A REINVESTIGATION OF THE THEORETICAL BASIS FOR
THE CALCULATION OF
ISOTHERMAL-ISOBARIC MASS TRANSFER IN GEOCHEMICAL SYSTEMS
INVOLVING AN AQUEOUS PHASE

by

ERNEST HENRY PERKINS
B.Sc., the University of British Columbia, 1975

A THESIS SUBMITTED IN PARTIAL FULFILMENT OF
THE REQUIREMENTS FOR THE DEGREE OF
MASTER OF SCIENCE

in
THE FACULTY OF GRADUATE STUDIES
Department of Geological Sciences

we accept this thesis as conforming
to the required standard

THE UNIVERSITY OF BRITISH COLUMBIA
May 1980

© Ernest Henry Perkins, 1980
In presenting this thesis in partial fulfilment of the requirements for an advanced degree at the University of British Columbia, I agree that the Library shall make it freely available for reference and study. I further agree that permission for extensive copying of this thesis for scholarly purposes may be granted by the Head of my Department or by his representatives. It is understood that copying or publication of this thesis for financial gain shall not be allowed without my written permission.

Department of Geological Sciences

The University of British Columbia
2075 Wesbrook Place
Vancouver, Canada
V6T 1W5

Date May 16, 1980
ABSTRACT

Many geochemical processes involve the reaction of an aqueous phase with minerals with which the aqueous phase is not in equilibrium. Prediction of the change in the composition and in the number of moles of phases and of aqueous species as the system proceeds toward overall equilibrium is made possible by differential equations formed from mass balance, mass action, ionic strength and activity of water equations. The equations developed by Helgeson, Brown, Nigrini and Jones (1970) have been examined and alternate forms of the differential equations which constrain reaction progress have been proposed. These new equations include correct terms for the change in the mass of water, the change in the activity of water and the change in the number of moles of each endmember of the solid solution phases. The equations have been formulated to allow a more efficient algorithm for numerical evaluation. General forms for all equations are presented. A FORTRAN program for the calculation of mass transfer in an isothermal and isobaric system and a description of the program are given.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>ii</td>
</tr>
<tr>
<td>TABLE OF CONTENTS</td>
<td>iii</td>
</tr>
<tr>
<td>LIST OF EQUATIONS</td>
<td>iv</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>v</td>
</tr>
<tr>
<td>LIST OF SYMBOLS</td>
<td>vi</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>viii</td>
</tr>
<tr>
<td>INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>CHOICE AND NUMBER OF COMPONENTS</td>
<td>2</td>
</tr>
<tr>
<td>THEORETICAL CONCEPTS</td>
<td>6</td>
</tr>
<tr>
<td>Mass Balance</td>
<td>8</td>
</tr>
<tr>
<td>Mass Action</td>
<td>11</td>
</tr>
<tr>
<td>Activity Coefficients</td>
<td>13</td>
</tr>
<tr>
<td>Activity Of Water</td>
<td>17</td>
</tr>
<tr>
<td>Solid Solution Minerals</td>
<td>19</td>
</tr>
<tr>
<td>THE GENERAL SOLUTION</td>
<td>25</td>
</tr>
<tr>
<td>The First Derivative</td>
<td>26</td>
</tr>
<tr>
<td>Higher Order Derivatives</td>
<td>32</td>
</tr>
<tr>
<td>Initial Solution Composition</td>
<td>33</td>
</tr>
<tr>
<td>Prediction Of Saturation</td>
<td>34</td>
</tr>
<tr>
<td>CONCLUDING REMARKS</td>
<td>36</td>
</tr>
<tr>
<td>SELECTED REFERENCES</td>
<td>37</td>
</tr>
<tr>
<td>APPENDIX 1</td>
<td>39</td>
</tr>
<tr>
<td>Ionic Strength</td>
<td>41</td>
</tr>
<tr>
<td>Mass Balance</td>
<td>42</td>
</tr>
<tr>
<td>Activity Of Water</td>
<td>43</td>
</tr>
<tr>
<td>Mass Action</td>
<td>46</td>
</tr>
<tr>
<td>APPENDIX 2</td>
<td>52</td>
</tr>
<tr>
<td>The Program PATH</td>
<td>52</td>
</tr>
<tr>
<td>Data Stucture For Unit 3</td>
<td>55</td>
</tr>
<tr>
<td>Data Structure For Unit 5</td>
<td>63</td>
</tr>
<tr>
<td>Restarting PATH</td>
<td>69</td>
</tr>
<tr>
<td>Error Messages</td>
<td>70</td>
</tr>
<tr>
<td>Example</td>
<td>72</td>
</tr>
<tr>
<td>APPENDIX 3</td>
<td>93</td>
</tr>
</tbody>
</table>
# LIST OF EQUATIONS

| Equation (1) | 4 |
| Equation (2) | 8 |
| Equation (3) | 9 |
| Equation (4) | 9 |
| Equation (5) | 10 |
| Equation (6) | 10 |
| Equation (7) | 11 |
| Equation (8) | 12 |
| Equation (9) | 12 |
| Equation (10) | 14 |
| Equation (11) | 15 |
| Equation (12) | 15 |
| Equation (13) | 15 |
| Equation (14) | 16 |
| Equation (15) | 16 |
| Equation (16) | 18 |
| Equation (17) | 18 |
| Equation (18) | 18 |
| Equation (19) | 20 |
| Equation (20) | 20 |
| Equation (21) | 21 |
| Equation (22) | 21 |
| Equation (23) | 22 |
| Equation (24) | 22 |
| Equation (25) | 23 |
| Equation (26) | 25 |
| Equation (27) | 27 |
| Equation (28) | 30 |
| Equation (29) | 30 |
| Equation (30) | 30 |
| Equation (31) | 30 |
| Equation (32) | 30 |
| Equation (33) | 32 |
| Equation (34) | 33 |
| Equation (1-A) | 40 |
| Equation (1-B) | 40 |
| Equation (1-C) | 41 |
| Equation (1-D) | 42 |
| Equation (1-E) | 43 |
| Equation (1-F) | 44 |
| Equation (1-G) | 45 |
| Equation (1-H) | 47 |
| Equation (1-I) | 48 |
| Equation (1-J) | 48 |
| Equation (1-K) | 48 |
| Equation (1-L) | 48 |
| Equation (1-M) | 49 |
| Equation (1-N) | 49 |
| Equation (1-O) | 50 |
| Equation (1-P) | 51 |
LIST OF TABLES

Table I ................................................................. 6
Table II ..................................................................... 46
Table III ................................................................. 62
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>A, B</td>
<td>Molal Debye-Huckel Parameters</td>
</tr>
<tr>
<td>a_c, a_j, a_s</td>
<td>Activity of the c\textsuperscript{th} component, of the j\textsuperscript{th} solid solution species, of the s\textsuperscript{th} aqueous species and of the i\textsuperscript{th} endmember of the \phi\textsuperscript{th} mineral, respectively</td>
</tr>
<tr>
<td>a_i, \phi</td>
<td>Ion size parameter of the \phi\textsuperscript{th} mineral</td>
</tr>
<tr>
<td>g_s</td>
<td>The derivative of ( \omega_e ) for the s\textsuperscript{th} aqueous species</td>
</tr>
<tr>
<td>c_s</td>
<td>Number of solid solution species of the \phi\textsuperscript{th} solid phase</td>
</tr>
<tr>
<td>end_\phi</td>
<td>True ionic strength of the aqueous solution</td>
</tr>
<tr>
<td>K_s</td>
<td>Equilibrium constant for the equilibrium reaction between the s\textsuperscript{th} aqueous species and the components</td>
</tr>
<tr>
<td>m_s</td>
<td>Molality of the s\textsuperscript{th} aqueous species</td>
</tr>
<tr>
<td>n_c, T</td>
<td>Total number of moles of the c\textsuperscript{th} component</td>
</tr>
<tr>
<td>n_i, \phi, n_r, n_s</td>
<td>Number of moles of the i\textsuperscript{th} endmember of the \phi\textsuperscript{th} mineral, the r\textsuperscript{th} reactant, the s\textsuperscript{th} aqueous species, and of water in the system, respectively</td>
</tr>
<tr>
<td>N_C \cdot</td>
<td>Total number of components</td>
</tr>
<tr>
<td>N_C _p</td>
<td>Number of components which are described by solid solution species</td>
</tr>
<tr>
<td>N_C _sp</td>
<td>Number of components described by aqueous species</td>
</tr>
<tr>
<td>N_P</td>
<td>Number of solid phases in equilibrium with the system</td>
</tr>
<tr>
<td>N_R</td>
<td>Number of phases reacting with the system</td>
</tr>
<tr>
<td>N_S</td>
<td>Number of aqueous species in the system</td>
</tr>
<tr>
<td>R</td>
<td>Number of non-component mass action equations</td>
</tr>
<tr>
<td>R</td>
<td>Gas Constant</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in Kelvins</td>
</tr>
<tr>
<td>w_e</td>
<td>For a charged species, the Deviation function; for a neutral species, a constant which when multiplied by the true ionic strength is equal to the activity coefficient of the species. Typically modeled using the activity coefficients of carbon dioxide.</td>
</tr>
</tbody>
</table>
$WG_1, WG_2$ Margules excess energy parameters for the first and second solid solution species in a binary solid solution, respectively

$WG_{1,\phi}, WG_{2,\phi}$ Margules excess energy parameters for the first and second solid solution species in the $\phi$th solid phase, respectively

$x_j, x_{1,\phi}, x_{2,\phi}$ Mole fraction of the $j$th solid solution species and of the first and second solid solution species in the $\phi$th mineral, respectively

$Z_s$ Charge on the $s$th aqueous species

$\tilde{I}_1, \tilde{I}_2$ Activity coefficients of CO$_2$ in water at ionic strengths of $\tilde{I}_1$ and $\tilde{I}_2$, respectively

$\gamma_s$ Activity coefficient of the $s$th aqueous species

$\lambda_{i,\phi}$ Activity coefficient of the $i$th solid solution species of the $\phi$th phase

$\xi$ Reaction progress variable

$v_{i,\phi,c}$ Number of moles of the $c$th component in one mole of the $i$th solid solution species of the $\phi$th phase.

$v_{r,c}$ Number of moles of the $c$th component in one mole of the $r$th reactant phase.

$v_{s,c}$ Number of moles of the $c$th component in one mole of the $s$th aqueous species.
ACKNOWLEDGEMENTS

The author wishes to express his sincere thanks to Dr. T.H. Brown, under whose supervision this thesis was written. His assistance, helpful comments and criticisms have helped this thesis immensely. Comments by Dr. H.J. Greenwood have also been of benefit.

The author is particularly grateful to his wife, Laurie, for her patience and moral support.

This research was funded by Natural Science and Engineering Research Counsel operating grant number A-8842.
INTRODUCTION

Any chemical system in partial equilibrium will tend to approach total equilibrium by transferring mass among the phases in the system. The total amount of mass transferred at any given stage of the reaction is a measure of the progress of the reaction. If no kinetic constraints exist, the progress of the system towards equilibrium can be analyzed by equilibrium thermodynamics even though reaction progress is path dependent and irreversible.

Although the concept of reaction progress has been present in the chemical literature for many years (De Donder, 1920; De Donder and Van Rysselberghe, 1936; Prigogine and Defay, 1954), only recently has it been applied to geological systems. Garrels and Mackenzie (1967) simulated the evaporative concentration of spring water by a distribution of species method, a non-linear and iterative approach. Unfortunately, this method has the major disadvantage that complete events (the saturation and subsequent dissolution of a phase) may be overlooked. Helgeson (Helgeson, 1968; Helgeson, Brown, Nigrini and Jones, 1970) recognized that the derivatives of the mass action and mass balance equations which constrain reaction progress form a system of linear equations. Helgeson modeled reaction progress as a continuous function by a power series in the derivatives, a method that can be solved by linear techniques. Subsequent work on mass transfer theory (for example: Fouillac, Michard and Bocquier, 1976) has generally been based on Helgeson's work although Karpov, Kay'min and Kashik (1973) and Parkhurst, Plummer and Thorstenson (1978) have used methods similar to Garrels and Mackenzie.
Application of mass transfer theory to geological systems (for example: Helgeson, Garrels and Mackenzie, 1969; Helgeson, 1970; Fouillac, Michard and Bocquier, 1976; Pfeifer, 1977; Villas and Norton, 1977) has shown that many different geochemical processes can be modeled by mass transfer calculations, thus leading to a better understanding of geochemical systems.

The purpose of this paper is to supplement and to make corrections to the theoretical basis of isothermal-isobaric mass transfer involving an aqueous phase as presented by Helgeson et al (1970). Modifications of the mass balance and mass action equations to correctly allow for the changing mass of water, a simple method to calculate the changing activity of water, and improved methods for the numerical solution of the mass transfer equations will be presented.

CHOICE AND NUMBER OF COMPONENTS

Generally elements, oxides, simple ionic species and electrons are used as components although any phase or species, real or imaginary, may be used equally well. The only constraint upon the nature and the number of components is that the components must form an independent basis for the compositional space of all possible phases and species in the system.

The maximum number of components needed to describe any system is the number of elements present in the system plus one. A reduction in the number of components (NC) occurs when there is a linear dependence between any two (or more) members of the component basis or when a component is not present in any of the phases or species.
Even though there is no unique choice of components and any independent basis will suffice to describe the system, a judicious choice of components often simplifies conceptual difficulties and shortens computations. For example, we have found that computations are made more efficient if some or all of the components have fixed chemical potentials. This will be discussed below.

In any system each stoichiometric phase\(^1\) in equilibrium with the system will fix one chemical potential at a given temperature and pressure, and each \(n\) component solid solution phase will arbitrarily fix \(n\) independent chemical potentials at a given temperature, pressure and composition. In this paper minerals in equilibrium with the system will be chosen as part of the component basis. Each stoichiometric mineral will be chosen as one of the components, and each \(n\) component solid solution mineral will be chosen as \(n\) of the \(NC\) components that describe the system. For increased accuracy during computations, the remaining components will be chosen from the most abundant independent aqueous species. Water will generally be chosen as a component because of its abundance.

When a phase or species is chosen as a component the component has the same composition and activity as that phase or species. If the bulk composition of the system lies outside of the convex space enclosed by the composition of the components, the total number of moles of some of the components may be negative. This can occur even though the phase, species or endmember which describes that component

\(^1\)Throughout this paper the term "stoichiometric phase" or "stoichiometric mineral" will be used to indicate phases that do not exhibit compositional variation.
is present in the system. When discussing the properties (number of moles, activity or molality) of a phase or species chosen to describe a component, the phrase "component phase or species" or the phrase "component species" will be used. A "non-component species" is any species or phase that is not a descriptor of the component basis.

Because a mineral may only be in equilibrium with the system during a portion of a reaction, the component basis will change each time a new mineral becomes saturated with respect to an aqueous phase or a mineral dissolves completely into the aqueous phase. Matrix operations (Greenwood, 1975) offer a simple method to change from one component basis to another.

In any system at equilibrium there are $NC$ mass balance equations, one for each component, and $R$ independent mass actions equations, one for each non-component phase or species in the system. $R$ is defined by:

$$R = NS - NC_{sp} + \sum_{\phi=1}^{NP} end_{\phi} - NC_p$$

(1)

$NS$ is the number of aqueous species in the system and $NP$ is the number of minerals in equilibrium with the system. $NC_{sp}$ and $NC_p$ are the number of components that are described by aqueous species and by solid solution species of minerals in equilibrium with the system, respectively. $end_{\phi}$ is the number of solid solution species of the $\phi$th mineral. If the $\phi$th mineral is stoichiometric, $end_{\phi}$ is equal to one; if it is a binary solid solution, $end_{\phi}$ is equal to two. Generally $NC_p$ is equal to the total number of endmembers of minerals present, but it will not be under two conditions: when any of the minerals have more
solid solution species than solid solution components, or when one of the solid solution components is already present as part of the basis.

All phases, species and endmembers present in the system can be easily related to the components by writing the system in a matrix format. Table I is a simple example in which the component basis is potassium feldspar, quartz, potassium ion, hydrogen ion and water. These components have been used to describe a variety of non-component aqueous species.

In Table I the $s$th column in the matrix contains the coefficients of the components ($v_{s,c}$) in the balanced chemical equation which describes the equilibrium between the component phases and species, and one mole of the $s$th species. These coefficients are also coefficients of the components in the mass action equation for that species. The last $R$ columns in the matrix are one set of the $R$ independent mass action equations. The $c$th row in the matrix in Table I contains the coefficients for the mass balance equation of the $c$th component. The $s$th position in the $c$th row is the number of moles of the $c$th component in one mole of the $s$th species ($v_{c,s}$) and this is multiplied by the total number of moles of the $s$th species to obtain the total number of moles of the $c$th component present because of that species.
Table I

<table>
<thead>
<tr>
<th></th>
<th>KAlSi$_3$O$_8$</th>
<th>SiO$_2$</th>
<th>K$^+$</th>
<th>H$^+$</th>
<th>H$_2$O</th>
<th>H$_4$SiO$_4$</th>
<th>H$_3$SiO$_4$</th>
<th>KOH</th>
<th>Al$^{+++}$</th>
<th>Al(OH)$^{+++}$</th>
<th>Al(OH)$_2$</th>
<th>Al(OH)$_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>KAlSi$_3$O$_8$</td>
<td>1 0 0 0 0 0 0</td>
<td>0 1 0 0 0 1</td>
<td>1 1 0 -3 -3 -3</td>
<td>0 0 1 -1 -1 -1</td>
<td>0 0 1 -1 -1 -1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SiO$_2$</td>
<td>0 1 0 0 0 1 0</td>
<td>1 1 0 -3 -3 -3</td>
<td>0 0 1 -1 -1 -1</td>
<td>0 0 1 -1 -1 -1</td>
<td>0 0 1 -1 -1 -1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K$^+$</td>
<td>0 0 1 0 0 0</td>
<td>0 0 1 0 0 0</td>
<td>0 0 1 -1 -1 -1</td>
<td>0 0 1 -1 -1 -1</td>
<td>0 0 1 -1 -1 -1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H$^+$</td>
<td>0 0 0 1 0 0</td>
<td>0 0 0 1 0 0</td>
<td>0 0 1 -1 -1 -1</td>
<td>0 0 1 -1 -1 -1</td>
<td>0 0 1 -1 -1 -1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H$_2$O</td>
<td>0 0 0 0 0 1</td>
<td>0 0 0 2 1 -2</td>
<td>0 0 1 -1 -1 -1</td>
<td>0 0 1 -1 -1 -1</td>
<td>0 0 1 -1 -1 -1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The components are potassium feldspar, quartz, potassium ion, hydrogen ion and water. Phases and species considered include H$_4$SiO$_4$, H$_3$SiO$_4$, KOH, Al$^{+++}$, Al(OH)$^{+++}$, Al(OH)$_2$ and Al(OH)$_3$ as well as the components.

The coefficients for the mass action equation of one mole of any phase or species to the component phases and species can be read from the column of the matrix corresponding to that phase or species. For example, the mass action equation for aluminum ion to the components can be written from the coefficients in the aluminum column. It is

$$
\ln K_{\text{Al}^{+++}} = -1 \ln a_{\text{Al}^{+++}} + \ln a_{\text{KAlSi}_3\text{O}_8} - 3 \ln a_{\text{SiO}_2} - 1 \ln a_{\text{K}^+} + 4 \ln a_{\text{H}^+} - 2 \ln a_{\text{H}_2\text{O}}
$$

In a similar fashion, the coefficients for the mass balance equation of each component is read across the row corresponding to that component. For example, the total amount of water in the system is

$$
n_{\text{H}_2\text{O},T} = n_{\text{H}_2\text{O}} + 2 n_{\text{H}_4\text{SiO}_4} + 1 n_{\text{H}_3\text{SiO}_4} + 1 n_{\text{KOH}} - 2 n_{\text{Al}^{+++}}
$$

The symbol for the coefficient of the $c$th component phase or species in the mass action equation for the $s$th species is $v_{c,s}$. The symbol for the coefficient describing the number of moles of the $s$th species in the mass balance equation of the $c$th component is $v_{s,c}$. Because the matrix method has been used to obtain these coefficients, their numerical value is identical.
THEORETICAL CONCEPTS

Helgeson showed that the progress of a reaction can be modeled as a Taylor's expansion in the derivatives of the mass action and mass balance equations taken with respect to reaction progress. The progress variable ($\xi$) was defined by DeDonder (1920), DeDonder and Van Rysselberghe (1936), and Prigogine and Defay (1954). The change in the number of moles of the phases and species ($dn/d\xi$) is calculated, and this change is added to the total number of moles of each phase and species. Various techniques exist to approximate nonlinear equations using their derivatives (Taylor's expansion, Predictor-Corrector, Runge-Kutta, Gear, etc) and the advantages and disadvantages of each type is reviewed in many standard numerical texts. The accuracy of these techniques increases with the number of derivatives used, but for typical mass transfer calculations; no more than three derivatives are usually needed.

Molalities and activities of aqueous species in hydrothermal systems commonly range from $10^{-10}$ to 3, but ranges of $10^{250}$ to 6 are not unusual. The derivatives of these molalities and activities with respect to reaction progress ($dm/d\xi$, $da/d\xi$) will have a similar range. To avoid ill-conditioned matrices these derivatives are solved as logarithmic derivatives. The change in the number of moles of a mineral with respect to reaction progress ($dn/d\xi$) can be calculated either as a "normal" or as a logarithmic derivative, although under certain conditions which are discussed later, there is an advantage using a "normal" derivative. By the use of the identity 

\[ n \, d\ln n = dn \]

the "normal" derivative can be easily calculated.
from the logarithmic derivative.

Mass Balance

The total number of moles of the $c$th component ($n_{c,T}$) in any geochemical system can be expressed as

$$n_{c,T} = \sum_{\phi=1}^{NR} \sum_{i=1}^{n\phi} v_{i,\phi, c} n_{i,\phi} + \sum_{s=1}^{NS} v_{s, c} n_s + \sum_{r=1}^{NR} v_{r, c} n_r$$

(2)

$NR$ is the number of phases reacting with the system. $n_s$, $n_{i,\phi}$, and $n_r$ are the number of moles of the $s$th aqueous species, of the $i$th endmember of the $\phi$th mineral in equilibrium with the system, and of the $r$th reactant, respectively. $v_{s, c}$, $v_{r, c}$, and $v_{i,\phi, c}$ are the number of moles of the $c$th component in one mole of the $s$th aqueous species, in one mole of the $r$th reactant phase, and in one mole of the $i$th endmember of the $\phi$th phase in equilibrium with the system, respectively. In a stoichiometric phase the number of endmembers is one, and the number of moles of that endmember equals the total number of moles of that phase.

The derivative of equation (2) with respect to reaction progress is
In a system closed with respect to mass equation (3) is equal to zero. If the system is not closed to some or all of the components (e.g., if the fluid phase flows through the system), then the change of mass of those components must be specified. This can be done in several ways. For example, the change of these components can be defined as a known function of reaction progress, or an equal number of other variables in the system can be specified. In the third alternative, additional equations which constrain reaction progress in an open system can be added to the system of equations, and then the change of these components with respect to reaction progress can become unknowns to be calculated.

