE      BMS4 130
    IF (K) 600,600,45                                          BMS4 131
115 YKALA1 = YKALA(IY,KZ)*(1.0 - FRY) + YKALA(IY+1,KZ)*FRY      BMS4 132
    YKALA2 = YKALA(IY,KZ+1)*(1.0 - FRY) + YKALA(IY+1,KZ+1)*FRY      BMS4 133
    YKALA3 = YKALA1*(1.0 - FRZ) + YKALA2*FRZ                      BMS4 134
    CKALA = YKALA3 * YLASF                                         BMS4 135
    YKAPR1 = YKAPR(IY,KZ)*(1.0 - FRY) + YKAPR(IY+1,KZ)*FRY      BMS4 136
    YKAPR2 = YKAPR(IY,KZ+1)*(1.0 - FRY) + YKAPR(IY+1,KZ+1)*FRY      BMS4 137
    YKAPR3 = YKAPR1*(1.0 - FRZ) + YKAPR2*FRZ                      BMS4 138
    CKAPR = YKAPR3 * YPRSF                                         BMS4 139
    YKAND1 = YKAND(IY,KZ)*(1.0 - FRY) + YKAND(IY+1,KZ)*FRY      BMS4 140
    YKAND2 = YKAND(IY,KZ+1)*(1.0 - FRY) + YKAND(IY+1,KZ+1)*FRY      BMS4 141
    YKAND3 = YKAND1*(1.0 - FRZ) + YKAND2*FRZ                      BMS4 142
    CKAND = YKAND3 * YNDSF                                         BMS4 143
    YKASM1 = YKASM(IY,KZ)*(1.0 - FRY) + YKASM(IY+1,KZ)*FRY      BMS4 144
    YKASM2 = YKASM(IY,KZ+1)*(1.0 - FRY) + YKASM(IY+1,KZ+1)*FRY      BMS4 145
    YKASM3 = YKASM1*(1.0 - FRZ) + YKASM2*FRZ                      BMS4 146
    CKASM = YKASM3 * YSMSF                                         BMS4 147
    TOTK = CKTLA + CKTPR + CKTND + CKTSM                          BMS4 148
    HNO3K = CKALA + CKAPR + CKAND + CKASM                          BMS4 149
    TMAQ = TMOR/TOTK                                              BMS4 150
    AMAQ = AMOR/HNO3K                                             BMS4 151
    REMAQ = TMAQ - AMAQ                                           BMS4 152
    IF (REMAQ) 120,120,125                                       BMS4 153
120 PRINT 514, TMAQ,AMAQ,REMAQ,HNO3K                             BMS4 154
    IF (K) 600,600,45                                          BMS4 155
125 BLAPR = 0.8187 - 0.1106*TMOR                                BMS4 156
    BPRPR = 1.0                                                  BMS4 157
    BNDPR = 1.0448 + 0.09874*TMOR                                BMS4 158
    BSMPR = -0.3795 + 0.9214*TMOR                                BMS4 159
    DEMS = XLAMOR/BLAPR + PRMOR/BPRPR + XNDMOR/BNDPR + SMMOR/BSMPR      BMS4 160
    XLAMAQ = XLAMOR*REMAQ/(BLAPR*DEMS)                            BMS4 161
    PRMAQ = PRMOR*REMAQ/(BPRPR*DEMS)                              BMS4 162
    XNDMAQ = XNDMOR*REMAQ/(BNDPR*DEMS)                            BMS4 163
    SMMAQ = SMMOR*REMAQ/(BSMPR*DEMS)                              BMS4 164
    XHNO3 = AMAQ/TMAQ                                             BMS4 165
    XLA = XLAMAQ/TMAQ                                             BMS4 166
    XPR = PRMAQ/TMAQ                                              BMS4 167
    XND = XNDMAQ/TMAQ                                             BMS4 168
    XSM = SMMAQ/TMAQ                                              BMS4 169
    XRE = REMAQ/TMAQ                                              BMS4 170
    XLASF = XLAMAQ/REMAQ                                          BMS4 171
    XPRSF = PRMAQ/REMAQ                                          BMS4 172
    XNDSF = XNDMAQ/REMAQ                                          BMS4 173
    XSMSF = SMMAQ/REMAQ                                          BMS4 174
    SXA = XHNO3 + XLA + XPR + XND + XSM                          BMS4 175
    IF (0.9999 - SXA) 130,140,135                                BMS4 176
130 IF (1.0001 - SXA) 135,140,140                                BMS4 177
135 PRINT 515, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ      BMS4 178
    IF (K) 600,600,45                                          BMS4 179
140 SXREA = XLASF + XPRSF + XNDSF + XSMSF                        BMS4 180
    IF (0.9999 - SXREA) 145,155,150                              BMS4 181
145 IF (1.0001 - SXREA) 150,155,155                              BMS4 182
150 PRINT 516, TMAQ,AMAQ,XLAMAQ,PRMAQ,XNDMAQ,SMMAQ,REMAQ      BMS4 183
    IF (K) 600,600,45                                          BMS4 184
155 IF (L - M) 165,160,165                                       BMS4 185
160 PRINT 517                                                    BMS4 186

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Figure 45. (Continued)

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165  PRINT 518,L,TMAQ,AMAO,XLAMAO,PRMAQ,XNDMAQ,SMMAO,REMAQ,XHNO3,XLA,XPBMS4 187
1R,XND,XSM,XRE,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 = ((XLAMAO - ROLAM)*RSC/S) + S1LAM BMS4 192
PRMOR = ((PRMAQ - ROPRM)*RSC/S) + S1PRM BMS4 193
XNDMOR = ((XNDMAQ - RONDM)*RSC/S) + S1NDM BMS4 194
SMMOR = ((SMMAO - ROSMM)*RSC/S) + S1SMM BMS4 195
GO TO 180 BMS4 196
175  TMOR = TMAQ*REX/S - F1M*F/S - ROTM*RSC/S + S1TM BMS4 197
AMOR = AMAQ*REX/S - FAM*F/S - ROAM*RSC/S + S1AM BMS4 198
XLAMOR = XLAMAO*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 = SMMAO*REX/S - FSMH*F/S - ROSMM*RSC/S + S1SMM BMS4 202
180  REMOR = TMOR - AMOR BMS4 203
SOM = MIN1F(TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMR) BMS4 204
IF (SOM) 185,185,190 BMS4 205
185  PRINT 519, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMR 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/REMR BMS4 214
YPRSF = PRMOR/REMR BMS4 215
YNDSE = XNDMOR/REMR BMS4 216
YSMSF = SMMOR/REMR 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,REMR 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
IF (1.0001 - SYREO) 215,220,220 BMS4 225
210  PRINT 521, TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMR BMS4 226
IF (K) 600,600,45 BMS4 227
220  LL = L + 1 BMS4 228
PRINT 522, LL,TMOR,AMOR,XLAMOR,PRMOR,XNDMOR,SMMOR,REMR,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 REXBMS4 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/REBMS4 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 (8HJYKTR=016F6.3,F6.4,F6.3)	BMS4 252
513	FORMAT (8HJYKAR=016F6.3,F6.4,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 POINT)	BMS4 257
518	FORMAT (2HJRI2,7F8.4,10F6.3)	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 261
521	FORMAT (18HJSYREO NOT EQUAL 17F10.4)	BMS4 262
522	FORMAT (2H SI2,7F8.4,10F6.3)	BMS4 263
523	FORMAT (6HJTMOR=F10.4)	BMS4 264
600	STOP 89	BMS4 265
	END	BMS4 266

Figure 45. (Continued)