The molality of the \( s \)th aqueous species \( (m_s) \) is related to the number of moles of the \( s \)th aqueous species and the number of moles of solvent water \( (n_{H_2O}) \) by

\[
m_s = \frac{n_s}{n_{H_2O}} \cdot 55.51
\]

Rearranging equation (4) to solve for the number of moles of the aqueous species and taking the logarithmic derivative with respect to the progress variable, gives
Because solution compositions are generally expressed in terms of molalities, equation (5) can be combined with equation (3) and rearranged to obtain

\[
\frac{dn_s}{d\xi} = \frac{n_{H_2O}}{55.51} \frac{m_s}{d\xi} \ln m_s + \frac{m_s n_{H_2O}}{55.51} \frac{dln n_{H_2O}}{d\xi}
\]

(5)

Equation (6) is the general derivative of the mass balance equation with respect to reaction progress. From equation (4) the molality of water is a constant, and its derivative with respect to reaction progress is zero. Therefore, the last summation begins at \(s=2\) because \(s=1\) has been reserved for water.

Equations (4) to (6), inclusive, can be directly compared to equations (61) to (63), inclusive, of Helgeson et al (1970). In addition to the different notation, a conceptual difference exists as well. Helgeson et al (1970) references molalities and masses of minerals to a constant amount of solvent water (1000 grams). Thus,
during any reaction which changes the amount of solvent water, the number of moles of each component (referenced to 1000 grams of solvent water) must change in response. The total number of moles of each solid phase (both reactant phases and those in equilibrium with the system) and the molality of each aqueous species must also change to remain referenced to 1000 grams of solvent water. The number of moles of solvent water remains constant which results in an increase in the total number of moles of water in the system.

In contrast, the equations presented here assume the number of moles of each component to be constant, and if solvent water is removed from the aqueous phase, only the molality of the aqueous species and the number of moles of solvent water will change in response.

**Mass Action**

The activity of any phase, species or endmember can be calculated from the activity of the component phases and species using the Law of Mass Action. For the $s$th aqueous species, the Law of Mass Action can be written as

$$
\ln k_s = \ln a_s + \sum_{c=1}^{N_C} v_{c,s} \ln a_c
$$

(7)

where $a_c$ and $a_s$ are the activities of the $c$th component phase or species and the $s$th non-component species, respectively. $v_{s,c}$ is the reaction coefficient of the $c$th component phase or species in the $s$th reaction. $k_s$ is the equilibrium constant for the reaction between the
$s$th aqueous species and the component phases and species. The activity of a solid phase or of a solid solution species in a solid phase is calculated using an equation identical in form to equation (7). The subscript "s" is replaced by the subscript "i,φ", where the new subscript indicates the $i$th endmember of the $φ$th mineral.

The relationship between the activity and the molality of an aqueous species is

$$a_s = \gamma_s m_s$$

where $\gamma_s$ is the activity coefficient of the $s$th aqueous species.

Equation (7) does not differentiate between the different types of components. However, it can be rewritten such that $NP$ minerals are part of the component basis. $NC_{sp} - 1$ aqueous species and water make up the remaining portion of the component basis. Combining equation (8) with this rewritten form of equation (7) and taking the derivative with respect to reaction progress, gives

$$\frac{d\ln K_s}{d\xi} = \frac{d\ln \gamma_s}{d\xi} + \frac{d\ln m_s}{d\xi} + \sum_{φ=1}^{NP} \sum_{i=1}^{end_φ} \nu_{i,φ,s} \frac{d\ln a_{i,φ}}{d\xi}$$

$$+ \nu_{H_2O,s} \frac{d\ln a_{H_2O}}{d\xi} + \sum_{c=2}^{NC_{sp}} \nu_{c,s} \frac{d\ln m_c}{d\xi}$$

$$+ \sum_{c=2}^{NC_{sp}} \nu_{c,s} \frac{d\ln \gamma_c}{d\xi}$$

The derivatives of the molalities of the aqueous component species are summed beginning with $c=2$ to allow the derivative of the activity of
water to be treated separately. If water is not a component species, then the water term is dropped and the aqueous component species are summed beginning with $c=1$. If the $i$th endmember of the $\phi$th mineral is not a component species, then $\nu_{i,\phi,s}$ (the coefficient of the $i$th endmember of the $\phi$th mineral in the $s$th reaction) is zero. If the number of endmembers of a solid phase is greater than the number of components of that phase, then a mass action equation similar in form and derivation to equation (9) exists to calculate the derivative of the activity of those endmembers.

Although advances have been made in the theoretical treatment of activity coefficients of aqueous species as a function of pressure and temperature (Helgeson and Kirkham, 1976), considerable uncertainty still exists about the activity coefficients of many aqueous complexes as a function of pressure and temperature. Owing to this only isobaric isothermal mass transfer will be considered. Thus, the derivative of the equilibrium constant with respect to reaction progress is zero, and equation (9) is equal to zero.

Activity Coefficients

The activity coefficient for any aqueous species is generally some function of the ionic strength, and as the ionic strength changes, the activity coefficient of the aqueous species changes. In some geochemical systems the mass transfer between the solid phases and the aqueous phase is large (for example, rain water falling on and reacting with surface material); in others, a significant amount of water may be consumed or released during a reaction. In both of these cases the
Ionic strength can change significantly during the reaction, and, thus, necessitate the calculation of the derivative of the activity coefficient with respect to reaction progress.

In some geochemical systems which involve concentrated brines, the ionic strength of the aqueous phase is essentially constant, and, consequently, the derivative of the activity coefficient with respect to reaction progress is approximately zero. This derivative should still be calculated, however, because including it will minimize numerical errors.

Many different methods exist to calculate activity coefficients, each with their own merits. The extended Debye-Hückel model will be used as an example, however, any other method could be used equally well.

Helgeson (1969) proposed that for a given temperature the activity coefficient for the $s$th aqueous species could be approximated by

$$\ln \gamma_s = \frac{-2.303 A Z_s^2 \sqrt{I}}{1 + \frac{a_s}{B} \sqrt{I}} + 2.303 w_e \frac{I}{I}$$

(10)

Where $I$ is the true ionic strength of the solution (defined below), and $A$ and $B$ are the molal Debye-Hückel parameters. $a_s$ and $Z_s$ are the ion size parameter and the charge on the $s$th aqueous species, respectively. For any neutral aqueous species $w_e$ is a function of the ionic strength of the solution and is assigned a value such that $\gamma_s$ is equal to the activity coefficient of carbon dioxide in water. For any charged species $w_e$ is the deviation function and is independent of ionic strength.
The true ionic strength of any aqueous system is defined as

$$
\bar{I} = \frac{1}{2} \sum_{s=2}^{NS} z_s^2 m_s
$$

(11)

Again the summation begins at $s=2$ because $s=1$ has been reserved for water.

The derivative of equation (10) with respect to reaction progress is

$$
\frac{d \ln \gamma_s}{d \xi} = 2.303 \left( C_s - \frac{A z_s^2}{2 \sqrt{\bar{I} \left[ 1 + \frac{A z_s^2}{B \sqrt{\bar{I}}} \right]} \right) \frac{d \bar{I}}{d \xi}
$$

(12)

where for the $s$th charged species $C_s$ is equal to the deviation function. For the $s$th neutral species $C_s$ is the derivative of $W_e$ with respect to ionic strength. The nature of this derivative depends on the functional form representing $W_e$. Typically, $W_e$ is interpolated from a matrix of values at different ionic strengths. Thus for a neutral species equation (12) would reduce to

$$
\frac{d \ln \gamma_s}{d \xi} = \left[ \frac{\left( \ln \gamma_{CO_2} - \ln \gamma_{CO_2} \right)}{(I_2 - I_1)} \right] \frac{d \bar{I}}{d \xi}
$$

(13)

$I_2$ and $I_1$ are known activity coefficients of carbon dioxide at ionic strengths $\bar{I}_2$ and $\bar{I}_1$, respectively, where $\bar{I}_2$ and $\bar{I}_1$ bound the ionic strength of the solution. Usually these coefficients are modeled using
the activity coefficient for carbon dioxide in water.

Equation (12) for charged species (or (13) for neutral species) can now be substituted for the derivative of the activity coefficient of all aqueous species in equation (9). This results in

$$
0 = \frac{d \ln m_s}{d \xi} + \sum_{c=2}^{N_C} \nu_{c,s} \frac{d \ln m_c}{d \xi} + \nu_{H_2O,s} \frac{d \ln a_{H_2O}}{d \xi} + 2.303 \left( c_s + \sum_{c=2}^{N_C} \nu_{c,s} c_s \right) + \\
\frac{A}{2 \sqrt{I}} \left[ \frac{z_s^2}{1 + a_s B \sqrt{I}} \right] + \sum_{c=2}^{N_C} \nu_{c,s} \frac{z_c^2}{1 + a_c B \sqrt{I}} \left[ d \frac{A \sqrt{I}}{d \xi} \right]
$$

Thus the derivative of the molality of any non-component species can be written in terms involving only the molalities and activities of the component species and of the derivative of ionic strength.

The derivative of equation (11), the ionic strength equation, with respect to reaction progress is

$$
0 = -\frac{1}{2} \sum_{s=2}^{NS} z_s^2 \frac{d \ln m_s}{d \xi} + \frac{d \bar{I}}{d \xi}
$$

From this it can be seen that the derivative of ionic strength with respect to reaction progress is a function of the molalities of all aqueous species and not just of the component species.
Equation (15) could now be substituted for the derivative of ionic strength with respect to reaction progress in equation (14), the mass balance equation. Rather than make this substitution which results in a derivation similar to that of Helgeson et al (1970), equation (15) will be introduced as a new constraining equation. The derivative of ionic strength with respect to reaction progress will be treated as a new unknown.

By avoiding the substitution of equation (15), the R mass action equations (equation (14)) are functions only of the derivatives of the molalities, of the number of moles of the components, and of the ionic strength. The implications of this will be discussed below; but briefly, this allows a more efficient algorithm to be used to predict the progress of the reaction.

Activity of Water

In many geochemical processes a concentrated brine reacts with phases in the system. During this process the activity of water is essentially constant, and its derivative with respect to reaction progress is approximately zero. However, for numerical reasons, this derivative should still be considered.

In those systems where the composition of the aqueous phase changes notably (for example, during the evolution of a salt lake), the change in the activity of water with respect to reaction progress must be known to adequately predict the solution path.

The activity of water in any system is dependent upon the number of moles of water and on the number of moles and activities of all
other species in the aqueous phase. A form of the isothermal isobaric Gibbs-Duham equation for the aqueous phase can be written to describe this:

$$\sum_{s=1}^{NS} n_s \ln a_s = 0$$  \hspace{1cm} (16)

$n_s$ and $a_s$ are the number of moles and the activity of the $s$th aqueous species, respectively. Solving equation (16) for the logarithmic derivative of the activity of water yields

$$\frac{\ln a_{H_2O}}{d\xi} + \sum_{s=2}^{NS} \frac{n_s}{n_{H_2O}} \frac{\ln a_s}{d\xi} = 0$$  \hspace{1cm} (17)

Combining equations (8), (4) and (12) (or (13) for a neutral species) allows the derivative of the activity of water with respect to reaction progress to be written in the form

$$0 = \frac{\ln a_{H_2O}}{d\xi} + \sum_{s=2}^{NS} \frac{m_s}{55.51} \frac{\ln m_s}{d\xi}$$

$$+ \sum_{s=2}^{NS} \frac{m_s}{55.51} 2.303 \left( c_s - \frac{A z_s^2}{2 \sqrt{I} \left[ 1 + \frac{\alpha_s}{a_s} B \sqrt{I} \right]^2} \right) \frac{dI}{d\xi}$$  \hspace{1cm} (18)

The derivative of the activity of water is a function of the derivative of ionic strength and of the derivative of the molality of all aqueous species. Equation (18) could be substituted for the derivative of the
activity of water with respect to reaction progress in equation (14), the mass action equation. Rather than make this substitution, equation (18) will be introduced as a new constraining equation and the derivative of the activity of water with respect to reaction progress will be treated as a new unknown. The argument for this is the same as the reason for including the derivative of ionic strength as a new unknown and will be discussed in detail below.

Solid Solution Minerals

For the standard state adopted here, at any given temperature and pressure, the activity of any phase in internal equilibrium and in equilibrium with the system, is one. The activity of the component species describing this phase are generally less than or equal to one. An exception occurs when one of the components describing a phase is an aqueous species. In this case, the standard state used for aqueous species permits these activities to equal or exceed one. When a solid solution endmember is compositionally and crystallographically distinct and is a compositional extreme point in the set of all possible compositions of the solid solution phase. A solid solution species is compositional distinct with a unique structural symmetry in this space. The set of all solid solution species includes the set of all solid solution endmembers. Solid solution components are the set of components used to describe the solid solution phase. Typically, solid solution endmembers are chosen as descriptors for solid solution components. The number of solid solution species or of solid solution endmembers is always equal to or greater than the number of solid solution components (Brown and Greenwood, in preparation). In this paper the solid solution components are chosen as component species to describe the entire system whenever a solid solution phase is in equilibrium with the system. The situation of two or more solid phases in equilibrium with the system and sharing components will not modify the equations developed. It will modify the method in which these equations are solved however, and is discussed below.
component has the same composition as the phase it describes (as with any stoichiometric phase), then the activity of the component is equal to one.

Rather than solve explicitly for the activities of the components in a solid phase, these activities will be related to the mole fraction and, ultimately, to the total number of moles of the components in the solid phase.

The activity of the \( j \)th solid solution species \( (a_j) \) in a \( k \)-component solid solution mineral is given by

\[
a_j = \lambda_j x_j
\]

\( x_j \) and \( \lambda_j \) are the mole fraction and the activity coefficient of the \( j \)th solid solution species, respectively.

The mole fraction of the \( j \)th solid solution species in a \( k \)-component solid solution mineral is related to the number of moles of each species in the solid solution by

\[
x_j = \frac{n_j}{\sum_{i=1}^{k} n_i}
\]

The change in the activity of the \( k \)th solid solution species can be related to the change in the activity coefficient of that species and to the change in the number of moles of all solid solution species in the solid solution. By substituting equation (20) for the mole fraction term in equation (19) and taking the derivative with respect to reaction progress, yields
There is no generally accepted solid solution model for any mineral with greater than two solid solution species, and in most cases, there is insufficient data to make such models. Data exists for many binary solid solution minerals and the Margules model (Thompson, 1967) is commonly used to represent these phases. An asymmetric Margules model will be used to illustrate the derivation of the derivative of the activity coefficient taken with respect to reaction progress. Any other solution model could be used equally well, including those in which the number of solid solution species is greater than the number of solid solution components.

In a binary asymmetric solid solution, Thompson (1967, equation 80a) relates the activity coefficient and the mole fraction of the first solid solution species by

$$\frac{d\ln a_j}{d\xi} = \frac{d\ln \lambda_j}{d\xi} + \frac{d\ln n_j}{d\xi} - \sum_{i=1}^{k} x_i \frac{d\ln n_i}{d\xi}$$  \hspace{1cm} (21)$$

$$a R T \ln \lambda_1 = x_2^2 (W_{G_2} + 2 (W_{G_2} - W_{G_1}) x_1)$$  \hspace{1cm} (22)$$

$T$ is the temperature in Kelvins and $R$ is the gas constant. $a$ is the number of possible mixing sites. $W_{G_1}$ and $W_{G_2}$ are the Margules excess free energy parameters for the first and second species of a binary solid solution, respectively. Substituting equation (20) into equation (22) and taking the derivative with respect to the progress variable allows the derivative of the activity coefficient of the first solid solution species to be written in terms of the number of moles of both
component species:

\[
\frac{\text{dln} \lambda_1}{\text{d}\xi} = \frac{2 x_2^2 x_1}{a\, R\, T} \left[ 3 x_1 \, WG_2 + WG_1 - 3 x_1 \, WG_1 \right] \frac{\text{dln} n_2}{\text{d}\xi} \\
- \frac{2 x_2^2 x_1}{a\, R\, T} \left[ 3 x_1 \, WG_2 + WG_1 - 3 x_1 \, WG_1 \right] \frac{\text{dln} n_1}{\text{d}\xi}
\]  

(23)

The equation for the second species of a binary solid solution is identical in form to equation (23) with only the subscripts "1" and "2" interchanged. Simplifying equation (21) for a binary solid solution and substituting equation (23) for the derivatives of the activity coefficients allows the derivative of the activity of the first solid solution species with respect to reaction progress for a binary solid solution to be written as

\[
\frac{\text{dln} a_1}{\text{d}\xi} = \frac{\text{dln} n_2}{\text{d}\xi} \\
- \frac{2 x_2^2 x_1}{a\, R\, T} \left[ 3 x_1 \, WG_2 + WG_1 - 3 x_1 \, WG_1 \right] \frac{\text{dln} n_1}{\text{d}\xi}
\]

(24)

Equation (24) can be substituted for the activity of the components formed from species of solid solution phases in equation (14). The result is the general mass action equation for any non-component aqueous species when the component basis is composed of stoichiometric and binary solid solution minerals, aqueous species and water. The resulting equation is
Equation (25) has been derived using a binary solid solution model. If the phase being considered is a stoichiometric phase, then the solid solution term in equation (25) is zero. This can be accomplished by letting \( \text{end} \) equal one, the mole fraction of the first solid solution
species \( X_i, \psi \) equal one, and the second \( X_{3-i, \psi} \) equal zero.

It is important to note that when a solid solution phase is in equilibrium with the system all solid solution species are needed to calculate the derivative of the unknown aqueous species with respect to reaction progress. This is the case even though only one of the solid solution species may be involved directly in the reaction forming that aqueous species.

Equation (25) has been derived using the logarithmic derivative with respect to reaction progress for the solid phases. When the phase has reached saturation the logarithmic derivative of the change in mass of each component of a solid solution phase is infinite. If the normal derivative is used, the solid solution term is divided by the number of moles of that solid solution species present, and this results in an infinite coefficient. To avoid this difficulty a trivial amount of the phase is assumed to be formed when any solid solution phase reaches saturation. This amount is subtracted from the total amount of that phase when more of that phase has precipitated. The problem does not exist for any stoichiometric phase if the "normal" derivative is used because the activity of these phases is one and is not a function of composition.

Equation (25) assumes that all phases are in internal equilibrium and in equilibrium with the system and that a zoned crystal can not be present. This equation could be modified to allow zoning by assuming each packet of solid solution phase produced was independent of the previous packet. Then as the phase reacts it would be dissolved in the reverse order of the precipitation order.
THE GENERAL SOLUTION

The derivative of the number of moles or of the molality of all phases and species has been treated as only a function of reaction progress. All other variables (temperature, pressure and total number of moles of the components) have been assumed to be constant. Thus, given a known amount of a phase or species it is possible to calculate its amount at any subsequent stage of reaction by means of a series expansion in the derivatives with respect to the progress variable. With infinitely precise computations and an infinite number of derivatives the Taylor's Expansion is exact. Lack of these two conditions is a serious disadvantage shared to some extent by all methods. However the clarity of the Taylor's Expansion and its ease of expansion to any number of derivatives are the reasons for using it here. A Taylor's Expansion in the number of moles of a phase at a given value of reaction progress can be written as

\[ n_{\xi+\Delta \xi} = n_\xi + \Delta \xi \frac{dn}{d\xi} + \frac{(\Delta \xi)^2}{2!} \frac{d^2n}{d\xi^2} + \ldots \]

\[ + \frac{(\Delta \xi)^j}{j!} \frac{d^jn}{d\xi^j} \]  

where \( n_\xi \) is the total number of moles when the reaction progress variable has a value of \( \xi \); \( n_{\xi+\Delta \xi} \) will be the number of moles when the progress variable has a value of \( \xi + \Delta \xi \). \( \Delta \xi \) is equal to the change in the progress variable, \( \frac{d^jn}{d\xi^j} \) is the \( j \)th derivative of the number of moles with respect to reaction progress evaluated at \( n = n_\xi \).

Once all derivatives are known, the function can be predicted and
solved accurately using the Taylor's Expansion. The error produced by considering a finite number of terms is less than the value of the first term not considered. Therefore when following the function, an error limit can be established, and the series evaluated only to the order of derivative whose value is less than that or the error. This will help optimize calculations within the error limits established.

The First Derivative

The derivatives of the $NC$ mass balance equations, of the ionic strength equation, of the activity of water equation and of the $R$ mass action equations (equations 6, 15, 18, 25, respectively) form a system of $NC + 2 + R$ equations. These equations are linear with respect to the $NC$ derivatives of the number of moles of the components (or of the molality of the components), to the derivative of ionic strength, to the derivative of the activity of water, and to the $R$ derivatives of the molality of the non-component species. Because these equations are linear in the unknown derivatives, this system of equations and unknowns can be written and solved in matrix notation. Equation (27) and the following discussion indicates the format.
In matrix A and in vectors B and C, rows 1 to \( NC \) are formed from the derivatives of the Mass Balance equation (equation 6). Row \( NC + 1 \) is formed from the derivative of the Gibbs-Duhem equation constraining the activity of water (equation 18). Row \( NC + 2 \) is formed from the derivative of the equation constraining the ionic strength of the aqueous phase (equation 15). The remaining rows are formed from the \( R \) derivatives of the Mass Action equations for every non-component species (equation 25).

Matrix A contains the coefficients of the derivatives from equations (6), (18), (15) and (25). Columns 1 to \( NC - 1 \) contain the coefficients of the derivatives in the number of moles or molality of the component phases or species. Column \( NC \) is reserved for the
coefficients of the derivative of the number of moles of water and it
water is not a component, then the $NC$th component will be here. Column
$NC + 1$ is reserved for the coefficients of the derivative of the
activity of water; column $NC + 2$ is reserved for the coefficients of
the derivative of ionic strength. The remaining $R$ columns contain the
coefficients of the derivatives of the molalities of the non-component
species. Inspection of equation (25) shows that partition $Y$,
dimensioned $R$ by $R$ and located in lower left of matrix $A$, is an
identity matrix.

Vector $B$ contains all of the unknown derivatives that have been
taken with respect to the progress variable. The first $NC - 1$
positions in this vector are the derivatives of the number of moles
($d \ln n / d \xi$) or of the molalities ($d \ln m / d \xi$) of the component phases
and species. The $NC + 1$ position is the derivative of the activity of
water ($d \ln n_{H_2O} / d \xi$). The $NC + 2$ position is the derivative of ionic
strength ($d \tilde{I} / d \xi$). The remaining positions are the derivatives of the
log molalities of the non-component species ($d \ln m / d \xi$).

Vector $C$ contains the constant terms from each equation. The
first $NC$ positions are the change in the number of moles of each
component as a result of the decrease in the reactant minerals. The
remaining positions are zero. The individual terms in this vector are
on the left hand side of the equal sign in equations (6), (18), (15)
and (25).

If two or more phases in equilibrium with the system share
components or if a solid solution phase has more solid solution species
than solid solution components, partition $Y$ of matrix $A$ will not be the
identity matrix. However, by substituting equation (26) for those
particular non-component solid solution species, partition Y can be recast into an identity matrix. In general, recasting is not possible if a solid solution phase has two or more non-component species. Under these conditions partitions U, V and W of matrix A must be expanded to include the coefficients of the derivatives of these species and partition Y will be correspondingly smaller.

The unknown derivatives in vector B can be solved by inverting matrix A and multiplying by vector C (equation 27). Rather than directly inverting matrix A, the inverse can be calculated by a partitioning method which only involves the direct inverse of a matrix of dimensions $NC + 2$. Because the computer time used to directly invert a matrix is proportional to the cube of the matrix size, a substantial amount of time is saved.\(^1\) Inversion by partitioning is discussed in most matrix algebra texts (for example: Hadley, 1961).

Equations (28) to (32), inclusive, indicate the method of solution.

\(^1\)The inverse of the identity matrix is the identity matrix and any matrix multiplied by the identity matrix remains unchanged. Due to the introduction of the derivatives of the activity of water and of the ionic strength as unknown derivatives, partition Y of matrix A (equation 26) is the identity matrix. Equations (29) through (32) inclusive, take advantage of this. If partition Y was not the identity matrix, then each of these equations would have inverse terms, and would result in a method of solution which would involve the inverse of all elements of matrix A. There would be no savings of computer processing time in solving the problem.
where: \( J = (U - VW)^{-1} \)  
\[ (29) \]
and: \( L = -WJ \)  
\[ (30) \]
and: \( K = -JV \)  
\[ (31) \]
and: \( M = I - WK \)  
\[ (32) \]

Where I is the identity matrix and the superscript "-1" indicates the inverse of the specified matrix.

The derivative of the molalities of the non-component species can be independently calculated from equation (25) after the derivative of the molality and the number of moles of the component phases and species, the ionic strength and the activity of water are known. Thus, the derivatives of the molalities of the non-component species computed
from equations (28) to (32) can be compared with those calculated from equation (25) to allow an estimation of the numerical error. Appropriate action can be taken if this error is too large.

The complete inverse of matrix \( A \) does not need to be calculated because only the derivatives of the molalities and the number of moles of the component species and phases, the derivative of ionic strength and the derivative of the activity of water need to be known to completely determine the system. Instead, if only the \( J \) and \( K \) partitions of the inverse of matrix \( A \) are determined, then all other derivatives can be calculated from equation (25). This is the same as the rearrangement and substitution of equation (25) for the derivatives of the molalities of all of the non-component species in the mass balance, activity of water and ionic strength equations (equations 6, 18, and 15, respectively). This reduces the system to \( NC + 2 \) constraining equations and \( NC + 2 \) unknown derivatives.

If this substitution is made, and because these \( NC + 2 \) equations are linear and share variables, further rearrangement and substitution can take place to reduce the number of equations. With each level of reduction less information about the system is available, to this information must be calculated independently whenever it is needed. Because information about all of the component phases and species, ionic strength, and the activity of water are needed at each step to test for mineral saturation and to determine the size of the next step, no saving in the number of calculations are obtained by reducing the system below \( NC + 2 \) equations and unknowns.

By reducing the system to \( NC + 2 \) equations and unknowns considerable reduction in computer storage is realized. The
disadvantage in this reduction is that the numerical error can no longer be estimated.

Higher Order Derivatives

Higher order derivatives can be obtained by taking the derivative with respect to reaction progress of the preceding order of derivative. For example, to obtain the second derivative of the mass action equation, the derivative of equation (25) with respect to reaction progress is taken. The general form for any order of derivative of the mass action, mass balance, ionic strength and activity of water equations are given in appendix 1.

The equations constraining the higher order of derivatives can be solved in a manner identical to that for the first derivative. If the derivative of equation (27) is taken and rearranged to solve for the second derivative of the number of moles (or molality) of the components, the ionic strength, the activity of water and the molality of the component species (contained in the vector $B'$), we have

$$B' = A^{-1}(C - A'B)$$  \hspace{1cm} (33)

Where ' indicates the first derivative of the terms in that matrix. The derivative of equation (33) can be taken and rearranged to solve for the third derivatives of the number of moles (or molality) of the components, the ionic strength, the activity of water and the molality of the non-component species (contained in the vector $B''$). It is
\[ B'' = A^{-1} \left( C' - A''B + 2A'B' \right) \]  

(34)

Where " indicates the second derivative of the terms in that matrix. Successive derivatives can be found similarly. It is important to note that matrix A needs only to be inverted once and is used to solve any order of the derivatives. Each successive derivative of equation (27) introduces only one new term that must be calculated: the \( k \)th derivative of the terms in matrix A. All other terms have been computed or solved in the previous order of derivatives. Thus evaluating each order of derivatives is rapid, and, therefore, sufficient terms can be used to accurately represent the function.

Initial Solution Composition

Given the total number of moles or the activity of each of the component phases and species, the molality of each of the aqueous species can be calculated using the Mass Action and Mass Balance equations. Many different authors (Van Zeggern and Story, 1970; Ting-Po and Nancollas, 1972; Wolery and Walters, 1975) have presented different methods to solve this type of problem. In conjunction with the mass transfer calculations a modification of the method of Wolery and Walters (1975) has been found to be the most convenient for finding the distribution of species. The modification is the changing of the component basis to include solid phases in equilibrium with the solution, to include aqueous species whose activities are known and fixed, and to include constraints on the activity of water. The
remaining components are given by a chemical analysis and charge balance restrictions.

Generally, the initial solution composition includes elements from all phases in the system even if the amount is trivial. If it does not, then when the first amount of that element is dissolved into the aqueous phase a distribution of species calculation must be performed. This is necessary because on addition of a new element to the system, the function describing reaction progress is discontinuous in all derivatives at that point.

During the mass transfer calculations, error in the molality of each aqueous species gradually accumulates even though the total number of moles of each component is known exactly. This error is most significant in species present in low concentration. When this error becomes too large, a distribution of species can be done to correct the molality of each aqueous species. In addition, when a phase first becomes saturated with respect to the aqueous phase, a distribution of species can be calculated with that new phase as part of the component basis. This ensures that the solution is in equilibrium with the components and that it is still on the function constrained by the reaction.

Prediction of Saturation

The activity quotient of any stoichiometric phase can be calculated using equation (7). When this activity quotient is equal to the equilibrium constant, then the stoichiometric phase has saturated with respect to the aqueous phase. In a similar manner, the activities of all solid solution species of a phase can be calculated with
equation (7). Then by iterative techniques the entire compositional range of the solid solution must be checked for saturation. The above technique, however is iterative and is required at every step. Consequently, this checking consumes considerable computer processing time. Alternatively, a modification of the method of Brown and Skinner (1974) can be used and is much more efficient. When a solid solution phase saturates with respect to an aqueous phase, the chemical potential plane defined by the aqueous phase is tangential to the Gibbs free energy surface of the solid solution phase. Given this, only the points of the Gibbs free energy surface of the solid solution phase which have a parallel tangent to the chemical potential plane of the aqueous phase need to be tested for saturation.

The points on the Gibbs free energy surface of the solid solution phase which have tangents parallel to the chemical potential plane of the aqueous phase will change their position on this surface as the composition of the aqueous phase changes. However, once these points of tangency are known for a given value of reaction progress, they can be predicted at any future value using a Taylor's expansion similar to equation (26). This is a linear problem and is much faster than iteratively checking for saturation at each step of reaction progress.
CONCLUDING REMARKS

The equations developed above to describe isothermal-isobaric rock water interaction have several major advantages over existing methods. The principal of these, the correct inclusion of the changing activity and mass of water, allows dehydration reactions and evaporation to be considered correctly. The speed of the computational method presented is proportional to the number of components plus two \((NC + 2)\) and is relatively independent of the number of species and phases in the system. The method presented by Helgeson et al (1970) is proportional to the total number of species and phases in the system, which is often an order of magnitude greater than the number of components. The computation method presented here allows a substantial reduction in computer processing time and provides a saving in computer storage for any given problem, thus allowing consideration of more complex problems.

A computer program embodying these equations has been written in the FORTRAN language and is described in Appendix 2. A listing of the program comprises Appendix 3.
SELECTED REFERENCES


APPENDIX 1

The main body of this thesis has discussed the development of the first derivative of the mass action, mass balance, ionic strength and activity of water equations taken with to reaction progress and the methods used for the numerical solution of these equations. By examination of the Taylor's expansion (equation (26)), it is apparent that by increasing the number of derivatives used in the expansion, the error for a given step size will be smaller. Alternately, a large step size can be taken within a given error limit if more derivatives are used in calculating the expansion.

For these reasons, the general form for the \( k \)th derivative of the mass balance, mass action, ionic strength and activity of water equations are presented in this appendix. These equations have been derived and generalized in the simplest form possible. As a result of this simplification, many derivatives have been expressed as "normal" derivatives rather than "logarithmic" derivatives.

Some of the summation signs in this appendix use an expression to calculate the upper limit of the summation. Integer arithmetic must be used to calculate these limits.

The general form of many of the equations in this appendix have been written as functions of other equations. This has been done for reasons of space and clarity. Thus, to obtain the full general form, one equation must be substituted into another.

The first "normal" derivative can be related to the first "logarithmic" derivative by
\[
\frac{dn}{dn} = n \frac{d\ln n}{dn}
\]  

(1-A)

Higher order "normal" derivatives can be related to the corresponding "logarithmic" derivatives by

\[
d^k n = \sum_{i=1}^{k} \frac{(k - 1)!}{(k - i)! (i - 1)!} d^{k-i} n \frac{d^i \ln n}{dn}
\]

(1-B)

where \( d^0 n = n \). \( d^k n \) and \( d^k \ln n \) are the \( k \)th derivative and the \( k \)th logarithmic derivative of \( n \) taken with respect to the progress variable, respectively.
Ionic Strength

The first derivative on ionic strength taken with respect to reaction progress is given in equation (15). The $k$th derivative of ionic strength taken with respect to reaction progress can be written as

$$0 = -\frac{1}{\xi} \sum_{s=2}^{NS} 2^s \frac{d^k m_s}{d\xi^k} + \frac{d^k I}{d\xi^k} \tag{1-C}$$

The "normal" derivative of the molalities taken with respect to reaction progress can be converted to "logarithmic" derivatives by the substitution of equation (1-B) for the "normal" derivatives.
Mass Balance

The first derivative of the mass balance equation taken with respect to reaction progress has been presented previously as equation (6). The general form for the \(k\)th derivative of the mass balance equation taken with respect to reaction progress can be written as

\[
\sum_{r=1}^{NR} v_{r,c} \frac{55.51}{d} \frac{d^k n_r}{d \xi} = - \sum_{\phi=1}^{NP} \sum_{i=1}^{en\phi} 55.51 v_{i,\phi} c n_{i,\phi} \frac{d^k n_{i,\phi}}{d \xi}
\]

\[
= - \sum_{s=1}^{NS} v_{s,c} \sum_{j=1}^{k} \frac{k!}{(k - j)! j!} \frac{d^{k-j} m_s}{d \xi^{k-j}} \frac{d^j n_{H_2O}}{d \xi^j}
\]

\[
= - \sum_{s=2}^{NS} v_{s,c} \sum_{j=1}^{k} \frac{k!}{(k - j)! j!} \frac{d^{k-j} n_{H_2O}}{d \xi^{k-j}} \frac{d^j m_s}{d \xi^j}
\]

As before, the "logarithmic" derivative can be substituted for any "normal" derivative using equation (1-B).
Activity of Water

The first derivative of the activity of water taken with respect to reaction progress has been presented previously as equation (18). The general form for the $k$th derivative can be written as

$$
0 = \frac{d^k \ln a_{H_2O}}{d\xi^k} + \frac{1}{55.51} \sum_{s=2}^{NS} \frac{d^k m_s}{d\xi^k} + 2.303 \sum_{s=2}^{NS} \left( \sum_{i=1}^{k} \frac{(k-1)!}{(k-i)! (i-1)!} \frac{d^{(k-i)} m_s}{d\xi^{k-i}} \frac{d^i f(\tilde{I})}{d\xi^i} \right) (1-E)
$$

d$f^k(\tilde{I})$ corresponds to the $k$th derivative of the extended Debye-Hückel equation for activity coefficients in an aqueous solution. The following equation describes the $k$th derivative of the Debye-Hückel model where $k$ is less than or equal to four. The inequality following each term indicates the lowest order of derivative that the term can be used in.
\[ \frac{d^k f(\tilde{r})}{d\xi^k} = \left( C_s + \frac{d g(\tilde{r})}{d\xi} \right) \frac{d^k \tilde{r}}{d\xi^k} \]

\[ \begin{align*}
+ \frac{d^2 g(\tilde{r})}{d\xi^2} & \sum_{j=1}^{k/2} \frac{d^j \tilde{r}}{d\xi^j} \frac{d^{k-j} \tilde{r}}{d\xi^{k-j}} Q(j, k-j) \\
+ \frac{d^3 g(\tilde{r})}{d\xi^3} & \sum_{i=1}^{k/3} \frac{d^i \tilde{r}}{d\xi^i} \sum_{j=i}^{k-i} \frac{d^j \tilde{r}}{d\xi^j} \frac{d^{k-j-i} \tilde{r}}{d\xi^{k-j-i}} Q(i, j, k-j-i) \\
+ \frac{d^4 g(\tilde{r})}{d\xi^4} & \sum_{h=1}^{k/4} \frac{d^h \tilde{r}}{d\xi^h} \sum_{i=h}^{k-h} \frac{d^i \tilde{r}}{d\xi^i} \sum_{j=i}^{k-h-i} \frac{d^j \tilde{r}}{d\xi^j} \frac{d^{k-j-i-h} \tilde{r}}{d\xi^{k-j-i-h}} Q(h, i, j, k-j-i-h)
\end{align*} \]

\[ k \geq 1, \quad k \geq 2, \quad k \geq 3, \quad k \geq 4 \]

\( C_s \) was discussed and defined in the text following equation (12). To be consistent with this definition, second and higher order derivatives of \( C_s \) are zero and have not been included. \( Q(j, k-j) \), \( Q(i, j, k-j-i) \) and \( Q(h, i, j, k-j-i-h) \) are numerical constants and are defined in table II.

\( g^k(\tilde{r}) \) represents the leading terms of the derivatives of the extended Debye-Hückel equation. It is defined by
\[ \frac{d^k g(\overline{r})}{d \xi^k} = \frac{A z^2}{s} \sum_{h=0}^{k-1} K(h, k) \left( a_s B \right)^h (\overline{r})^{-h/2} \]

\[ \left( -2^k \right) \left[ 1 + \frac{a_s B}{\sqrt{s}} \frac{k+1}{k!} \right] \]

(1-G)

\( K(h, i) \) is a set of numerical constants and is defined in table II.
Table II

\[ Q(j, k-j) \] is defined by the following.

\[
\begin{array}{cccc}
  j & k-j & Q(j, k-j) \\
  1 & 1 & 1 \\
  1 & 2 & 3 \\
  1 & 3 & 4 \\
  2 & 2 & 3 \\
  1 & 4 & 5 \\
  2 & 3 & 10
\end{array}
\]

\[ Q(i, j, k-j-i) \] is defined by the following.

\[
\begin{array}{cccc}
  i & j & k-j-i & Q(i, j, k-j-i) \\
  1 & 1 & 1 & 1 \\
  1 & 2 & 6 & 10 \\
  1 & 1 & 3 & 15 \\
  1 & 2 & 2 & 15
\end{array}
\]

\[ Q(1,1,1,1) = 1 \quad Q(1,1,1,2) = 10 \quad Q(1,1,1,1,1) = 1 \]

\[ K(h, i) \] is defined in the following matrix.

\[
\begin{array}{cccccc}
  K( ,1) & K( ,2) & K( ,3) & K( ,4) & K( ,5) \\
  K(0, ) & 1 & 1 & 3 & 15 & 105 \\
  K(1, ) & - & 3 & 12 & 75 & 630 \\
  K(2, ) & - & - & 15 & 141 & 1530 \\
  K(3, ) & - & - & - & 105 & 1830 \\
  K(4, ) & - & - & - & - & 955
\end{array}
\]
Mass Action

The first derivative of the mass action equation taken with respect to reaction progress has been presented previously as equation (25). The general form corresponding to the kth derivative of the mass action equation can be written as

\[
0 = \frac{d \ln m}{d \xi^k} + \sum_{c=2}^{NCSP} v_{c,s} \frac{d \ln m_c}{d \xi^k} + v_{H_2O,s} \frac{d \ln a_{H_2O}}{d \xi^k} \\
+ 2.303 \sum_{c=2}^{NCSP} \frac{d^k f(I)}{d \xi^k} + 2.303 \frac{d^k f(I)}{d \xi^k} \\
+ \sum_{\phi=1}^{NP} \sum_{i=1}^{end_{\phi}} \left( \frac{d \ln \lambda_{i,\phi}}{d \xi^k} \right) + \sum_{h=1}^{k} \left( \frac{d^{k-h} x_{3-i,\phi}}{d \xi^{k-h}} \frac{d \ln n_{i,\phi}}{d \xi^h} \right) \\
- \left( \frac{d^{k-h} x_{3-i,\phi}}{d \xi^{k-h}} \frac{d \ln n_{3-i,\phi}}{d \xi^h} \right) \right) (1-H)
\]

The derivative of f(I) with respect to reaction progress is defined in equations (1-F) and (1-G). The general form for the kth derivative of the activity coefficient taken with respect to reaction progress can be written as
\[
\frac{d^k \ln \lambda_{i,\phi}}{d\xi^k} = \frac{d M(x_{i,\phi})}{d\xi} \frac{d^k x_{i,\phi}}{d\xi^k}
\]
\[k \geq 1\]

\[+ \frac{d^2 M(x_{i,\phi})}{d\xi^2} \sum_{j=1}^{k/2} \frac{d^j x_{i,\phi}}{d\xi^j} \frac{d^{k-j} x_{i,\phi}}{d\xi^{k-j}} Q(j, k-j)
\]
\[k \geq 2\]

\[+ \frac{d^3 M(x_{i,\phi})}{d\xi^3} \sum_{m=1}^{k/3} \frac{d^m x_{i,\phi}}{d\xi^m} \left( \sum_{j=m}^{k-m} \frac{d^j x_{i,\phi}}{d\xi^j} \right)
\]

\[\frac{d^{k-j-m} x_{i,\phi}}{d\xi^{k-j-m}} Q(m, j, k-j-m)
\]
\[k \geq 3\]

\[Q(j, k-j) \text{ and } Q(i, j, k-j-i) \text{ are numerical constants which are defined in Table II.}\]

The first four derivatives of \(M(x_1)\) can be written as

\[
\frac{d M(x_1)}{d\xi} = -6 WG_1(x_1)^2 + 8 WG_1 x_1 - 2 WG_1
\]
\[(1-J)\]

\[
+ 6 (x_1)^2 WG_2 - 6 x_1 WG_2
\]

\[
\frac{d^2 M(x_1)}{d\xi^2} = -12 WG_1 x_1 + 8 WG_1 + 12 WG_2 x_1 - 6 WG_2
\]
\[(1-K)\]

\[
\frac{d^3 M(x_1)}{d\xi^3} = -12 WG_1 + 12 WG_2
\]
\[(1-L)\]
The derivatives corresponding to the second solid solution species can be obtained by interchanging the subscripts "1" and "2". All derivatives of $M(x_1)$ of order four or greater are equal to zero. Therefore, equation (1-1) does not need additional terms to describe any higher order derivatives.

The first three derivatives of the mole fraction of the first solid solution species in a binary solid solution phase are defined in equations (1-N), (1-O), and (1-P). To obtain the derivatives of the mole fraction of the second solid solution species, the subscripts "1" and "2" should be interchanged. The first derivative is

$$
\frac{d}{dx_1} x_{1, \phi} = \sum_{i=0}^{1} \left( \frac{d^i n_{1, \phi}}{d \xi^i} \left( \frac{d^{1-i} n_{1, \phi}}{d \xi^{1-i}} + \frac{d^{1-i} n_{2, \phi}}{d \xi^{1-i}} \right) \right)
$$

$$
= \left( \frac{1!}{(1-i)! i!} \right) \left[ (-1)^{(1-i+1)} \left( \frac{1}{i+1} \right) \right] \left[ \frac{n_{1, \phi} + n_{2, \phi}}{n_{1, \phi} + n_{2, \phi}} \right]
$$

(1-N)
The second derivative is

\[
\frac{d^2 x_{1,\phi}}{d\xi^2} = \sum_{i=0}^{2} \left( \frac{d^i n_{1,\phi}}{d\xi^i} \sum_{j=0}^{2-i} \left( \frac{d^j n_{1,\phi}}{d\xi^j} + \frac{d^j n_{2,\phi}}{d\xi^j} \right) \right)
\]

\[
\left( \frac{d^{2-j-i} n_{1,\phi}}{d\xi^{2-j-i}} + \frac{d^{2-j-i} n_{2,\phi}}{d\xi^{2-j-i}} \right)
\]

\[
\left( \frac{2!}{(2-i-j)! j! i!} \right) \left[ (-1)^{((2-j-i+1)! + 1)} \right]
\]

\[
\left[ (-1)^{((j+1)! + 1)} \right] / \left[ n_{1,\phi} + n_{2,\phi} \right]
\]

\[1-0\]
The third derivative is

\[
\frac{d^3 \chi_{1, \phi}}{d \xi^3} = \sum_{i=0}^{3} \left( \frac{d^i n_{1, \phi}}{d \xi^i} \sum_{k=0}^{3-i} \left( \frac{d^k n_{1, \phi}}{d \xi^k} + \frac{d^k n_{2, \phi}}{d \xi^k} \right) \right)
\]

\[
\sum_{j=k}^{3-i-k} \left( \frac{d^j n_{1, \phi}}{d \xi^j} + \frac{d^j n_{2, \phi}}{d \xi^j} \right)
\]

\[
\left( \frac{d^{3-k-j-i} n_{1, \phi}}{d \xi^{3-k-j-i}} + \frac{d^{3-k-j-i} n_{2, \phi}}{d \xi^{3-k-j-i}} \right)
\]

\[
\left( \frac{3!}{(3-k-j-i)! \; k! \; j! \; i!} \right) \left[ (-1)^{(k+1)! + 1} \right] \left[ (-1)^{(j+1)! + 1} \right] \left[ (-1)^{(3-k-j-i+1)! + 1} \right]
\]

\[
\left( n_{1, \phi} + n_{2, \phi} \right)
\]

\[ (1-P) \]

These derivatives, especially the first two, would be much simpler if the expanded form was presented. However, they have been left in this notation to show the difference between each order of derivative and to facilitate the writing of the higher order of derivatives.
APPENDIX 2

The Program PATH

A computer program based on the equations developed in the main body of this thesis has been written in the FORTRAN language. The program PATH calculates the mass transfer between an aqueous solution and minerals which are not in equilibrium with the solution. It uses three derivatives in the Taylor's expansion to predict and follow the mass transfer process. Solid solution phases are not considered by the program.

Optionally, the program will perform only a distribution of species calculation.

The program will terminate before the calculations are completed if the user has set time or page limits that are too small. It will also terminate because of certain error conditions which are discussed below. If it is necessary to continue the calculations, the program can be restarted using the data printed in the final execution cycle as the input data for the following run.

Approximately 102 pages of virtual memory (exclusive of I/O files) are used to load the program under the MTS (Michigan Terminal System) Operating System executing on an AMDAHL V6 computer. The time used depends on the complexity of the run but will range from seconds to tens of minutes. The program has been run successfully on the following computers: AMDAHL 470 V/6, IBM 370/168, IBM 370/158, CDC 7600, CDC 6600. On the /370-type computers, IBM's FORTRAN G and
FORTRAN H compilers have been used.

To run the program at the University of British Columbia under the MTS Operating System, the following command is used.

$RUN XXXX:PATH.O 3=FILENAME1 5=FILENAME2 6=FILENAME3 19=FILENAME4

where:

PATH.O is the object code for the program PATH and, in the example, is stored on the I.D. XXXX.

Fortran Unit 3 is assigned to the file from which the thermodynamic and the compositional data for all minerals, aqueous species and gases are read. The format of this file is described below and a short example is given.

Fortran Unit 5 is assigned to the file from which the data specific to each run is read. If the program is executed in batch mode, then Unit 5 defaults to the card reader. If the default is allowed to take place, the data must be punched on cards and must immediately follow the "$RUN" card. In this case the data cards must have as a terminating card, "$ENDFILE". When Unit 5 is assigned to a file, the "$ENDFILE" is automatically supplied when all of the data has been read and the end of the file has been reached. When executed from a terminal, Unit 5 defaults to the terminal keyboard, however no messages prompting for the input data are sent to the keyboard.
printer/display. The format of this file is described in detail below and an example is given.

Fortran Unit 6 is assigned to a file or a device to which the program results are to be directed. If the program is executed in batch mode, the unit will default such that the results are printed. If it is run from a terminal, the unit will default such that the results will be directed to the terminal's output device. If a permanent record is desired, the unit should be assigned to a file stored on disc or on magnetic tape.

Fortran Unit 19 is automatically assigned by the program when running on the MTS system at the University of British Columbia but must be assigned to a file at other installations. This unit is used as a "core-to-core" buffer and is used to alter the form in which the character data is stored. When assigned to a file, it can be thought of as a one line file on which every "WRITE" is followed by a "REWIND", then by a "READ" and again by a "REWIND".
Data Structure for Unit 3

This file contains all of the compositional and thermodynamic data for all phases, aqueous species and gases that will be considered by the program. Generally this file does not change from run to run and is stored on disc or magnetic tape.

Record 1: The "A" Debye-Hückel term. One value is required for each of the temperatures 0.0, 25.0, 50.0, 150.0, 200.0, 250.0, 300.0 °C.

FORMAT(8F8.4)

Record 2: The "B" Debye-Hückel term. One value is required for each of the temperatures 0.0, 25.0, 50.0, 150.0, 200.0, 250.0, 300.0 °C.

FORMAT(8F8.4)

Record 3: The deviation function (B). One value is required for each of the temperatures 0.0, 25.0, 50.0, 150.0, 200.0, 250.0, 300.0 °C.

FORMAT(8F8.4)

Record 4: The activity coefficient of carbon dioxide in a NaCl solution at infinite dilution. It is used in calculating activity coefficients of neutral species. One value is required for each of the temperatures 0.0, 25.0, 50.0, 150.0, 200.0, 250.0, 300.0 °C.

FORMAT(8F8.4)
Record 5: The activity coefficient of carbon dioxide in a one molal NaCl aqueous solution. It is used in calculating the activity coefficients of neutral species. One value is required for each of the temperatures 0.0, 25.0, 50.0, 150.0, 200.0, 250.0, 300.0 °C.
FORMAT(8F8.4)

Record 6: The activity coefficient of carbon dioxide in a two molal NaCl aqueous solution. It is used in calculating the activity coefficients of neutral species. One value is required for each of the temperatures 0.0, 25.0, 50.0, 150.0, 200.0, 250.0, 300.0 °C.
FORMAT(8F8.4)

Record 7: The activity coefficient for carbon dioxide in a three molal NaCl aqueous solution. It is used in calculating the activity coefficients of neutral species. One value is required for each of the temperatures 0.0, 25.0, 50.0, 150.0, 200.0, 250.0, 300.0 °C.
FORMAT(8F8.4)

Record 8: The number of different chemical elements in the data records describing the atomic symbols (Record 9) and the atomic weights (Record m). This is program variable NCTZ.
FORMAT(1X,I3)

Record 9: NCTZ atomic symbols. There is one for each element which is
to be used in describing the composition of the phases of the species and of the gases in the data file. Seven symbols per record: each left justified in its field.

\texttt{FORMAT(7(4A1,4X))}

Record m: NCTZ atomic weights for the elements defined in Record 9. They must be in the same order as the atomic symbols. Seven values per record.

\texttt{FORMAT(7F10.5)}

Record n: A control record which will determine the nature of the composition and thermodynamic data following it. This data may be followed in turn by another control record and more composition and thermodynamic data. Only the following control records are possible: "**MINERAL DATA**", "**AQUEOUS SPECIES**", "**GASES**", "**REFERENCES**" and "**STOP**". Control records, with the exception of "**STOP**", can be used as often as needed and can occur in any order. The control records must be exactly as shown and must start in character position one. These records will be discussed in turn below.

\texttt{FORMAT(A1,5A4)}

**MINERAL DATA**

All records following this are treated as compositional and thermodynamic data for solid phases until another control record is encountered. The data records occur in pairs and
have the form

| NAME | FORMULA | ABV | REF # | DELTA | H | S | A | B | C | V |

and use the following format statements

FORMAT(1A1,25A4)
FORMAT(5X,6F10.3) ,
respectively.

For the record

| NAME | FORMULA | ABV | REF # |

which has the format (1A1,25A4),

NAME is the name of the mineral and starts in character position two. It can be of any length but only the first sixteen characters are used.

FORMULA is the mineral formula and is written in the form ZN(5)C(2)O(8)H(2). Real numbers (up to 4 figures with a decimal point) can be used instead of integers. The alphabetic characters corresponding to the atomic symbols must have been defined by Record 9. At least four blank spaces must separate NAME and FORMULA.

ABV is a abbreviation of the name and is used for plotting purposes. It can be any length, but only the first four characters are used. At least four blank spaces must separate FORMULA and ABV.

REF. # is any alphanumerical string for documentation purposes. REF. # is optional and is ignored by the program. At least four blank spaces must separate ABV and REF. #.

NAME, FORMULA and ABV must use less than one hundred and one
character positions.

For the record

```
DELTA H  S  A  B  C  V
```

which has the format (5X,6F10.3),

DELTA H is the delta enthalpy of formation from the elements for the phase. The units used are joules. If the enthalpy is greater than 999999., then the phase will not be considered.

S is the third law entropy, measured in joules.

A, B and C are the heat capacity terms for the Kelly-Meyer heat capacity function.

V is the volume in cubic centimeters.

**AQUEOUS SPECIES**

All records following this are treated as compositional and thermodynamic data for the aqueous species until another control record is encountered. Aqueous species data records must occur in pairs and have the form

```
NAME  FORMULA  REF #  c
DELTA H  S  A  a  CHARGE
```

and use the following format statements

```
FORMAT(1A1,25A4)
FORMAT(5X,6F10.3),
```

respectively. The format of these data records is exactly the same as that for the mineral data, except there is no abbreviation of the name (ABV) and there are no B and C heat
capacity terms. Two new terms have been added:
"$\tilde{a}$" is the Debye-Hückel size term for each ion and complex.
CHARGE is the charge on the ion or species. If the charge is
greater than 9.9, then the charge is assumed to equal
zero, and an activity coefficient of one is used for
that species.

**GASES**

All records following this are treated as compositional and
thermodynamic data for the gas species until another control
record is encountered. Gas data records must occur in pairs
and have the form

```
NAME FORMULA ABV REF #
DELTA H S A B C
```

and use the following format statements

```
FORMAT(1A1,25A4)
FORMAT(5X,6F10.3)
```

respectively. The format of these data records is exactly
the same as for the mineral data. Note that there is no
volume term (V) for gases.

**REFERENCES**

All records following this control record are ignored by the
program unless a control record or an $ENDFILE$ is
encountered. Usually, data references (see example in Table
III) are listed in this portion of the file but any
information, including blank lines, can be a part of this
section.
**STOP**

When this control record is encountered, reading of the data file is terminated. This record is optional and, generally, a $ENDFILE is used instead.
**Table III**

Example of Unit 3 Data Structure

<p>| | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4884</td>
<td>0.5095</td>
<td>0.5471</td>
<td>0.6019</td>
<td>0.6915</td>
<td>0.8127</td>
<td>0.9907</td>
<td>1.2979</td>
<td></td>
</tr>
<tr>
<td>0.3241</td>
<td>0.3284</td>
<td>0.3347</td>
<td>0.3425</td>
<td>0.3536</td>
<td>0.3659</td>
<td>0.3807</td>
<td>0.4010</td>
<td></td>
</tr>
<tr>
<td>0.0174</td>
<td>0.0410</td>
<td>0.0440</td>
<td>0.0460</td>
<td>0.0470</td>
<td>0.0470</td>
<td>0.0340</td>
<td>0.0</td>
<td></td>
</tr>
<tr>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td></td>
</tr>
<tr>
<td>1.3100</td>
<td>1.2700</td>
<td>1.2300</td>
<td>1.2000</td>
<td>1.1900</td>
<td>1.2300</td>
<td>1.3400</td>
<td>1.5000</td>
<td></td>
</tr>
<tr>
<td>1.6700</td>
<td>1.5700</td>
<td>1.4900</td>
<td>1.4400</td>
<td>1.4000</td>
<td>1.4700</td>
<td>1.6700</td>
<td>2.0000</td>
<td></td>
</tr>
<tr>
<td>2.0600</td>
<td>1.9300</td>
<td>1.7800</td>
<td>1.7400</td>
<td>1.7000</td>
<td>1.7400</td>
<td>1.8600</td>
<td>2.2900</td>
<td></td>
</tr>
</tbody>
</table>

**MINERAL DATA**

**AQUEOUS DATA**

**GASES**

**REFERENCES**

Ref. #1 HELGESON 1977 SUPCRIT DATA SET
Ref. #2 BROWN 1976 CALCULATED
Ref. #3 HELGESON 1969 A.J.S. VOL. 267, P 729-408
A normal data base may consist of hundreds of phases, aqueous species and gases but to simplify the example in Table III, it has only three phases, three aqueous species and two gases.

The first eight line images in the example correspond to program records 1 to 8. The following line image is the number of chemical elements (NCTZ) and is followed by six line images containing the 37 (NCTZ) atomic symbols. These are followed by six line images of the 37 (NCTZ) atomic weights. The atomic symbols and the atomic weights are in the same order and correspond to each other.

The data images "**MINERAL DATA**, **AQUEOUS DATA** and **GASES** and the data images following them are self-explanatory from the data record description. The **REFERENCE** information is never used or even printed by the program. In this example, however, the REF. # from the data section corresponds to the data sources given in the **REFERENCE** data images and is for the investigator's own information.

Data Structure for Unit 5

This file contains all of the data for a specific execution. Unlike Unit 3 on which the data is generally static, the data in this file will change from one modeling attempt to another. When executing this program with a given set of data on this unit for the first time, it is recommended that the maximum step size be set to one and the results examined for correctness.

Record 1: Title card 1
FORMAT(20A4)

Record 2: Title card 2

FORMAT(20A4)

Record 3: T, P, NRT, AMH20, NDLINC, MAXI, IMX, ISX, IGX

FORMAT(2F10.3,I5,F10.3,5I5)

T is the temperature in degrees Celsius.
P is the pressure in bars. Use 1 bar because the program does not consider aqueous species at other pressures.
NRT is the number of initial reactants. If NRT is equal to 0, then only a distribution of species calculation is done.
AMH20 is currently not used. Leave this field blank.
NDLINC is the number of steps between each print cycle. There will automatically be a report each quarter of a log unit once log is greater than -6.0.
MAXI is the maximum number of steps in the execution. If this field is blank, it defaults to 10000.
IMX, ISX, IGX are the number of minerals, aqueous solution species and gases, respectively, from Unit 3 that will not be considered during this run. The names of the excluded phases and species will be specified in Records m, n and o.

Record 4: NION
The name of the ion used for electrical balance. This ion must be a charged aqueous species and must be present in the **AQUEOUS SPECIES** section of the data read from Unit 3. This ion must be one of the component species, and the data for this ion must be given as a molality. Assigning this ion as a component species with a given molality will be discussed in Record p. The molality given by the user on Record p will be varied by the distribution of species subroutine until the aqueous solution is electrically balanced. Thus, the initial molality of this ion is used as a first guess for deriving the final, calculated molality. It must be left justified in the "A" format field.

Record 5: RR, AM, NAM

FORMAT(F5.3,5X,F10.5,5X,5A4)

This record is repeated NRT times, once for each reactant mineral. If NRT (see Record 3) is zero, this record is not needed.

RR is the reaction rate of the reactant mineral relative to the progress variable. Use 1.0 as a default value.

AM is the amount, in grams, of the reactant mineral.

NAM is the name of the reactant mineral as it appears in the data records on Unit 3. NAM must be left justified in the "A" format field.

Record m: IM
FORMAT(3(5A4,5X))

Names of the minerals to be suppressed. There must be IMX (see Record 3) names, 3 per record, left justified in the "A" format field. If IMX is equal to 0, this record is not needed. The names must be identical to the names as they appear in the data records on Unit 3.

Record n: IS

FORMAT(4(2A4,12X))

Names of the aqueous species to be suppressed. There must be ISX (see Record 3) names, 4 per record, left justified in the "A" format field. If ISX equal to is 0, this record is not needed. The names must be identical to the names of the aqueous species as they appear on Unit 3.

Record o: IG

FORMAT(3(5A4,5X))

Names of the gases to be suppressed. There must be IGX (see Record 3) names, 3 per record, left justified in the "A" format field. If IGX is equal to 0, this record is not needed. The names must be identical to the names of the gases as they appear on Unit 3.

Record p: MOA, NDX, TOTM, NAM, FORM

FORMAT(2I2,E10.3,60A1)

This set of records specifies the set of component phases,
species and gases used during the distribution of species calculation and defines the compositional space of the system. There are $NC - 1$ records, where $NC$ is the number of components needed to describe the system. Each of the records describes one component in the system which is to be constrained. Water is automatically added as a constraint by the program. In a non-redox system composed of $N$ elements, the user must supply $N - 1$ constraints. In any redox system composed of $N$ elements, the user must supply $N$ constraints. All constraints (including water) must be linearly independent!

If executing in batch mode, the last record must be an "$ENDFILE". If this data is being read from a file, the "$ENDFILE" will be supplied automatically.

The variables are described in an order different than that required for the data record in order to simplify the explanation.

NAM is the name of the component phase, species or gas and is left justified in the "A" format field. It must start in column 15. The name must be identical to the name as given on Unit 3.

FORM is the formula of the component phase, species or gas and follows the form given for formulas discussed in the data records for Unit 3 (see Unit 3, **MINERAL DATA**). There must be four blank spaces between NAM and FORM.

NDX indicates whether the state of the component is a aqueous species ($NDX = 0$), stoichiometric solid phase ($NDX = 1$),
solid solution phase (NDX = 2, this code is currently not used), or a gas (NDX = 3). See below for the relationship among NDX, TOTM and MOA.

TOTM is the number of grams, the molality, the log activity or the log fugacity of the component phase, species or gas.

MOA indicates whether the data in TOTM is moles/molality (MOA = 00) or log activity/fugacity (MOA = 01).

If NDX is 01, indicating a solid phase, then TOTM is assumed to equal the total number of grams of that phase regardless of the setting of MOA. If NDX is 03, indicating a gas, then MOA must be equal to 01 and TOTM will contain the log fugacity of that gas.

The following example is the data assigned to Unit 5 to model the reaction of potassium feldspar with a one molal sodium chloride solution at 25 C. and one bar total pressure. The initial amount of potassium feldspar present is ten grams. The initial pH is 5.5 and the solution is saturated with respect to quartz (i.e., quartz is in equilibrium with the solution). This example uses chloride ion to maintain electrical neutrality within the solution. This data deck specifies there will be a print cycle each 100 steps, and that the run will stop after 10000 steps or sooner if the solution comes to equilibrium. The first record in the example data deck is the title record indicating " TEST RUN ...... " and the last is the record specifying the potassium ion molality.
TEST RUN OF DISSOLUTION OF K-FELDSPAR IN ONE MOLAL NA(CL) SOLUTION AT 25 DEGREES

298.15 1.0 1 10010000

CL-
1.0 10.0 K-FELDSPAR
00001.0 NA+ NA(1)
00001.0 CL- CL(1)
0100-5.5 H+ H(1)
010110.0 ALPHA-QUARTZ SI(1)O(2)
0000 0.5E-10AL+++ AL(1)
00000.05 K+ K(1)

Restarting PATH

To restart the program, the data records used for Unit 5 are identical with the initial data used with two major exceptions.

The amount in grams of the reactant phases will have changed, thus in record 5, AM will be different for each reactant phase. One or more of the reactants may have been consumed, in which case NRT must be decreased by one (or more) in Record 3 and there will be one (or more) less Record 5's required.

The molalities of the component aqueous species and the number of grams of the component phases will have changed. The component basis has most likely changed as well. The component basis existing during the final print cycle can be read and these components used as data records for Unit 5. Use activities in constraining all of the component aqueous species except for the component species chosen for charge balance. It must be given as a molality.
Error Messages

The following are error messages commonly encountered while using the program. Possible causes are listed with the messages.

"SINGULAR MATRIX RETURNED FROM INVERSE ROUTINE. THE COMPONENTS PASSED TO IT FOR THE NEW BASIS MUST NOT BE INDEPENDENT. THESE COMPONENTS ARE ............"

Check input data because initial components chosen by user are not independent. Remember that water is automatically assigned as a component by the system.

"A CONSTRAINING PHASE CONTAINS TWO OXIDATION STATES - BUT THERE IS NO REDOX COUPLE. YOU MUST HAVE A REDOX COUPLE IF YOU HAVE TWO OXIDATION STATES."

Check your input data as per error message.

"IMPROPERLY FORMATED DATA BANK. LINE IN ERROR IS ...... "

Error in the thermodynamic data file on Unit 3. Line with error is shown. Correct and rerun.

"PHASE BOUNDARY NOT FOUND IN XXXX HALVINGS"

This indicates that the program, for reasons due to numerical rounding, can not find the exact point at which the phase has become saturated. Typically this can solved by restarting the program using data from the preceding step.

" THE SPECIES "----" CHOSEN AS THE ION TO BE BALANCED ON COULD NOT BE FOUND "

or
"COMPONENT "----" COULD NOT BE FOUND. CHECK IF COMPONENT IS PRESENT IN DATA DECK AND THAT YOU HAVE SPELLED IT THE SAME AND THAT IT IS LEFT JUSTIFIED IN THE INPUT FIELD."  
"ALSO CHECK THAT THIS PHASE DOES NOT HAVE TWO OXIDATION STATES IF THE SOLUTION CONSTRAINTS ONLY ONE. "  

Self explanatory.

"CONCENTRATION OF ION DRIVEN NEGATIVE WHILE TRYING TO ACHIEVE ELECTRICAL BALANCE "  

Choose ion with opposite charge to the present one for the charge balance ion.

"IMPOSSIBLE CONSTRAINTS FOR DISTRIBUTION OF SPECIES "----" DRIVEN NEGATIVE "  
or  
"FAILURE TO CONVERGE ON CONCENTRATION IN 25 CYCLES. "  

The data defines a solution composition that is impossible. Reconsider Unit 5 data.

"STEP SIZE HAS GONE TO SMALL. "  
The program can no longer follow the mass transfer function, because the error has gotten too large. This is also the result of numerical rounding techniques. By restarting the program at the previous step, this error can be corrected.

"THIS RUN HAS BEEN TERMINATED BECAUSE THE INITIAL SOLUTION IS SUPERSATURATED WITH RESPECT TO ONE OR MORE PHASES. "  

Self explanatory. Examine input data for Unit 5 and lower some of the activities or molalities of the components.
Example

This example simulates the reaction of potassium feldspar with an aqueous solution in equilibrium with quartz. It uses the same input data for Unit 5 as was given above.

This example was run on an AMDAHL 470 V/6 Model II computer under the Michigan Terminal System (MTS) and took 2.9 CPU seconds. There may be slight numerical differences between this example and the same executed on another type of computer because of the possible differences in word length, exponentiation and rounding.
Test run of dissolution of K-feldspar in one molal NaCl solution at 25 degrees.

Temperature (Kelvin) of this run is 298.15
Pressure (bars) of this run is 1.00

Maximum number of steps is 10000
Number of steps between each print out is 100

Ion chosen for electrical balance is Cl-
Moles of solvent H2O in system is 55.508250

*********** Initial Reactants ***********

<table>
<thead>
<tr>
<th>Ratio Present</th>
<th>Grams Present</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-feldspar</td>
<td>1.00000</td>
</tr>
</tbody>
</table>

*********** Initial Solution Constraints ***********

- 1.0000000E+01 molality Na+ Na(1) (aqueous species)
- 1.0000000E+01 molality Cl- Cl(1) (aqueous species)
- -0.5500000E+01 log act. H+ H(1) (aqueous species)
- 0.10000000E+01 grams Alpha-quartz Si(1)O(2) (solid)
- 0.50000000E-10 molality Al+++ Al(1) (aqueous species)
- 0.50000000E-01 molality K+ K(1) (aqueous species)
TEST RUN OF DISSOCIATION OF K-FELDSPAR IN ONE MOHAL NACL SOLUTION AT 25 DEGREES

DISTRIBUTION OF SPECIES CALLED AT STEP 0

<table>
<thead>
<tr>
<th>AQUEOUS SPECIES</th>
<th>SPECIES</th>
<th>MOLALITY</th>
<th>LOG MOL</th>
<th>ACTIVITY</th>
<th>LOG ACT</th>
<th>ACT COEF</th>
<th>LG ACT C</th>
<th>GRAMS/KGM H2O</th>
<th>PPM</th>
<th>LOG PPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>AL+++</td>
<td>0.17413E-10</td>
<td>-10.759</td>
<td>0.13109E+11</td>
<td>-11.882</td>
<td>0.75284E-01</td>
<td>-1.123</td>
<td>0.46984E-09</td>
<td>1840.650</td>
<td>3.265</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>0.50000E+00</td>
<td>-1.301</td>
<td>0.30354E+01</td>
<td>-1.518</td>
<td>0.60708E+00</td>
<td>-0.217</td>
<td>0.19551E+01</td>
<td>2164.997</td>
<td>3.265</td>
<td></td>
</tr>
<tr>
<td>Na</td>
<td>0.10000E+00</td>
<td>0.0</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.22990E+02</td>
<td>8.308</td>
<td>0.919</td>
<td></td>
</tr>
<tr>
<td>H4SiO4</td>
<td>0.91812E+04</td>
<td>-4.037</td>
<td>0.91812E+04</td>
<td>-4.037</td>
<td>0.10000E+01</td>
<td>0.0</td>
<td>0.88246E-02</td>
<td>35046.605</td>
<td>4.545</td>
<td></td>
</tr>
<tr>
<td>Cl</td>
<td>0.10500E+01</td>
<td>0.021</td>
<td>0.63734E+00</td>
<td>-0.196</td>
<td>0.63734E+00</td>
<td>-0.217</td>
<td>0.37226E+02</td>
<td>0.000</td>
<td>4.103</td>
<td></td>
</tr>
<tr>
<td>OH</td>
<td>0.49256E-08</td>
<td>-8.308</td>
<td>0.31317E+00</td>
<td>-8.504</td>
<td>0.63589E+00</td>
<td>-0.197</td>
<td>0.37772E-07</td>
<td>0.000</td>
<td>4.103</td>
<td></td>
</tr>
<tr>
<td>H*</td>
<td>0.18596E-05</td>
<td>-5.413</td>
<td>0.31623E+00</td>
<td>-5.500</td>
<td>0.81932E+00</td>
<td>-0.087</td>
<td>0.38904E-05</td>
<td>0.000</td>
<td>2.436</td>
<td></td>
</tr>
<tr>
<td>H2O</td>
<td>0.55508E+02</td>
<td>1.744</td>
<td>0.96287E+00</td>
<td>-0.016</td>
<td>0.17346E+01</td>
<td>-1.761</td>
<td>0.10000E+04</td>
<td>944146.436</td>
<td>5.974</td>
<td></td>
</tr>
<tr>
<td>Al(CH)++</td>
<td>0.32490E-10</td>
<td>-10.488</td>
<td>0.72961E+11</td>
<td>-11.137</td>
<td>0.22456E+00</td>
<td>-0.649</td>
<td>0.14292E-08</td>
<td>0.000</td>
<td>5.871</td>
<td></td>
</tr>
<tr>
<td>Al(CH)4-</td>
<td>0.56247E-13</td>
<td>-13.017</td>
<td>0.63666E+13</td>
<td>-13.196</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.91445E-11</td>
<td>0.000</td>
<td>8.065</td>
<td></td>
</tr>
<tr>
<td>H3SiO4-</td>
<td>0.55851E-08</td>
<td>-8.253</td>
<td>0.36944E+08</td>
<td>-8.432</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.53118E-06</td>
<td>0.001</td>
<td>3.301</td>
<td></td>
</tr>
<tr>
<td>HCl</td>
<td>0.11462E+11</td>
<td>-11.941</td>
<td>0.14729E+11</td>
<td>-11.832</td>
<td>0.12850E+01</td>
<td>0.109</td>
<td>0.41792E-10</td>
<td>0.000</td>
<td>7.405</td>
<td></td>
</tr>
</tbody>
</table>

IONIC STRENGTH = 0.105000E+01  ELECTRICAL BALANCE = 0.732650E-15

NAME | LOG K | ACTIVITY | LOG ACTIVITY
STRAW | 1.50517 | 0.30068E-01 | -1.52160

THE LOG K FOR MUSCOVITE HAS BEEN EXCEEDED AT STEP 1

LOG K = 10.3095251  LOG Q = 10.7906963
### Reactants

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Cumulative Gram Change</th>
<th>Log Cumault</th>
<th>Cumulative Mole Change</th>
<th>Log Cumult</th>
<th>Reaction Coefficient</th>
<th>Log of Solubility Product</th>
<th>Log of Ion Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-Feldspar</td>
<td>-0.248075E-05</td>
<td>-5.605</td>
<td>-0.891276E-08</td>
<td>-8.050</td>
<td>0.100000E+01</td>
<td>0.672030E+01</td>
<td>0.609356E+01</td>
</tr>
</tbody>
</table>

### Products

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Cumulative Gram Change</th>
<th>Log Cumault</th>
<th>Cumulative Mole Change</th>
<th>Log Cumult</th>
<th>Reaction Coefficient</th>
<th>Log of Solubility Product</th>
<th>Log of Ion Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha-Quartz</td>
<td>-0.100000E+01</td>
<td>0.000</td>
<td>0.166432E-01</td>
<td>-1.779</td>
<td>0.299517E+01</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Minerals

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Log K</th>
<th>Log Q</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha-Quartz</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Analcime</td>
<td>9.809</td>
<td>7.4454200</td>
</tr>
<tr>
<td>Andalusite</td>
<td>9.674</td>
<td>4.2324007</td>
</tr>
<tr>
<td>A-Cristobalite</td>
<td>0.270</td>
<td>0.0</td>
</tr>
<tr>
<td>Beta-Quartz</td>
<td>0.138</td>
<td>0.0</td>
</tr>
<tr>
<td>Bournite</td>
<td>4.150</td>
<td>2.1079848</td>
</tr>
<tr>
<td>B-Cristobalite</td>
<td>0.376</td>
<td>0.0</td>
</tr>
<tr>
<td>Coesite</td>
<td>0.810</td>
<td>0.0</td>
</tr>
<tr>
<td>Corundum</td>
<td>10.490</td>
<td>4.2324007</td>
</tr>
<tr>
<td>Dehydrated</td>
<td>14.516</td>
<td>7.4318511</td>
</tr>
<tr>
<td>Diaspore</td>
<td>3.305</td>
<td>2.1079848</td>
</tr>
<tr>
<td>Giessite</td>
<td>2.515</td>
<td>2.095537</td>
</tr>
<tr>
<td>Halite</td>
<td>1.432</td>
<td>-0.3750500</td>
</tr>
<tr>
<td>High Sanidine</td>
<td>7.292</td>
<td>6.0935556</td>
</tr>
<tr>
<td>High Albite</td>
<td>10.941</td>
<td>7.4318511</td>
</tr>
<tr>
<td>Jadeite</td>
<td>11.249</td>
<td>7.4318511</td>
</tr>
<tr>
<td>Kalsilite</td>
<td>9.899</td>
<td>6.0935556</td>
</tr>
<tr>
<td>Kaolinite</td>
<td>4.532</td>
<td>4.1995308</td>
</tr>
<tr>
<td>Kyanite</td>
<td>9.400</td>
<td>4.2324007</td>
</tr>
<tr>
<td>K-Feldspar</td>
<td>6.720</td>
<td>6.0935556</td>
</tr>
<tr>
<td>Low Albite</td>
<td>9.623</td>
<td>7.4318511</td>
</tr>
<tr>
<td>Muscovite</td>
<td>10.310</td>
<td>10.3095251</td>
</tr>
<tr>
<td>Nepheline</td>
<td>12.664</td>
<td>7.4318511</td>
</tr>
<tr>
<td>Taragonite</td>
<td>14.069</td>
<td>11.6478206</td>
</tr>
<tr>
<td>Potassium Oxide</td>
<td>86.316</td>
<td>7.9547105</td>
</tr>
<tr>
<td>Pyrophyllite</td>
<td>6.157</td>
<td>4.2159696</td>
</tr>
<tr>
<td>Sillimanite</td>
<td>10.033</td>
<td>4.2324007</td>
</tr>
</tbody>
</table>
### GASES

<table>
<thead>
<tr>
<th>NAME</th>
<th>LOG K</th>
<th>ACTIVITY</th>
<th>LOG ACT</th>
<th>ACT COEF</th>
<th>LOG ACT C</th>
<th>GRAMS/KGM H2O</th>
<th>PPM</th>
<th>LOG PPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEAM</td>
<td>1.50517</td>
<td>0.30088E-01</td>
<td>-1.52160</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### AQUEOUS SPECIES

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>MOLALITY</th>
<th>LOG MOL</th>
<th>ACTIVITY</th>
<th>LOG ACT</th>
<th>ACT COEF</th>
<th>LOG ACT C</th>
<th>GRAMS/KGM H2O</th>
<th>PPM</th>
<th>LOG PPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>AL+++</td>
<td>0.31056E-08</td>
<td>-8.508</td>
<td>0.23398E-09</td>
<td>-9.631</td>
<td>0.75284E-01</td>
<td>-1.123</td>
<td>0.83794E-07</td>
<td>0.000</td>
<td>-4.103</td>
</tr>
<tr>
<td>K+</td>
<td>0.50000E-01</td>
<td>-1.301</td>
<td>0.30354E-01</td>
<td>-1.518</td>
<td>0.60708E+00</td>
<td>-0.217</td>
<td>0.19551E+01</td>
<td>1840.650</td>
<td>3.265</td>
</tr>
<tr>
<td>NA+</td>
<td>0.10000E+01</td>
<td>-0.000</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.22990E+02</td>
<td>2164.997</td>
<td>4.335</td>
</tr>
<tr>
<td>H4Si04</td>
<td>0.91812E-04</td>
<td>-4.637</td>
<td>0.91812E-04</td>
<td>-4.037</td>
<td>0.10002E+01</td>
<td>0.0</td>
<td>0.88246E-02</td>
<td>8.308</td>
<td>0.919</td>
</tr>
<tr>
<td>CL-</td>
<td>0.10500E+01</td>
<td>-0.021</td>
<td>0.63748E+00</td>
<td>-0.196</td>
<td>0.60708E+00</td>
<td>-0.217</td>
<td>0.37225E+02</td>
<td>3504.605</td>
<td>4.585</td>
</tr>
<tr>
<td>OH-</td>
<td>0.49638E-08</td>
<td>-8.304</td>
<td>0.31560E-08</td>
<td>-8.501</td>
<td>0.63580E+00</td>
<td>-0.197</td>
<td>0.84422E-07</td>
<td>0.000</td>
<td>-4.100</td>
</tr>
<tr>
<td>H+</td>
<td>0.38299E-05</td>
<td>-5.417</td>
<td>0.31380E-05</td>
<td>-5.503</td>
<td>0.81932E+00</td>
<td>-0.087</td>
<td>0.38604E-05</td>
<td>0.004</td>
<td>-2.440</td>
</tr>
<tr>
<td>H2O</td>
<td>0.55508E+02</td>
<td>1.744</td>
<td>0.96287E+00</td>
<td>-0.016</td>
<td>0.17346E-01</td>
<td>-1.761</td>
<td>0.10002E+04</td>
<td>941460.436</td>
<td>5.974</td>
</tr>
<tr>
<td>AL(CH)++</td>
<td>0.56395E-08</td>
<td>-8.234</td>
<td>0.13111E-08</td>
<td>-8.882</td>
<td>0.22455E+00</td>
<td>-0.649</td>
<td>0.25687E-06</td>
<td>0.000</td>
<td>-3.166</td>
</tr>
<tr>
<td>AL(CH)4-</td>
<td>0.17704E-10</td>
<td>-10.752</td>
<td>0.17711E-10</td>
<td>-10.931</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.53530E-06</td>
<td>0.001</td>
<td>-3.298</td>
</tr>
<tr>
<td>H3Si04-</td>
<td>0.56294E-08</td>
<td>-8.250</td>
<td>0.37202E-08</td>
<td>-8.429</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.53530E-06</td>
<td>0.001</td>
<td>-3.298</td>
</tr>
<tr>
<td>HCl</td>
<td>0.11374E-11</td>
<td>-11.544</td>
<td>0.14615E-11</td>
<td>-11.835</td>
<td>0.12850E+00</td>
<td>0.109</td>
<td>0.41470E-10</td>
<td>0.000</td>
<td>-7.408</td>
</tr>
</tbody>
</table>

### TOTAL MOLES

- **H2O**: 0.00000 0.13268E+01 0.23935E-01 -0.45194E+06 -0.81257E+04 -0.51818E+12 -0.93352E+10
- **TOTAL ACTIVITIES**: 0.00000 0.25642E+01 0.26631E-01 -0.90596E+04 -0.94089E+04 -0.10172E+11 -0.10564E+11

**DI/DXI IS 0.16805E+01**

**TOTAL EQUATIONS**

- **55,508,250.20 moles**

<table>
<thead>
<tr>
<th>COMPONENTS</th>
<th>TOTAL MOLALITY</th>
<th>LOG TOTAL MOLALITY</th>
<th>TOTAL GRAMS/KGM H2O</th>
<th>TOTAL PPM</th>
<th>TOTAL LOG PPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na+</td>
<td>0.10000E+01</td>
<td>-0.0000</td>
<td>0.22989E+02</td>
<td>0.21644E+06</td>
<td>5.3353</td>
</tr>
</tbody>
</table>

---

*Note: The image contains a table with various columns including species, log k, activity, log activity, and other chemical properties. The table is related to aqueous species and gases, including calculations for molality, log molality, and activity coefficients.*
<table>
<thead>
<tr>
<th>Ion</th>
<th>Moles (g)</th>
<th>Moles (g)</th>
<th>Moles (g)</th>
<th>Moles (g)</th>
<th>Moles (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-Feldspar</td>
<td>-0.8913E-08</td>
<td>0.2481E-05</td>
<td>0.0</td>
<td>0.0</td>
<td>0.3593E-01</td>
</tr>
<tr>
<td>Alpha-Quartz</td>
<td>0.2669E-07</td>
<td>0.1604E-05</td>
<td>0.0</td>
<td>0.0</td>
<td>0.1664E-01</td>
</tr>
</tbody>
</table>

**Total number of Delxi increments forward = 1**

**Ionic strength = 0.105000E+01**

**Electrical balance = 0.653474E-15**

**Total number of phase boundaries presently being considered = 1**
### Reactants

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Cumulative Gram Change</th>
<th>Log Cumult Mole Change</th>
<th>Reaction Coefficient</th>
<th>Log of Solubility Product</th>
<th>Log of Ion Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-Feldspar</td>
<td>-0.161249E-03</td>
<td>-3.793</td>
<td>-0.579330E-06</td>
<td>-6.237</td>
<td>0.100000E+01</td>
</tr>
</tbody>
</table>

### Products

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Cumulative Gram Change</th>
<th>Log Cumult Mole Change</th>
<th>Reaction Coefficient</th>
<th>Log of Solubility Product</th>
<th>Log of Ion Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha-Quartz</td>
<td>0.100007E+01</td>
<td>0.000</td>
<td>0.166443E-01</td>
<td>-1.779</td>
<td>0.199995E+01</td>
</tr>
<tr>
<td>Muscovite</td>
<td>0.760190E-04</td>
<td>-4.119</td>
<td>0.190852E-06</td>
<td>-6.719</td>
<td>0.334697E+00</td>
</tr>
</tbody>
</table>

### Minerals

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Log K</th>
<th>Log Q</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha-Quartz</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Alumina</td>
<td>6.372</td>
<td>4.0085973</td>
</tr>
<tr>
<td>Andalusite</td>
<td>2.801</td>
<td>-2.6703051</td>
</tr>
<tr>
<td>A-Cristobalite</td>
<td>0.270</td>
<td>0.000</td>
</tr>
<tr>
<td>Beta-Quartz</td>
<td>0.138</td>
<td>0.000</td>
</tr>
<tr>
<td>Boehmite</td>
<td>0.714</td>
<td>-1.3433681</td>
</tr>
<tr>
<td>B-Cristobalite</td>
<td>0.376</td>
<td>0.000</td>
</tr>
<tr>
<td>Coesite</td>
<td>0.810</td>
<td>0.000</td>
</tr>
<tr>
<td>Coesite</td>
<td>3.617</td>
<td>-2.6703051</td>
</tr>
<tr>
<td>Dehydro Alumina</td>
<td>11.079</td>
<td>4.0250284</td>
</tr>
<tr>
<td>Dehydrated Alumina</td>
<td>-0.131</td>
<td>-1.3433681</td>
</tr>
<tr>
<td>Gypsum</td>
<td>-0.922</td>
<td>-3.597992</td>
</tr>
<tr>
<td>Halite</td>
<td>1.432</td>
<td>-0.3750500</td>
</tr>
<tr>
<td>High Sanidine</td>
<td>4.483</td>
<td>2.6867362</td>
</tr>
<tr>
<td>High Aelite</td>
<td>7.504</td>
<td>4.0250284</td>
</tr>
<tr>
<td>Jadeite</td>
<td>7.913</td>
<td>4.0250284</td>
</tr>
<tr>
<td>Kalsilite</td>
<td>6.663</td>
<td>2.6867362</td>
</tr>
<tr>
<td>Kaolinite</td>
<td>-2.341</td>
<td>-2.7031673</td>
</tr>
<tr>
<td>Kyanite</td>
<td>2.526</td>
<td>-2.6703051</td>
</tr>
<tr>
<td>K-Feldspar</td>
<td>3.284</td>
<td>2.6867362</td>
</tr>
<tr>
<td>Low Aelite</td>
<td>6.186</td>
<td>4.0250284</td>
</tr>
<tr>
<td>Muscovite</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Nepheline</td>
<td>1.227</td>
<td>4.0250284</td>
</tr>
<tr>
<td>Paragonite</td>
<td>3.760</td>
<td>1.3382922</td>
</tr>
<tr>
<td>Potassium Oxide</td>
<td>84.316</td>
<td>8.0437776</td>
</tr>
<tr>
<td>Pyrophyllite</td>
<td>-0.716</td>
<td>-2.6867362</td>
</tr>
<tr>
<td>Species</td>
<td>Molarity</td>
<td>Log Molar Activity</td>
</tr>
<tr>
<td>---------------</td>
<td>----------</td>
<td>--------------------</td>
</tr>
<tr>
<td>AL+++</td>
<td>0.22065E-08</td>
<td>-8.656</td>
</tr>
<tr>
<td>K+</td>
<td>0.50000E-01</td>
<td>-1.301</td>
</tr>
<tr>
<td>Na+</td>
<td>0.10000E+01</td>
<td>-0.000</td>
</tr>
<tr>
<td>H4SiO4</td>
<td>0.91812E-04</td>
<td>-4.037</td>
</tr>
<tr>
<td>H+</td>
<td>0.37567E-05</td>
<td>-5.548</td>
</tr>
<tr>
<td>H2O</td>
<td>0.5556E+02</td>
<td>-1.744</td>
</tr>
<tr>
<td>Al(OH)++</td>
<td>0.45970E-08</td>
<td>-8.338</td>
</tr>
<tr>
<td>Al(OH)++</td>
<td>0.18955E-10</td>
<td>-10.722</td>
</tr>
<tr>
<td>H3SiO4-</td>
<td>0.6235E-08</td>
<td>-8.205</td>
</tr>
<tr>
<td>HCl</td>
<td>0.10265E-11</td>
<td>-11.989</td>
</tr>
</tbody>
</table>

**AQUEOUS SPECIES**

**TOTAL MOLES**

- H2O: 55.50825020

**ACTIVITIES**

- H2O: 55.50825020

**DI/DXI is -0.56516E-02**

**TOTAL MOLES OF WATER IN THE SYSTEM IS 55.50825020 MOLES**
<table>
<thead>
<tr>
<th>MINERAL PHASES</th>
<th>AMOUNT OF REACTANT DESTROYED</th>
<th>AMOUNT OF REACTANT PRODUCED</th>
<th>AMOUNT OF PRODUCT PRODUCED</th>
<th>AMOUNT OF PRODUCT DESTROYED</th>
<th>NET AMOUNT IN THE SYSTEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-FELDSPAR</td>
<td>-0.5793E-06, 0.1612E-03</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.3593E-01, 0.1000E+02</td>
</tr>
<tr>
<td>ALPHA-QUARTZ</td>
<td></td>
<td>0.1165E-05, 0.6999E-04</td>
<td>0.0</td>
<td>0.0</td>
<td>0.1664E-01, 0.1000E+01</td>
</tr>
<tr>
<td>MUSCOVITE</td>
<td></td>
<td>0.1909E-06, 0.7602E-04</td>
<td>0.0</td>
<td>0.0</td>
<td>0.1909E-06, 0.7602E-04</td>
</tr>
</tbody>
</table>

NUMER OF DELXI INCREMENTS FORWARD = 2

IONIC STRENGTH = 0.010500E+01  ELECTRICAL BALANCE = 0.740647E-15

TOTAL NUMBER OF PHASE BOUNDARIES PRESENTLY BEING CONSIDERED = 2
### Reactants

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Cumulative Gram Change</th>
<th>Log Cumulant Gram Change</th>
<th>Cumulative Mole Change</th>
<th>Log Cumulant Mole Change</th>
<th>Reaction Coefficient</th>
<th>Log of Solubility Product</th>
<th>Log of Ion Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-Feldspar</td>
<td>-0.278337E-03</td>
<td>-3.955</td>
<td>-0.100000E-05</td>
<td>-6.000</td>
<td>0.100000E+01</td>
<td>0.100000E+10</td>
<td>0.271081E+01</td>
</tr>
</tbody>
</table>

### Products

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Cumulative Gram Change</th>
<th>Log Cumulant Gram Change</th>
<th>Cumulative Mole Change</th>
<th>Log Cumulant Mole Change</th>
<th>Reaction Coefficient</th>
<th>Log of Solubility Product</th>
<th>Log of Ion Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha-Quartz</td>
<td>0.100012E+01</td>
<td>0.000</td>
<td>0.166451E-01</td>
<td>-1.779</td>
<td>0.199539E+01</td>
<td>0.300000E+01</td>
<td>0.00</td>
</tr>
<tr>
<td>Muscovite</td>
<td>0.132050E-03</td>
<td>-3.079</td>
<td>0.331524E-06</td>
<td>-6.479</td>
<td>0.334475E+00</td>
<td>0.300000E+01</td>
<td>0.00</td>
</tr>
</tbody>
</table>

### Minerals

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Log K</th>
<th>Log Q</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha-Quartz</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Analcime</td>
<td>6.372</td>
<td>4.0326672</td>
</tr>
<tr>
<td>Andalusite</td>
<td>2.801</td>
<td>-2.6943775</td>
</tr>
<tr>
<td>A-Cristobalite</td>
<td>0.270</td>
<td>0.0</td>
</tr>
<tr>
<td>Beta-Quartz</td>
<td>0.138</td>
<td>0.0</td>
</tr>
<tr>
<td>Boehmite</td>
<td>0.714</td>
<td>-1.3554043</td>
</tr>
<tr>
<td>B-Cristobalite</td>
<td>0.376</td>
<td>0.0</td>
</tr>
<tr>
<td>Coesite</td>
<td>0.810</td>
<td>0.0</td>
</tr>
<tr>
<td>Ccundum</td>
<td>3.617</td>
<td>-2.6943775</td>
</tr>
<tr>
<td>Dehydrated Analcime</td>
<td>11.079</td>
<td>4.0490983</td>
</tr>
<tr>
<td>Diaspore</td>
<td>0.213</td>
<td>0.0</td>
</tr>
<tr>
<td>Gibbsite</td>
<td>0.778</td>
<td>-1.3718354</td>
</tr>
<tr>
<td>Halite</td>
<td>1.132</td>
<td>-0.3750500</td>
</tr>
<tr>
<td>High Sanidine</td>
<td>4.483</td>
<td>2.7108086</td>
</tr>
<tr>
<td>High Albite</td>
<td>7.504</td>
<td>4.0490983</td>
</tr>
<tr>
<td>Jadeite</td>
<td>7.813</td>
<td>4.0490983</td>
</tr>
<tr>
<td>Kalsilite</td>
<td>6.463</td>
<td>2.7108086</td>
</tr>
<tr>
<td>Katoinite</td>
<td>-2.341</td>
<td>-2.7272397</td>
</tr>
<tr>
<td>Kyanite</td>
<td>2.526</td>
<td>-2.6943775</td>
</tr>
<tr>
<td>K-Feldspar</td>
<td>3.284</td>
<td>2.7108086</td>
</tr>
<tr>
<td>Low Albite</td>
<td>6.168</td>
<td>4.0490983</td>
</tr>
<tr>
<td>Muscovite</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Nepheline</td>
<td>9.227</td>
<td>4.0490983</td>
</tr>
<tr>
<td>Paragonnite</td>
<td>3.660</td>
<td>1.3382897</td>
</tr>
<tr>
<td>Potassium Oxide</td>
<td>84.316</td>
<td>8.1159946</td>
</tr>
<tr>
<td>Fylosphilit</td>
<td>0.716</td>
<td>-2.7108086</td>
</tr>
</tbody>
</table>
**TOTAL MOLES**

<table>
<thead>
<tr>
<th>NAME</th>
<th>LOG K</th>
<th>ACTIVITY</th>
<th>LOG ACTIVITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEAM</td>
<td>1.50517</td>
<td>0.30088E-01</td>
<td>-1.52160</td>
</tr>
</tbody>
</table>

**AGUAUS SPECIES**

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>MOLALITY</th>
<th>LOG MOL</th>
<th>ACTIVITY</th>
<th>LOG ACT</th>
<th>ACT COEF</th>
<th>LG ACT C</th>
<th>GRAMS/KGM</th>
<th>H2O</th>
<th>PPM</th>
<th>LOG PPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>AL+++</td>
<td>0.16724E-08</td>
<td>-8.777</td>
<td>0.12591E-09</td>
<td>-9.900</td>
<td>0.75258E-01</td>
<td>-1.123</td>
<td>0.45125E-07</td>
<td>0.000</td>
<td>4.372</td>
<td></td>
</tr>
<tr>
<td>K+</td>
<td>0.50001E-01</td>
<td>-1.301</td>
<td>0.30354E-01</td>
<td>-1.518</td>
<td>0.60708E+00</td>
<td>-0.217</td>
<td>0.19551E+01</td>
<td>1840.674</td>
<td>3.265</td>
<td></td>
</tr>
<tr>
<td>Na+</td>
<td>0.10000E+01</td>
<td>-0.000</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.22990E+02</td>
<td>21643.996</td>
<td>4.335</td>
<td></td>
</tr>
<tr>
<td>H4SiO4</td>
<td>0.91812E-04</td>
<td>-4.037</td>
<td>0.91812E-04</td>
<td>-4.037</td>
<td>0.10000E+01</td>
<td>0.0</td>
<td>0.88246E-02</td>
<td>8.308</td>
<td>0.919</td>
<td></td>
</tr>
<tr>
<td>Cl-</td>
<td>0.10500E+01</td>
<td>0.021</td>
<td>0.63744E+00</td>
<td>-0.196</td>
<td>0.60708E+00</td>
<td>-0.217</td>
<td>0.37226E+02</td>
<td>35046.604</td>
<td>4.585</td>
<td></td>
</tr>
<tr>
<td>OH-</td>
<td>0.27575E-08</td>
<td>-8.224</td>
<td>0.37994E-08</td>
<td>-8.420</td>
<td>0.63580E+00</td>
<td>-0.197</td>
<td>0.10163E-06</td>
<td>0.000</td>
<td>4.019</td>
<td></td>
</tr>
<tr>
<td>H+</td>
<td>0.31809E-05</td>
<td>-5.497</td>
<td>0.26062E-05</td>
<td>-5.594</td>
<td>0.81932E-06</td>
<td>-0.087</td>
<td>0.32063E-05</td>
<td>0.003</td>
<td>-2.520</td>
<td></td>
</tr>
<tr>
<td>H2O</td>
<td>0.55508E+02</td>
<td>1.744</td>
<td>0.96207E+00</td>
<td>0.016</td>
<td>0.17364E+00</td>
<td>-1.761</td>
<td>0.10000E+04</td>
<td>94140.413</td>
<td>5.974</td>
<td></td>
</tr>
<tr>
<td>Al (CH)++</td>
<td>0.3764E-08</td>
<td>-8.422</td>
<td>0.35787E-09</td>
<td>-9.070</td>
<td>0.22456E+00</td>
<td>-0.649</td>
<td>0.16656E-06</td>
<td>0.000</td>
<td>-3.805</td>
<td></td>
</tr>
<tr>
<td>Al (CH)++</td>
<td>0.20035E-10</td>
<td>-10.698</td>
<td>0.13253E+00</td>
<td>-10.878</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.19036E-08</td>
<td>0.000</td>
<td>-5.747</td>
<td></td>
</tr>
<tr>
<td>H3SiO4-</td>
<td>0.67755E-08</td>
<td>-8.169</td>
<td>0.44820E-08</td>
<td>-8.349</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.64443E-06</td>
<td>0.001</td>
<td>-3.217</td>
<td></td>
</tr>
<tr>
<td>HCl</td>
<td>0.54465E-12</td>
<td>-12.025</td>
<td>0.12139E-09</td>
<td>-11.916</td>
<td>0.12850E+01</td>
<td>0.109</td>
<td>0.3443E-10</td>
<td>0.000</td>
<td>-7.489</td>
<td></td>
</tr>
</tbody>
</table>

**SPECIES**

<table>
<thead>
<tr>
<th>NAME</th>
<th>LOG K</th>
<th>LOG C</th>
<th>N EAR</th>
<th>D2M</th>
<th>D2LN M/DXI</th>
<th>D3 M/DXI</th>
<th>D3LN M/DXI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na+</td>
<td>0.0</td>
<td>0.0</td>
<td>0.14827E-03</td>
<td>0.14827E-03</td>
<td>-0.76440E+01</td>
<td>0.19106E+08</td>
<td>0.19106E+08</td>
</tr>
<tr>
<td>Cl-</td>
<td>0.0</td>
<td>0.0</td>
<td>0.15588E-03</td>
<td>0.15588E-03</td>
<td>-0.80255E+00</td>
<td>0.20061E+08</td>
<td>0.19106E+08</td>
</tr>
<tr>
<td>H+</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00000E+00</td>
<td>-0.65505E+00</td>
<td>-0.18950E+06</td>
<td>0.36596E+11</td>
<td>0.12591E-09</td>
</tr>
<tr>
<td>K+</td>
<td>0.0</td>
<td>0.0</td>
<td>0.66555E+00</td>
<td>0.66555E+00</td>
<td>0.13311E+02</td>
<td>0.72705E+04</td>
<td>0.12591E-09</td>
</tr>
<tr>
<td>Al+++</td>
<td>0.1746</td>
<td>8.1746</td>
<td>0.13938E-02</td>
<td>0.67362E-06</td>
<td>0.12199E+12</td>
<td>0.14686E+09</td>
<td>0.91347E+16</td>
</tr>
<tr>
<td>H4SiO4</td>
<td>4.0042</td>
<td>4.0042</td>
<td>0.32487E-07</td>
<td>0.35384E-03</td>
<td>0.39874E+03</td>
<td>0.36596E+11</td>
<td>0.32063E+06</td>
</tr>
<tr>
<td>Cl-</td>
<td>13.9878</td>
<td>13.9878</td>
<td>0.10421E-02</td>
<td>0.18950E+06</td>
<td>0.39874E+03</td>
<td>0.36596E+11</td>
<td>0.32063E+06</td>
</tr>
<tr>
<td>Al (CH)++</td>
<td>-3.4365</td>
<td>-3.4365</td>
<td>0.20327E-02</td>
<td>0.42418E+06</td>
<td>0.50626E+03</td>
<td>0.85391E+11</td>
<td>0.32063E+06</td>
</tr>
<tr>
<td>H3SiO4-</td>
<td>15.0734</td>
<td>15.0734</td>
<td>0.23946E-05</td>
<td>0.12633E+06</td>
<td>0.76498E+00</td>
<td>0.24398E+11</td>
<td>0.91347E+16</td>
</tr>
<tr>
<td>HCl</td>
<td>13.8996</td>
<td>13.8997</td>
<td>0.11816E-02</td>
<td>0.18950E+06</td>
<td>0.45218E+03</td>
<td>0.16596E+11</td>
<td>0.25761E+09</td>
</tr>
</tbody>
</table>

**TOTAL MOLES**

<table>
<thead>
<tr>
<th>NAME</th>
<th>LOG K</th>
<th>ACTIVITY</th>
<th>LOG ACTIVITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2O</td>
<td>0.0</td>
<td>0.00000E+00</td>
<td>-0.82304E-02</td>
</tr>
<tr>
<td>H2O</td>
<td>0.0</td>
<td>0.00000E-03</td>
<td>-0.17035E-03</td>
</tr>
</tbody>
</table>

**DG/DXI IS -0.38321E-02**

**TOTAL MOLES OF WATER IN THE SYSTEM IS 55.50825019 MOLES**

**CONCENTRATIONS**

<table>
<thead>
<tr>
<th>TOTAL MOLALITY</th>
<th>LOG TOTAL MOLALITY</th>
<th>TOTAL GRAMS/KGM</th>
<th>H2O</th>
<th>TOTAL PPM</th>
<th>LOG TOTAL PPM</th>
</tr>
</thead>
</table>

- **SILLIMANITE:** 3.16G, -2.6943775
- **SODIUM OXIDE:** 6247, 10.7925741
- **SYLVEITE:** 1.223, -7.1133398
### Mineral Phases

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Reactant Destroyed</th>
<th>Reactant Produced</th>
<th>Product Produced</th>
<th>Product Destroyed</th>
<th>Net Amount in the System</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-Feldspar</td>
<td>-0.10000E-05</td>
<td>0.2783E-03</td>
<td>0.0</td>
<td>0.0</td>
<td>0.3593E-01 0.1000E+02</td>
</tr>
<tr>
<td>Alpha-Quartz</td>
<td>0.2004E-05</td>
<td>0.1204E-03</td>
<td>0.0</td>
<td>0.0</td>
<td>0.1665E-01 0.1000E+01</td>
</tr>
<tr>
<td>Muscovite</td>
<td>0.3315E-06</td>
<td>0.1321E-03</td>
<td>0.0</td>
<td>0.0</td>
<td>0.3315E-06 0.1321E-03</td>
</tr>
</tbody>
</table>

**Number of Delxi Increments Forward = 3**

**Ionic Strength = 0.10500E+01**

**Electrical Balance = 0.10462E-14**

**Total Number of Phase Boundaries Presently Being Considered = 2**
### Reactants

<table>
<thead>
<tr>
<th>MINERAL</th>
<th>CUMULATIVE GRAM CHANGE</th>
<th>LOG CUMULAT GRAM CHANGE</th>
<th>CUMULATIVE MOLE CHANGE</th>
<th>LOG CUMULAT MOLE CHANGE</th>
<th>REACTION COEFFICIENT</th>
<th>LOG OF SOLUBILITY PRODUCT</th>
<th>LOG OF ION PRODUCT</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-FELDSPAR</td>
<td>-0.494960E-03</td>
<td>-3.305</td>
<td>-0.177828E-05</td>
<td>-5.750</td>
<td>0.100000E+01</td>
<td>0.328379E+01</td>
<td>0.276151E+01</td>
</tr>
</tbody>
</table>

### Products

<table>
<thead>
<tr>
<th>MINERAL</th>
<th>CUMULATIVE GRAM CHANGE</th>
<th>LOG CUMULAT GRAM CHANGE</th>
<th>CUMULATIVE MOLE CHANGE</th>
<th>LOG CUMULAT MOLE CHANGE</th>
<th>REACTION COEFFICIENT</th>
<th>LOG OF SOLUBILITY PRODUCT</th>
<th>LOG OF ION PRODUCT</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALPHA-QUARTZ</td>
<td>0.100021E+01</td>
<td>0.000</td>
<td>0.166467E-01</td>
<td>-1.779</td>
<td>0.199578E+01</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>MUSCOVITE</td>
<td>0.235650E-03</td>
<td>-3.628</td>
<td>0.591619E-06</td>
<td>-6.228</td>
<td>0.334181E+00</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Minerals

<table>
<thead>
<tr>
<th>MINERAL</th>
<th>LOG K</th>
<th>LOG Q</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALPHA-QUARTZ</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>ANTHACITE</td>
<td>6.372</td>
<td>4.0833668</td>
</tr>
<tr>
<td>ANDALUSITE</td>
<td>2.801</td>
<td>-2.7450815</td>
</tr>
<tr>
<td>A-CRISTOFOELITE</td>
<td>0.270</td>
<td>0.0</td>
</tr>
<tr>
<td>BETA-QUARTZ</td>
<td>0.138</td>
<td>0.0</td>
</tr>
<tr>
<td>BOWMITE</td>
<td>0.714</td>
<td>-1.3807563</td>
</tr>
<tr>
<td>B-CRISTOFOELITE</td>
<td>0.376</td>
<td>0.0</td>
</tr>
<tr>
<td>COSEITE</td>
<td>0.810</td>
<td>0.0</td>
</tr>
<tr>
<td>COBUNDUM</td>
<td>3.617</td>
<td>2.7450815</td>
</tr>
<tr>
<td>DEHYDRATED ANTHACITE</td>
<td>11.079</td>
<td>4.0997979</td>
</tr>
<tr>
<td>DIASPHERE</td>
<td>-0.131</td>
<td>1.3807563</td>
</tr>
<tr>
<td>GILESITE</td>
<td>-0.922</td>
<td>-1.3971874</td>
</tr>
<tr>
<td>HALITE</td>
<td>1.432</td>
<td>-0.3750560</td>
</tr>
<tr>
<td>HIGH SANIDINE</td>
<td>4.483</td>
<td>2.7615126</td>
</tr>
<tr>
<td>HIGH ALBITE</td>
<td>7.504</td>
<td>4.0997979</td>
</tr>
<tr>
<td>JADEITE</td>
<td>7.813</td>
<td>4.0997979</td>
</tr>
<tr>
<td>KALSILITE</td>
<td>6.463</td>
<td>2.7615126</td>
</tr>
<tr>
<td>KAOLINITE</td>
<td>-2.341</td>
<td>-2.7779437</td>
</tr>
<tr>
<td>Kyanite</td>
<td>2.526</td>
<td>-2.7450815</td>
</tr>
<tr>
<td>K-FELDSPAR</td>
<td>3.284</td>
<td>2.7615126</td>
</tr>
<tr>
<td>LOW ALBITE</td>
<td>6.186</td>
<td>4.0997979</td>
</tr>
<tr>
<td>MUSCOVITE</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>NaClH2O</td>
<td>-2.227</td>
<td>4.0997979</td>
</tr>
<tr>
<td>PARAGONITE</td>
<td>3.760</td>
<td>1.3382652</td>
</tr>
<tr>
<td>POTASSIUM OXIDE</td>
<td>84.316</td>
<td>8.2681068</td>
</tr>
<tr>
<td>PHYTOPHYLLITE</td>
<td>-2.716</td>
<td>-2.7615126</td>
</tr>
</tbody>
</table>
### Gases

#### Name

<table>
<thead>
<tr>
<th>Log K</th>
<th>Activity</th>
<th>Log Activity</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEAM</td>
<td>1.50517</td>
<td>-1.52160</td>
</tr>
</tbody>
</table>

### Aqueous Species

#### Species

<table>
<thead>
<tr>
<th>Species</th>
<th>Molality</th>
<th>Log Mol</th>
<th>Activity</th>
<th>Log Act</th>
<th>Act Coef</th>
<th>Log Act C</th>
<th>Grams/Kg H2O</th>
<th>PPM</th>
<th>Log PPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>AL+++</td>
<td>-0.9332E-09</td>
<td>-0.303</td>
<td>0.70233E-10</td>
<td>-10.153</td>
<td>0.75284E-01</td>
<td>-1.123</td>
<td>0.25171E+07</td>
<td>0.000</td>
<td>-4.625</td>
</tr>
<tr>
<td>K+</td>
<td>-0.5000E-01</td>
<td>0.000</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.22990E+02</td>
<td>2163.996</td>
<td>4.335</td>
</tr>
<tr>
<td>Na+</td>
<td>0.1000E+01</td>
<td>-0.303</td>
<td>0.33655E-01</td>
<td>-1.518</td>
<td>0.60708E+00</td>
<td>-0.217</td>
<td>0.19551E+01</td>
<td>1840.693</td>
<td>3.265</td>
</tr>
<tr>
<td>H4SiO4</td>
<td>-0.91812E-04</td>
<td>0.000</td>
<td>0.91812E-04</td>
<td>-4.037</td>
<td>0.91812E-04</td>
<td>0.000</td>
<td>0.88246E-02</td>
<td>8.308</td>
<td>0.919</td>
</tr>
<tr>
<td>H+</td>
<td>-0.26695E-05</td>
<td>0.573</td>
<td>0.21876E-05</td>
<td>-5.660</td>
<td>0.1932E+00</td>
<td>-0.097</td>
<td>0.26912E+05</td>
<td>0.003</td>
<td>-2.596</td>
</tr>
<tr>
<td>H20</td>
<td>-0.55058E+02</td>
<td>1.744</td>
<td>0.96287E+00</td>
<td>-0.016</td>
<td>0.1746E+00</td>
<td>-0.761</td>
<td>0.10000E+04</td>
<td>941460.396</td>
<td>5.974</td>
</tr>
<tr>
<td>Al(OH)++</td>
<td>-0.25164E-08</td>
<td>-0.899</td>
<td>0.56508E-09</td>
<td>-9.248</td>
<td>0.22456E+00</td>
<td>-0.694</td>
<td>0.11069E+06</td>
<td>0.000</td>
<td>-3.982</td>
</tr>
<tr>
<td>Al(OH)4-</td>
<td>-0.2251E-10</td>
<td>10.648</td>
<td>0.14893E-10</td>
<td>-10.827</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.21392E+08</td>
<td>0.000</td>
<td>-5.696</td>
</tr>
<tr>
<td>H3SiO4-</td>
<td>0.80718E-08</td>
<td>-8.693</td>
<td>0.53393E-08</td>
<td>-8.273</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.76769E+06</td>
<td>0.001</td>
<td>-3.141</td>
</tr>
<tr>
<td>HCl</td>
<td>0.7929E-12</td>
<td>-12.101</td>
<td>0.10189E-11</td>
<td>-11.992</td>
<td>0.12850E+01</td>
<td>0.109</td>
<td>0.28910E-10</td>
<td>0.000</td>
<td>-7.565</td>
</tr>
</tbody>
</table>

#### Additional Information
- **Component**: Total Moles, Total Molality, Total Grams/Kg H2O, Total PPM, Log PPM
- **Di/Dxi** is -0.10921E-02
- **Total Moles of Water in the System**: 55.50825019 Moles

---

**Note**: The table contains detailed chemical compositions and activities, along with various logarithmic and other derived values that are typical in thermodynamic and chemical equilibrium calculations. The data includes species of interest such as sodium, potassium, aluminum, and their various compounds, along with associated activity coefficients and equilibrium constants.
### TOTAL MASS TRANSFER IN THE SYSTEM

<table>
<thead>
<tr>
<th>MINERAL PHASES</th>
<th>AMOUNT OF REACTANT DESTROYED</th>
<th>AMOUNT OF REACTANT PRODUCED</th>
<th>AMOUNT OF PRODUCT PRODUCED</th>
<th>AMOUNT OF PRODUCT DESTROYED</th>
<th>NET AMOUNT IN THE SYSTEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-FELDSPAR</td>
<td>-0.1778E-05 0.4950E-03</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.3593E-01 0.1000E+02</td>
</tr>
<tr>
<td>ALPHA-QUARTZ</td>
<td></td>
<td>0.3557E-05 0.2138E-03</td>
<td>0.0</td>
<td>0.0</td>
<td>0.1665E-01 0.1000E+01</td>
</tr>
<tr>
<td>MUSCOVITE</td>
<td></td>
<td>0.5916E-06 0.2356E-03</td>
<td>0.0</td>
<td>0.0</td>
<td>0.5916E-06 0.2356E-03</td>
</tr>
</tbody>
</table>

**NUMBER OF DELXI INCREMENTS FORWARD = 5**

**IONIC STRENGTH = 0.105000E+01**

**ELECTRICAL BALANCE = 0.119726E-14**

**TOTAL NUMBER OF PHASE BOUNDARIES PRESENTLY BEING CONSIDERED = 2**
### NEW STEEP SUMMARY

<table>
<thead>
<tr>
<th>DELXI</th>
<th>XI</th>
<th>LOG XI</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.966057E-07</td>
<td>0.316228E-05</td>
<td>-5.500</td>
</tr>
</tbody>
</table>

### REACTANTS

<table>
<thead>
<tr>
<th>MINERAL</th>
<th>CUMULATIVE GRAM CHANGE</th>
<th>LOG CUMULATIVE GRAM CHANGE</th>
<th>CUMULATIVE MOLE CHANGE</th>
<th>LOG CUMULATIVE MOLE CHANGE</th>
<th>REACTION COEFFICIENT</th>
<th>LOG OF SOLUBILITY PRODUCT</th>
<th>LOG OF ION PRODUCT</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-FELDSPAR</td>
<td>-0.880176E-03</td>
<td>-3.055</td>
<td>-0.316228E-05</td>
<td>-5.500</td>
<td>0.100000E+01</td>
<td>0.328379E+01</td>
<td>0.288200E+01</td>
</tr>
</tbody>
</table>

### PRODUCTS

<table>
<thead>
<tr>
<th>MINERAL</th>
<th>CUMULATIVE GRAM CHANGE</th>
<th>LOG CUMULATIVE GRAM CHANGE</th>
<th>CUMULATIVE MOLE CHANGE</th>
<th>LOG CUMULATIVE MOLE CHANGE</th>
<th>REACTION COEFFICIENT</th>
<th>LOG OF SOLUBILITY PRODUCT</th>
<th>LOG OF ION PRODUCT</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALPHA-QUARTZ</td>
<td>0.100038E+01</td>
<td>0.00</td>
<td>0.166495E-01</td>
<td>-1.779</td>
<td>0.199458E+01</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>MUSCovITE</td>
<td>0.419704E-03</td>
<td>-3.377</td>
<td>0.105370E-05</td>
<td>-5.977</td>
<td>0.333725E+00</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### MINERALS

<table>
<thead>
<tr>
<th>MINERAL</th>
<th>LOG R</th>
<th>LOG Q</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALEHa-QUArTZ</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>ANALCIME</td>
<td>6.372</td>
<td>4.2038432</td>
</tr>
<tr>
<td>ANDALUSITE</td>
<td>2.801</td>
<td>-2.8655660</td>
</tr>
<tr>
<td>A-CRISTOBALITE</td>
<td>0.270</td>
<td>0.0</td>
</tr>
<tr>
<td>BETA-QUARTZ</td>
<td>0.138</td>
<td>0.0</td>
</tr>
<tr>
<td>BOEHMITE</td>
<td>0.714</td>
<td>-1.4409985</td>
</tr>
<tr>
<td>B-CRISTOBALITE</td>
<td>0.376</td>
<td>0.0</td>
</tr>
<tr>
<td>COESITE</td>
<td>0.810</td>
<td>0.0</td>
</tr>
<tr>
<td>CORUNUM</td>
<td>3.617</td>
<td>-2.8655660</td>
</tr>
<tr>
<td>DEHYDRATED ANALCIME</td>
<td>11.079</td>
<td>4.2202743</td>
</tr>
<tr>
<td>DIASPHERE</td>
<td>-0.131</td>
<td>-1.4409985</td>
</tr>
<tr>
<td>GIBBESITE</td>
<td>-0.922</td>
<td>-1.4574296</td>
</tr>
<tr>
<td>BACLITE</td>
<td>1.432</td>
<td>-0.3750500</td>
</tr>
<tr>
<td>HIGH SANIDINE</td>
<td>4.483</td>
<td>2.8819971</td>
</tr>
<tr>
<td>HIGH ALEITE</td>
<td>7.504</td>
<td>4.2202743</td>
</tr>
<tr>
<td>JADEITE</td>
<td>7.813</td>
<td>4.2202743</td>
</tr>
<tr>
<td>KALSIITE</td>
<td>6.463</td>
<td>2.8819971</td>
</tr>
<tr>
<td>KACLINITE</td>
<td>-2.341</td>
<td>-2.8984282</td>
</tr>
<tr>
<td>KYANITE</td>
<td>2.526</td>
<td>-2.8655660</td>
</tr>
<tr>
<td>K-FELDSPAR</td>
<td>3.284</td>
<td>2.8819971</td>
</tr>
<tr>
<td>LOW ALEITE</td>
<td>6.186</td>
<td>4.2202743</td>
</tr>
<tr>
<td>MUSCovITE</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>NEPHELINE</td>
<td>9.227</td>
<td>4.2202743</td>
</tr>
<tr>
<td>PARAGNITE</td>
<td>3.760</td>
<td>1.33282772</td>
</tr>
<tr>
<td>POTASSIUM OXIDE</td>
<td>84.316</td>
<td>8.6295602</td>
</tr>
<tr>
<td>FLYROHYLLITE</td>
<td>-0.716</td>
<td>-2.8819971</td>
</tr>
</tbody>
</table>
### Gases

<table>
<thead>
<tr>
<th>NAME</th>
<th>LOG K</th>
<th>ACTIVITY</th>
<th>LOG ACTIVITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEAM</td>
<td>1.50517</td>
<td>0.30088E-01</td>
<td>-1.52160</td>
</tr>
</tbody>
</table>

### Aqueous Species

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>MOLALITY</th>
<th>LOG MOL</th>
<th>ACTIVITY</th>
<th>LOG ACT</th>
<th>ACT COEF</th>
<th>LOG ACT C</th>
<th>GRAMS/KGM H2O</th>
<th>PPM</th>
<th>LOG PPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>AL+++</td>
<td>0.23304E-09</td>
<td>-9.633</td>
<td>0.1754E-10</td>
<td>-10.756</td>
<td>0.7528E-01</td>
<td>-1.123</td>
<td>0.6287E+08</td>
<td>0.000</td>
<td>-5.228</td>
</tr>
<tr>
<td>K+</td>
<td>0.50002E-01</td>
<td>-1.301</td>
<td>0.3035E-01</td>
<td>-1.518</td>
<td>0.6070E+00</td>
<td>-0.217</td>
<td>0.1955E+01</td>
<td>1840.727</td>
<td>3.265</td>
</tr>
<tr>
<td>Na+</td>
<td>0.1000E+01</td>
<td>0.000</td>
<td>0.6614E-00</td>
<td>-0.179</td>
<td>0.6614E+00</td>
<td>-0.179</td>
<td>0.2299E+02</td>
<td>2164.995</td>
<td>4.335</td>
</tr>
<tr>
<td>H2O</td>
<td>0.9181E-04</td>
<td>-4.037</td>
<td>0.9181E-04</td>
<td>-4.037</td>
<td>0.1000E+01</td>
<td>0.000</td>
<td>0.8824E-02</td>
<td>8.308</td>
<td>0.919</td>
</tr>
<tr>
<td>Cl-</td>
<td>0.1050E+01</td>
<td>0.021</td>
<td>0.6374E-00</td>
<td>-0.196</td>
<td>0.6070E+00</td>
<td>-0.217</td>
<td>0.3722E+02</td>
<td>3506.603</td>
<td>4.545</td>
</tr>
<tr>
<td>OH-</td>
<td>0.1079E+06</td>
<td>-7.967</td>
<td>0.6860E-08</td>
<td>-8.164</td>
<td>0.6358E+00</td>
<td>-0.197</td>
<td>0.1835E+06</td>
<td>0.000</td>
<td>-3.763</td>
</tr>
<tr>
<td>H+</td>
<td>0.1761E-05</td>
<td>-5.754</td>
<td>0.1442E-05</td>
<td>-5.841</td>
<td>0.8193E+00</td>
<td>-0.087</td>
<td>0.1775E-05</td>
<td>0.000</td>
<td>-2.777</td>
</tr>
<tr>
<td>H2O</td>
<td>0.5550E+02</td>
<td>1.744</td>
<td>0.9628E+00</td>
<td>-0.016</td>
<td>0.1734E+01</td>
<td>-1.761</td>
<td>0.1000E+04</td>
<td>94140.364</td>
<td>5.974</td>
</tr>
<tr>
<td>Al(OH)+</td>
<td>0.9530E-09</td>
<td>-9.021</td>
<td>0.2410E-09</td>
<td>-9.670</td>
<td>0.2245E+00</td>
<td>-0.649</td>
<td>0.4192E-07</td>
<td>0.000</td>
<td>-4.404</td>
</tr>
<tr>
<td>Al(OH)+</td>
<td>0.2970E+07</td>
<td>-10.527</td>
<td>0.1965E+07</td>
<td>-10.707</td>
<td>0.6614E+00</td>
<td>-0.179</td>
<td>0.2822E-08</td>
<td>0.000</td>
<td>-5.576</td>
</tr>
<tr>
<td>H3O4-</td>
<td>0.1223E+07</td>
<td>-7.912</td>
<td>0.8092E+08</td>
<td>-8.092</td>
<td>0.6614E+00</td>
<td>-0.179</td>
<td>0.1163E+05</td>
<td>0.000</td>
<td>-2.960</td>
</tr>
<tr>
<td>HCl</td>
<td>0.5230E+01</td>
<td>-12.282</td>
<td>0.6720E+02</td>
<td>-12.173</td>
<td>0.1285E+01</td>
<td>0.109</td>
<td>0.1906E-10</td>
<td>0.000</td>
<td>-7.746</td>
</tr>
</tbody>
</table>

### Species

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>LOG K</th>
<th>LOG Q</th>
<th>N FAR</th>
<th>DLN M/DXI</th>
<th>D2 M/DXI</th>
<th>D2LN M/DXI</th>
<th>D3 M/DXI</th>
<th>D3LN M/DXI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na+</td>
<td>0.0</td>
<td>0.0</td>
<td>0.2475E+00</td>
<td>0.2475E+00</td>
<td>0.1400E+03</td>
<td>0.1400E+03</td>
<td>0.1713E+09</td>
<td>0.1713E+09</td>
</tr>
<tr>
<td>Cl-</td>
<td>0.0</td>
<td>0.0</td>
<td>0.2601E+00</td>
<td>0.2477E+00</td>
<td>0.1408E+03</td>
<td>0.1408E+03</td>
<td>0.1799E+09</td>
<td>0.1713E+09</td>
</tr>
<tr>
<td>H+</td>
<td>0.0</td>
<td>0.0</td>
<td>0.6556E+00</td>
<td>0.3593E+00</td>
<td>0.3832E+04</td>
<td>0.1270E+12</td>
<td>0.6548E+10</td>
<td>0.8695E+17</td>
</tr>
<tr>
<td>K+</td>
<td>0.0</td>
<td>0.0</td>
<td>0.3593E+00</td>
<td>0.3593E+00</td>
<td>0.1270E+12</td>
<td>0.6548E+10</td>
<td>0.8695E+17</td>
<td></td>
</tr>
<tr>
<td>Al+++</td>
<td>-8.176</td>
<td>-8.175</td>
<td>0.3140E+03</td>
<td>0.1197E+07</td>
<td>0.2651E+03</td>
<td>0.4563E+03</td>
<td>0.4838E+08</td>
<td>0.9769E+09</td>
</tr>
<tr>
<td>Al(OH)+</td>
<td>0.4004</td>
<td>0.4004</td>
<td>0.5234E-07</td>
<td>0.6343E-07</td>
<td>0.3408E-01</td>
<td>0.3408E-01</td>
<td>0.4079E+05</td>
<td>0.4482E+09</td>
</tr>
<tr>
<td>OH-</td>
<td>-13.978</td>
<td>-13.980</td>
<td>0.3742E-02</td>
<td>0.3593E+06</td>
<td>0.2668E+04</td>
<td>0.1270E+12</td>
<td>0.2815E+10</td>
<td>0.8695E+17</td>
</tr>
<tr>
<td>Al(OH)+</td>
<td>-3.4365</td>
<td>-3.4365</td>
<td>0.8677E+03</td>
<td>0.8384E+06</td>
<td>0.4209E+03</td>
<td>0.2964E+12</td>
<td>0.4842E+08</td>
<td>0.2029E+18</td>
</tr>
<tr>
<td>Al(OH)+</td>
<td>-15.0734</td>
<td>-15.0735</td>
<td>0.6951E+05</td>
<td>0.2395E+06</td>
<td>0.4123E-01</td>
<td>0.4123E-01</td>
<td>0.8469E+11</td>
<td>0.5879E+17</td>
</tr>
<tr>
<td>H3O4-</td>
<td>-13.6026</td>
<td>-13.6098</td>
<td>0.4244E+02</td>
<td>0.3593E+06</td>
<td>0.3025E+04</td>
<td>0.1270E+12</td>
<td>0.3192E+10</td>
<td>0.8695E+17</td>
</tr>
<tr>
<td>HCl</td>
<td>6.1363</td>
<td>6.1363</td>
<td>0.1947E+08</td>
<td>0.3593E+06</td>
<td>0.1137E-02</td>
<td>0.1270E+12</td>
<td>0.1947E+04</td>
<td>0.8695E+17</td>
</tr>
</tbody>
</table>

**TOTAL MOLES**

| FLUID | 0.0 | 0.0000 | -0.1374E-01 | -0.2475E-03 | -0.7754E+04 | -0.1400E+03 | -0.9510E+10 | -0.1713E+09 |

**ACTIVITIES**

| FLUID | 0.0 | 0.0000 | -0.3053E-03 | -0.3171E-03 | -0.1787E+03 | -0.1856E+03 | -0.2139E+09 | -0.2221E+09 |

**D2/DXI** is 0.64437E-02

**Total moles of water in the system is 55.50825017 moles**

<table>
<thead>
<tr>
<th>COMPONENTS</th>
<th>TOTAL</th>
<th>LOG TOTAL</th>
<th>GRAMS/KGM H2O</th>
<th>TOTAL</th>
<th>LOG TOTAL</th>
<th>GRAMS/KGM H2O</th>
</tr>
</thead>
</table>

SILLIMANITE | 3.160 | -2.8655660 | | | | |
SODIUM OXIDE | 67.427 | 11.3061147 | | | | |
SYLVE | 1.293 | -1.7133273 | | | | |
TOTAL MASS TRANSFER IN THE SYSTEM

<table>
<thead>
<tr>
<th>MINERAL PHASES</th>
<th>AMOUNT OF REACTANT DESTROYED</th>
<th>AMOUNT OF REACTANT PRODUCED</th>
<th>AMOUNT OF PRODUCT PRODUCED</th>
<th>AMOUNT OF PRODUCT DESTROYED</th>
<th>NET AMOUNT IN THE SYSTEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-FELDSPAR</td>
<td>-0.3162E-05 -0.8802E-03 0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.3592E-01 0.9999E+01</td>
</tr>
<tr>
<td>ALPHA-QUARTZ</td>
<td>0.6319E-05 0.3797E-03 0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.1665E-01 0.1000E+01</td>
</tr>
<tr>
<td>MUSCOVITE</td>
<td>0.1054E-05 0.4197E-03 0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.1054E-05 0.4197E-03</td>
</tr>
</tbody>
</table>

NUMBER OF DELXI INCREMENTS FORWARD = 10

IONIC STRENGTH = 0.105000E+01

ELECTRICAL BALANCE = 0.981612E-15

TOTAL NUMBER OF PHASE BOUNDARIES PRESENTLY BEING CONSIDERED = 2

DISTRIBUTION OF SPECIES CALLED AT STEP 21

THE LOG K FOR K-FELDSPAR HAS BEEN EXCEEDED AT STEP 24

LOG K = 3.2837942  LOG Q = 3.3074076

<table>
<thead>
<tr>
<th>NA+</th>
<th>0.100000E+01</th>
<th>0.0000</th>
<th>0.229898E+02</th>
<th>0.216440E+06</th>
<th>5.3353</th>
<th>89</th>
</tr>
</thead>
<tbody>
<tr>
<td>CL-</td>
<td>0.105000E+01</td>
<td>0.0212</td>
<td>0.372258E+02</td>
<td>0.350466E+06</td>
<td>5.546</td>
<td></td>
</tr>
<tr>
<td>MUSCOVITE</td>
<td>0.405255E-09</td>
<td>-9.3923</td>
<td>0.161419E-06</td>
<td>0.151969E-02</td>
<td>-2.8182</td>
<td></td>
</tr>
<tr>
<td>ALPHA-QUARTZ</td>
<td>0.918233E-04</td>
<td>-4.0370</td>
<td>0.551718E-02</td>
<td>0.519421E+02</td>
<td>1.7155</td>
<td></td>
</tr>
<tr>
<td>H+</td>
<td>0.174106E-05</td>
<td>-5.7592</td>
<td>0.175493E-05</td>
<td>0.165220E-01</td>
<td>-1.7819</td>
<td></td>
</tr>
<tr>
<td>K+</td>
<td>0.500021E-01</td>
<td>-1.3010</td>
<td>0.195518E+01</td>
<td>0.184073E+05</td>
<td>4.2650</td>
<td></td>
</tr>
<tr>
<td>H2O</td>
<td>0.555084E+02</td>
<td>1.7444</td>
<td>0.100000E+04</td>
<td>0.941463E+07</td>
<td>6.9738</td>
<td></td>
</tr>
</tbody>
</table>
EQUILIBRIUM HAS BEEN ATTAINED AND SOLUTION CHARACTERISTICS ARE OUTLINED BELOW

\[ \log_{10} \xi = 0.354948 \times 10^{-7} \]

\[ \log_{10} \xi = 0.519635 \times 10^{-5} \]

\[ \log_{10} \xi = -5.284 \]

### Products

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Cumulative Gram Change</th>
<th>Log Cumult Gram Change</th>
<th>Cumulative Mole Change</th>
<th>Log Cumult Mole Change</th>
<th>Reaction Coefficient</th>
<th>Log of Solubility Product</th>
<th>Log of Ion Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALPHA-QUARTZ</td>
<td>1.00062E+01</td>
<td>0.000</td>
<td>1.66535E-01</td>
<td>-1.778</td>
<td>0.194284E+01</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>MUSCOVITE</td>
<td>6.89915E-03</td>
<td>-3.161</td>
<td>1.73209E-05</td>
<td>-5.761</td>
<td>0.333356E+00</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Minerals

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Log K</th>
<th>Log Q</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALPHA-QUARTZ</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>ANALCIME</td>
<td>6.372</td>
<td>4.6056286</td>
</tr>
<tr>
<td>ANDALUSITE</td>
<td>2.801</td>
<td>-3.2673631</td>
</tr>
<tr>
<td>A-CRISTOEALITE</td>
<td>0.270</td>
<td>0.0</td>
</tr>
<tr>
<td>BETA-QUARTZ</td>
<td>0.138</td>
<td>0.0</td>
</tr>
<tr>
<td>BOSEKITE</td>
<td>0.714</td>
<td>-1.6418971</td>
</tr>
<tr>
<td>B-CRISTOEALITE</td>
<td>0.376</td>
<td>0.0</td>
</tr>
<tr>
<td>COESITE</td>
<td>0.810</td>
<td>0.0</td>
</tr>
<tr>
<td>COBUNDUM</td>
<td>3.617</td>
<td>-3.2673631</td>
</tr>
<tr>
<td>DEHYDRATED ANALCIME</td>
<td>11.079</td>
<td>4.6220597</td>
</tr>
<tr>
<td>DIASPORRE</td>
<td>-0.131</td>
<td>-1.6418971</td>
</tr>
<tr>
<td>GIBBSITE</td>
<td>-0.922</td>
<td>-1.6583262</td>
</tr>
<tr>
<td>HALITE</td>
<td>1.432</td>
<td>0.3759500</td>
</tr>
<tr>
<td>HIGH SANIDINE</td>
<td>4.483</td>
<td>3.2837942</td>
</tr>
<tr>
<td>HIGH ALBITE</td>
<td>7.504</td>
<td>4.6220597</td>
</tr>
<tr>
<td>JADEITE</td>
<td>7.813</td>
<td>4.6220597</td>
</tr>
<tr>
<td>KALSIILITE</td>
<td>6.463</td>
<td>3.2837942</td>
</tr>
<tr>
<td>KACLINITRE</td>
<td>-2.341</td>
<td>-3.3002253</td>
</tr>
<tr>
<td>KYANITE</td>
<td>2.526</td>
<td>-3.2673631</td>
</tr>
<tr>
<td>K-FELDSPAR</td>
<td>3.284</td>
<td>3.2837942</td>
</tr>
<tr>
<td>LOW ALBITE</td>
<td>6.186</td>
<td>4.6220597</td>
</tr>
<tr>
<td>MUSCOVITE</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>NASHILINE</td>
<td>9.227</td>
<td>4.6220597</td>
</tr>
<tr>
<td>PARAGONITE</td>
<td>3.760</td>
<td>1.3382655</td>
</tr>
<tr>
<td>POTASSIUM OXIDE</td>
<td>84.316</td>
<td>9.8349515</td>
</tr>
<tr>
<td>ROYOPHILLITE</td>
<td>-0.716</td>
<td>-3.2673631</td>
</tr>
<tr>
<td>SILLIMANITE</td>
<td>3.160</td>
<td>-3.2673631</td>
</tr>
<tr>
<td>SODIUM OXIDE</td>
<td>67.427</td>
<td>12.5114825</td>
</tr>
<tr>
<td>SYLVITE</td>
<td>1.223</td>
<td>-1.7133155</td>
</tr>
</tbody>
</table>

### Gases

<table>
<thead>
<tr>
<th>NAME</th>
<th>Log K</th>
<th>Activity</th>
<th>Log Activity</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEAM</td>
<td>1.50517</td>
<td>0.30088E-01</td>
<td>-1.52160</td>
</tr>
</tbody>
</table>
### AQUEOUS SPECIES

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>MOLALITY</th>
<th>LOG MOL</th>
<th>ACTIVITY</th>
<th>LOG ACT</th>
<th>ACT COEF</th>
<th>LG ACT C</th>
<th>GRAMS/KGM H2O</th>
<th>PPM</th>
<th>LOG PPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2O</td>
<td>0.55580E+02</td>
<td>1.744</td>
<td>0.96287E+00</td>
<td>-0.016</td>
<td>0.17346E-01</td>
<td>-1.761</td>
<td>0.000010E+04</td>
<td>941460.316</td>
<td>5.974</td>
</tr>
<tr>
<td>AL (OH)++</td>
<td>0.37398E-10</td>
<td>-10.427</td>
<td>0.83982E-11</td>
<td>-11.076</td>
<td>0.22456E+00</td>
<td>-0.649</td>
<td>0.16451E-08</td>
<td>0.000</td>
<td>-5.810</td>
</tr>
<tr>
<td>AL (OH)++</td>
<td>0.74949E-10</td>
<td>-10.125</td>
<td>0.49578E-10</td>
<td>-10.305</td>
<td>0.66147E+00</td>
<td>-0.179</td>
<td>0.46627E-05</td>
<td>0.000</td>
<td>-2.358</td>
</tr>
<tr>
<td>HCl</td>
<td>0.13056E-12</td>
<td>-12.088</td>
<td>0.16777E-12</td>
<td>-12.775</td>
<td>0.12850E+00</td>
<td>0.109</td>
<td>0.47604E-11</td>
<td>0.000</td>
<td>-8.349</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>LOG M</th>
<th>LOG Q</th>
<th>N EAR</th>
<th>DLM M/DXI</th>
<th>D2 M/DXI</th>
<th>D2LN M/DXI</th>
<th>D3 M/DXI</th>
<th>D3LN M/DXI</th>
</tr>
</thead>
<tbody>
<tr>
<td>K+</td>
<td>0.0</td>
<td>0.0</td>
<td>-0.29687E-02</td>
<td>0.29687E-02</td>
<td>0.60504E+04</td>
<td>0.14987E+11</td>
<td>0.14987E+11</td>
<td></td>
</tr>
<tr>
<td>Cl-</td>
<td>0.0</td>
<td>0.0</td>
<td>-0.31178E-02</td>
<td>0.25690E-02</td>
<td>0.63529E+04</td>
<td>0.15736E+11</td>
<td>0.15736E+11</td>
<td></td>
</tr>
<tr>
<td>H+</td>
<td>0.0</td>
<td>0.000000000</td>
<td>-0.55887E+00</td>
<td>-0.12167E+07</td>
<td>0.21878E+06</td>
<td>-0.10040E+13</td>
<td>0.54357E+12</td>
<td>-0.68034E+16</td>
</tr>
<tr>
<td>AL+++</td>
<td>-8.1746</td>
<td>-8.1745</td>
<td>-0.10715E-04</td>
<td>-0.40557E+07</td>
<td>0.34614E+03</td>
<td>-0.10040E+13</td>
<td>0.54357E+12</td>
<td>-0.68034E+16</td>
</tr>
<tr>
<td>H4SiO4</td>
<td>4.0042</td>
<td>4.0042</td>
<td>-0.70978E-06</td>
<td>-0.77308E-06</td>
<td>-0.14470E+01</td>
<td>-0.15760E+05</td>
<td>-0.35835E+07</td>
<td>-0.39303E+11</td>
</tr>
<tr>
<td>OH-</td>
<td>13.9878</td>
<td>13.9878</td>
<td>0.50535E-01</td>
<td>0.12167E+07</td>
<td>0.10281E+06</td>
<td>0.10040E+13</td>
<td>0.25435E+12</td>
<td>0.68034E+18</td>
</tr>
<tr>
<td>AL (OH)++</td>
<td>-3.4936</td>
<td>-3.4935</td>
<td>-0.11760E-03</td>
<td>-0.83902E+07</td>
<td>0.23680E+03</td>
<td>-0.23428E+13</td>
<td>-0.18705E+09</td>
<td>-0.15875E+19</td>
</tr>
<tr>
<td>HCl</td>
<td>6.1363</td>
<td>6.1363</td>
<td>-0.16597E-06</td>
<td>-0.12167E+07</td>
<td>0.64973E-01</td>
<td>-0.10040E+13</td>
<td>0.16143E+06</td>
<td>-0.68034E+18</td>
</tr>
</tbody>
</table>

**TOTAL MOLES**

- **H2O**: 0.0
- **H2C**: 0.0

**DI/DXI** is **0.1047E+00**

**TOTAL MOLES OF WATER IN THE SYSTEM** is **55.5825007 MOLES**

### COMPONENTS

<table>
<thead>
<tr>
<th>COMPONENTS</th>
<th>TOTAL MOALITY</th>
<th>LOG TOTAL MOALITY</th>
<th>TOTAL GRAMS/KGM H2O</th>
<th>TOTAL PPM</th>
<th>LOG PPM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na+</td>
<td>0.10000E+01</td>
<td>0.0000000000</td>
<td>0.22989E+02</td>
<td>0.21644E+06</td>
<td>5.3353</td>
</tr>
<tr>
<td>Cl-</td>
<td>0.10500E+01</td>
<td>0.0212000000</td>
<td>0.37225E+02</td>
<td>0.35046E+06</td>
<td>5.5446</td>
</tr>
<tr>
<td>H2SiO4</td>
<td>0.32000E-10</td>
<td>-10.417800000</td>
<td>0.12829E+07</td>
<td>0.19289E-03</td>
<td>-3.8438</td>
</tr>
<tr>
<td>K+</td>
<td>0.50000E+01</td>
<td>-1.301000000</td>
<td>0.19552E+01</td>
<td>0.18407E+05</td>
<td>4.2560</td>
</tr>
<tr>
<td>H2O</td>
<td>0.55000E+02</td>
<td>1.7444000000</td>
<td>0.10000E+00</td>
<td>0.94163E+07</td>
<td>6.9738</td>
</tr>
</tbody>
</table>
TOTAL MASS TRANSFER IN THE SYSTEM

<table>
<thead>
<tr>
<th>MINERAL PHASES</th>
<th>AMOUNT OF REACTANT DESTROYED</th>
<th>AMOUNT OF REACTANT PRODUCED</th>
<th>AMOUNT OF PRODUCT PRODUCED</th>
<th>AMOUNT OF PRODUCT DESTROYED</th>
<th>NET AMOUNT IN THE SYSTEM</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>MOLES</td>
<td>GRAMS</td>
<td>MOLES</td>
<td>GRAMS</td>
<td>MOLES</td>
</tr>
<tr>
<td>ALPH-A-QUARTZ</td>
<td>0.1035E-04</td>
<td>0.6220E-03</td>
<td>0.0</td>
<td>0.0</td>
<td>0.1665E-01</td>
</tr>
<tr>
<td>MUSCOVITE</td>
<td>0.1732E-05</td>
<td>0.6899E-03</td>
<td>0.0</td>
<td>0.0</td>
<td>0.1732E-05</td>
</tr>
<tr>
<td>K-FELDSPAR</td>
<td>0.0</td>
<td>0.0</td>
<td>-0.5196E-05</td>
<td>-0.1446E-02</td>
<td>0.3592E-01</td>
</tr>
</tbody>
</table>

NUMBER OF DELXI INCREMENTS FORWARD = 24

IONIC STRENGTH = 0.105000E+01       ELECTRICAL BALANCE = 0.283738E-15

TOTAL NUMBER OF PHASE BOUNDARIES PRESENTLY BEING CONSIDERED = 2
APPENDIX 3
INLElCIT REAL*8 (A - H, O - Z)
COMMON / P A T D A T / NDX (200, 2), COPM (20, 200), AZERO (200), GMIN (200),
1 GSOL (200), GCOM (20, 10), COHS (20, 200), Z (200), BR (20),
2 COMEG (20, 10), WGHTM (200), WGHTS (200), WGT (10), GMEXT (4),
3 F, T, ADH, BDH, GT, MNRW, ALSTHY, NAM (5, 200),
4 NAMES (2, 200), NAM (10), NAMER (5, 20), MOA (20),
5 IREACT (20), NMT, NST, NC, NGAS, NET, MAX, NDLINC, INCN,
6 COM/N / A A A / A A A (200), ALG (200), ACT (200), ALA (200), C (200),
1 ALG (200), B (20, 200), TOTM (20), XPPM (200), TN (200),
2 GSP (200), ALGAS (20), AGAS (20), OX, ELECT, XIPRT, DELXIT
COMMON / C A R A Y / QM (200), QS (200), BB (20, 200), A (20, 20), DN (200),
1 CC (200, 20), X (200, 4), CV (200), UCV (200), CSVE (200), DC (200),
2 WS (20, 20), W (20, 200), XD (200, 4), ASYS (200), AMDE (200),
3 ADEST (200), AO, OX, DEDI, IPEOD (20), NDELD, ISAT, NPT,
4 NOD, IFIN, IPRINT
DIMENSION GRMTOT (40), XTFPM (40)
IFIN = 0
DELXIT = 0.0D0
DA 10 I = 1, 200
AMADE (I) = 0.0D0
ADEST (I) = 0.0D0
ASYS (I) = 0.0D0
10 CONTINUE
XIPRT = -6.0D0
NFT = 0
NDELDI = 0
C ALL DATA (ICTM)
CALL DREAD (E, ASYS)
DELXIT = 1.0D-10
NINC = NDLINC
NOD = 1
NC1 = NC - 1
NPT = 0
DA 20 I = 1, NC1
IF (NDX I, 2) .EQ. 0 OR. NDX I, 2) .EQ. 3) GO TO 20
NFT = NFT + 1
K = NDX I, 1
IPEOD (NFT) = K
ASYS (K) = TOTM (I) / WGHTM (K)
20 CONTINUE
IF (NFT .LT. 1) GO TO 40
DA 30 I = 1, NFT
K = IREACT (I)
ASYS (K) = ASYS (K) / WGHTM (K)
30 CONTINUE
DA 40 CALL DIST
CALL SATCHK
IPRINT = 1
IF (NRT .LE. 1 .AND. NDELXI .EQ. 0) NRT = -2
IF (NRT .LT. 1 .AND. NDELXI .EQ. 0) GO TO 120
IF (ISAT .NE. 0 .AND. NDELXI .EQ. 0) GO TO 110
IF (NDELXI .NE. 0) GO TO 60
50 CALL FINDC
CALL ACTIV
CALL SETCOL
CALL SETMAT
60 IF (ISAT .NE. 0) CALL REACTN
IF (IFIN .NE. 0) GO TO 130
70 CALL MOVE
NDELXI = NDELXI + 1
CALL SAVCHK
CALL FINMV
IF (NINC .EQ. NDELXI) IPRINT = 1
IF (ISAT .NE. 0). IPRINT = 1
IF (NINC .EQ. NDELXI) NINC = NINC * NDLINC
IF (NDELXI .GE. MAXI) GO TO 140
IF (IPEINT .EQ. 1) CALL OUTPUT
IF (IPEINT .EQ. 1) GO TO 90
80 CONTINUE
90 IPRINT = 0
GO TO 60
100 CALL SOLSP3(GRMFOT, XTPPM)
CALL DIST
GO TO 60
110 CONTINUE
NRT = -1
120 CALL OUTPUT
STOP
130 CONTINUE
NRT = 0
140 CALL OUTPUT
STOP
END

SUBROUTINE CIST

THIS SUBROUTINE CALCULATES THE DISTRIBUTION OF SPECIES.

IMPLICIT REAL*8(A-H, O-Z)

TOTM(I) CONTAINS TOTAL MOALITY OF COMPONENT OR LOG ACTIVITY
OF COMPONENT SPECIES
MOA(I) IS THE SWITCH TO INDICATE MOALITY OR ACTIVITY
0 = TOTAL MOALITY  1 = LOG ACTIVITY

DIMENSION CSAVE(200), ASAVE(200), CSV(20), CBS(200),
1 NDXTALL(200,2), B1(20,200), NDXSOL(200,2), GSOL1(200)
COMMON /PATDAV/, MDX(200,2), COMPA(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GAS(10), COMPS(20,200), Z(200), R(20),
2 COMEG(20,10), WMTHM(200), GWHTS(200), GWHTS(10), GMIN(N),
3 PG, T, ADH, BDH, BDCT, ANH2O, ANH2O, NAMEM(5,200),
4 NAMES(2,200), NAMEG(5,10), NAMER(5,20), MOA(20),
5 IREACT(20), NMT, NST, NC, NGAS, NRT, MAXI, NDLINC, INION,
6  COMMON /CONCI/ G(200), ALG(200), ACT(200), ALA(200), C(200),
1 ALC(200), E(20,200), TOTM(20), XPM(200), TN(200),
2 GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXIT
COMMON /CARRAY/ QM(200), QS(200), BB(20,200), A(20,20), DN(200),
1 CC(200,20), X(200,4), CV(200), UCV(20), CSVE(200), DC(200),
2 WS(20,20), W(20,200), XD(200,4), ASYS(200), AMAD(200),
3 ADEST(200), A10, XL, DELXI, IPR(20), NDELI, ISAT, NPT,
4 NOD, IFIN, IPRINT
DATA IO2 /'OXYG'/
NC1 = NC - 1
DD = 10.0000
A10 = DLOG(DD)
WRITE (6,620) NDELI
NK2 = NK - 2
IF (NDELI . LT. 1) GO TO 20
EC 10 I = 1, NST
CBG(I) = ALC(I)
ASAVE(I) = ALA(I)
10 CONTINUE
20 CONTINUE
IF (NDELI . GT. 1) GO TO 40
EC 30 I = 1, NK2
IF (.INICN = NDX(1,1) . AND. NDX(I,2) . EQ. 0) GO TO 110
30 CONTINUE
40 IF (NGAS . LT. 1) GO TO 80
DO 50 I = 1, NGAS
IF (102 . NE. NAMEG(I,1)) GO TO 50
IQ = I
GO TO 60
50 CONTINUE
GO TO 80
60 ATEMP = 100.000
DO 70 I = 1, NC1
IF (NDX(I,2) . NE. 0) GO TO 70
IF (DABS(CMPG(I,IQ)) . LT. 1.0D-13) GO TO 70
LL = NDX(I,1)
IF (C(LL) . GT. ATEMP) GO TO 70
ATEMP = C(LL)
K = I
70 CONTINUE
NDX(K,1) = IQ
NDX(K,2) = 3
MOA(K) = 1
IRET = -1
CALL TRANS(E, IRET)
CALL ACTIV
80 ATEMP = 0.0000
DO 100 I = 1, NC1
IF (NDX(I,2) . NE. 0) GO TO 90
IF (MOA(I) . EQ. 1) GO TO 100
K = NDX(I,1)
IF (ATEMP . GT. C(K) . OR. DABS(Z(K)) . LE. 1.0D-5 . OR. Z(K) . GT. 9.99) GO TO 100
ATEMP = C(K)
10 IF = I
INICN = K
GO TO 100
50 IF (NDX (I, 2) .EQ. 1) MOA (I) = 1
100 CONTINUE
110 IEAL = IP
C
INITIALIZE
IF (NDELXI .GT. 1) GO TO 240
DO 120 I = 1, NC
CSV (I) = 0.0D00
120 CONTINUE
DO 130 I = 1, NST
CSAVE (I) = 0.0D00
G (I) = 1.0E00
ALG (I) = 0.0D00
130 CONTINUE
K = NEX (NC, 1)
ACT (K) = 1.0D00
ALA (K) = 0.01D0
C (K) = 1.0D00 / .01801534D00
ALC (K) = DLOG10 (C (K))
G (K) = .01801534D00
ALG (K) = DLOG10 (G (K))
DO 170 I = 1, NC1
IF (NDX (I, 2) .GT. 0) GO TO 150
K = NDX (I, 1)
IF (MOA (I) .EQ. 1) GO TO 140
C (K) = TOTM (I)
ALC (K) = DLOG10 (C (K))
ACT (K) = C (K)
ALA (K) = AIC (K)
GO TO 170
140 ALC (K) = TOTM (I)
C (K) = 10.0D00 ** ALC (K)
ACT (K) = C (K)
ALA (K) = ALC (K)
GO TO 170
150 IF (NDX (I, 2) .EQ. 1) GO TO 160
K = NEX (I, 1)
ALG AS (K) = TOTM (I)
AGAS (K) = 10.0D00 ** (ALG AS (K))
GO TO 170
160 CONTINUE
170 CONTINUE
IF (NDELXI .GT. 0) GO TO 240
DO 180 J = 1, NC
NDXALL (J, 1) = NDX (J, 1)
NDXALL (J, 2) = NDX (J, 2)
180 CONTINUE
CALL FLIP
NK2 = NK - 2
NX1 = NK - NC - 2
DO 190 J = 1, NK2
NDXSOL (J, 1) = NDX (J, 1)
NDXSOL (J, 2) = NDX (J, 2)
190 CONTINUE
DO 210 J = 1, NX1
DO 200 I = 1, NC
B1(I,J) = B(I,J)

CONTINUE

DO 220 J = 1, NST
   GSCL1(J) = GSOL(J)

CONTINUE

DO 230 J = 1, NC
   NDX(J,1) = NDXALL(J,1)
   NDX(J,2) = NDXALL(J,2)

CONTINUE

IRET = -1
CALL TRANS(E, IRET)

CONTINUE

NIC = 0
NX = NK - NC - 2
IF (NDELXI .LT. 1) GO TO 280
DO 260 J = 1, NX1
   DO 250 I = 1, NC
      B1(I,J) = B(I,J)
   CONTINUE

DO 270 K = 1, NK
   NDXSOI(K,1) = NDX(K,1)
   NDXSOI(K,2) = NDX(K,2)
   GSCL1(K) = GSOL(K)

CONTINUE

IF (NDELXI .GT. 0) GO TO 300
DO 290 I = 1, SC
   IF (NDX(I, 2) .EQ. 1) GO TO 400
CONTINUE

NSCC = 0
CONTINUE

DO 370 I = 1, NC1
   IF (NDXSOL(I,2) .NE. 0) GO TO 370
   K = NDXSOI(I,1)
   IF (MGA(I) .EQ. 1) GO TO 370
   ATEMP = 1.0D0

DO 360 J = 1, NX1
   IF (DABS(B1(I,J)) .LT. 1.0D-13) GO TO 360
   L = NDXSOI(NC + J,1)
   BTEMP = (B1(I,J) - 1.0D00) * ALA(K)
   BTEMP = BTEMP + ALG(K) - GSOL1(L) - ALG(L)
   DO 350 JJ = 1, NC
      IF (JJ .EQ. I) GO TO 350
      IF (DABS(B1(JJ,J)) .LT. 1.0D-13) GO TO 350
      IF (NDXSOL(JJ,2) .GT. 0) GO TO 330
      MM = NDXSOI(JJ,1)
      BTEMP = BTEMP + B1(JJ,J) * ALA(MM)
      GO TO 350
   CONTINUE

IF (NDXSOL(JJ,2) .EQ. 3) GO TO 340
GO TO 350

BTEMP = BTEMP + B1(JJ,J) * ALGAS(NDX(JJ,1))

CONTINUE

ATEMP = ATEMP + B1(I,J) * 10.0 ** BTEMP
CONTINUE
C(K) = TOTM(I) / ATEMP
IS = I
KI = K
IF (C(K) .LT. 0.0D00) GO TO 590
370 CONTINUE
380 XTTEST = 1.0D-9
KK = 0
NN = 0
DO 390 I = 1, NC
   IF (NDX(I,2) .NE. 0) GO TO 390
   IF (MCA(I) .EQ. 1) GO TO 390
   KK = KK + 1
   K = NDX(I,1)
   ATEMP = DASES((CSV(I) - C(K))/C(K))
   IF (ATEMP .LE. XTTEST) NN = NN + 1
   ALC(K) = DLOG10(C(K))
   CSV(I) = C(K)
   ALA(K) = ALC(K) + ALG(K)
   ACT(K) = 10.0D00 ** ALA(K)
390 CONTINUE
NSOC = NSOC + 1
IF (KK .NE. NN .AND. NSOC .LT. 50) GO TO 320
CALL XICALC(C, Z, ELECT, NST, XI)
CALL GAMMA(XI, ADA, BDH, BDOT, NST,,NC, AZERO, Z, GNEUT, G, C, 1
ACT, NEX, XL, ALG)
ATEMP = 0.0D00
DO 460 I = 1, NC
   IF (NDX(I,2) .NE. 0) GO TO 460
   IF (MCA(I) .EQ. 1) GO TO 450
   K = NDX(I,1)
   ALA(K) = AIC(K) + ALC(K)
   ACT(K) = 10.0 ** ALA(K)
   ATEMP = ATEMP + C(K)
450 CONTINUE
460 CONTINUE
C (K) = 10.0000 ** ALC(K)
ATEMP = ATEMP + C(K)

460 CONTINUE
DC 470 I = 1, NX
  K = NDX(NC + I, 1)
  ALC(K) = ALC(K) + ALG(K)
  ACT(K) = 10.0000 ** ALC(K)
  ATEMP = ATEMP + C(K)

470 CONTINUE
C
COMPUTE ACTIVITY OF H2O
IF (NDELXI .GT. 1) GO TO 480
IF (ATEMP .GT. 30) ATEMP = 30.
  K = NDX(NC, 1)
  ALC(K) = -ATEMP * .018015340000 / A10
  ACT(K) = 10.0000 ** ALC(K)
  G(K) = ACT(K) * .018015340000
  ALG(K) = DLOG10(G(K))
C
CORRECT CHARGE BALANCE
480 TOTM(IBAL) = TOTM(IBAL) - ELECT / Z(INION)
IF (TOTM(IBAL) .LT. 0.0) GO TO 570
  XTEST = 1.0D-7
  KK = 0
  DO 500 I = 1, NST
    IF (C(I) .EQ. 0.0000) ATEMP = CSAVE(I) - C(I)
    IF (C(I) .EQ. 0.0000) GO TO 490
    ATEMP = (CSAVE(I) - C(I)) / C(I)
  IF (DABS(ATEMP) .LT. XTEST) KK = KK + 1
  CSAVE(I) = C(I)
  500 CONTINUE
NTO = NTO + 1
  IF (KK .NE. NST .AND. NTO .LT. 50) GO TO 310
  IF (KK .NE. NST .AND. NTO .GE. 50)  GO TO 580
  CALL SOLSP1(NST, C, GS, WGHTS, XPPM)
  CALL ACTIV
  IF (NDELXI .LT. 1) GO TO 510
  CALL FINDC
  CALL ACTIV
  CALL SETCOL
  CALL SETMAT
  IF (NDELXI .GT. 1) GO TO 550
  510 WRITE(6,680)
    DC 530 I = 1, NST
    XLG = ALC(I)
    XLGACT = AIA(I)
    XLGG = ALG(I)
    IF (XPPM(I) .EQ. 0.0000) XLPPM = -1000.0000
    IF (XPPM(I) .EQ. 0.0000) GO TO 520
    XLPIM = DLOG10(XPPM(I))
    WRITE(6,690) NAMES(1,I), NAMES(2,I), C(I), XLG, ACT(I),
                 XLGACT, G(I), XLGG, GSP(I), XPPM(I), XLPPM
  520 CONTINUE
  WRITE(6,690) XI, ELECT
  IF (NGAS .LT. 1) GO TO 550
  WRITE(6,630)
    DO 540 J = 1, NGAS
      WRITE(6,640) (NAMEG(JJ,J), JJ=1,5), GGAS(J), AGAS(J), ALGAS(J)
    540 CONTINUE
550 DO 560 I = 1, NC
  MOA(I) = 0
560 CONTINUE
END
570 WHITE (6,670)
STOP
580 WHITE (6,660)
STOP
590 IF (NDLX1 .LT. 1) GO TO 610
  DO 600 I = 1, NST
    ALA(I) = ASAVE(I)
    ALC(I) = CEG(I)
    C(I) = 10.0D00 ** ALC(I)
 600 CONTINUE
  MOA(IS) = 1
  GO TO 80
610 WHITE (6,650) NAMES(1,KI), NAMES(2,KI)
STOP
C
620 FORMAT (" DISTRIBUTION OF SPECIES CALLED AT STEP ", I5)
630 FORMAT (" GASES", ", " ' " NAME", ", " NAME", " LOG K", " ACTIVITY", " LOG ACTIVITY", ", " NAME")
640 FORMAT (X, 5A4, 1X, F12.5, 1X, E12.5, 1X, F12.5)
650 FORMAT (" IMPOSSIBLE CONSTRAINTS FOR DISTRIBUTION OF SPECIES";
  " DRIVEN NEGATIVE")
660 FORMAT (" FAILURE TO CONVERGE ON CONCENTRATION IN 25 CYCLES;
  " DRIVEN NEGATIVE")
670 FORMAT (" CONCENTRATION OF ION DRIVEN NEGATIVE WHILE TRYING TO ACHIEVE ELECTRICAL BALANCE")
680 FORMAT (" AQUEOUS SPECIES", ", " SPECIES", ", " MOLALITY", ", " LOG MCI", ", " LOG PPM")
700 FORMAT (" IONIC STRENGTH = ", E13.6, " ELECTRICAL BALANCE = ", E13.6)
END
SUBROUTINE FLIP
IMPLICIT REAL*8(A - H, O - Z)
COMMON /PAIDAT/ NDX(200,2), COMPH (20,200), AZERO(200), GMIN(200),
  GSOL (200), GAAS(10), COMPS(20,200), Z(200), RB(20),
  CONFG(20,10), WGHTM(200), WGHTS(200), WGHTG(10), GNEUT(4),
  P, T, ADH, BDH, BDC, ALMH2O, ALMH2O, NAMER(5,200),
  NAMES(2,200), NAMERG(5,10), NAMER(5,20), MOA(20),
  IREA(20), NM, NST, NC, NGAS, NET, MAXI, NDLINC, INION,
  NK
COMMON /CONC/ G(200), ALG(200), ACT(200), ALA(200), C(200),
  ALC(200), P(20,200), TOTM(20), XPM(200), TN(200),
  GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXIT
NC2 = NC * 2
NX = NK - NC2
NC1 = NC - 1
IRET = 1
10 CONTINUE
DO 30 I = 1, NC1
  IF (NDX(I,2) .NE. 1) GO TO 30
  IF (NDX(I,2) .NE. 1) GO TO 30
SUBROUTINE SCLSP1(NST, C, GSP, WTSP, XPPM)
C THIS ROUTINE CALCULATES THE GRAINS AND PM'S OF THE SOLUTION SPECIES
IMPLICIT REAL*8 (A - H, O - Z)
DIMENSION C(200), GSP(200), WTSP(200), XPPM(200)
SGSF = 0.0E00
DO 10 I = 1, NST
  GSP(I) = C (I) * WTSP(I)
  10 SGSF = SGSF + GSP (I)
  ARTP = 1.0D-6 / (SGSF)
  DO 20 I = 1, NST
  XPIM(I) = GSP(I) * ARTP
  20 CONTINUE
RETURN...
END

SUBROUTINE GAMMA(XL, ADH, EDH, BDOT, NST, NC, AZERO, Z, GNEUT, G, ACT, NDX, XL, ALG)
C CALCULATES GAMMAS OF AQUEOUS SPECIES - NEUTRAL SPECIES
APPROXIMATED FROM KNOWN DATA FOR CO2 AT VARIOUS IONIC STRENGTHS
IMPLICIT REAL*8 (A - H, O - Z)
DIMENSION AZERO(200), Z(200), GNEUT(4), G(200), C(200), ACT(200),
1 NDX(200,2), ALG(200)
MM = 1
IF (XI .GT. 1.) MM = 2
IF (XI .GT. 2.) MM = 3
IF (XI .GT. 3) GO TO 10
XG = GNEUT(MM) (GNEUT(MM) - GNEUT(MM - 1)) * (XI - MM + 1)
GO TO 20
10 XG = GNEUT(MM) + (GNEUT(MM) - GNEUT(MM - 1)) * (XI - MM + 1)
20 XL = DLG10(XG)
SXI = XI ** 5.0D-01
ADT = ADH * SXI
BDT = EDH * SXI
DC 50 I = 1, NST
SXI = Z(I)
IF (DABS(SXI) .LT. 1.0D-5) GO TO 30
IF (SXI .GT. 9.99) GO TO 40
G(I) = 10. ** (-ADT*SXI*SXI/(1. + BDT*AZERO(I)) + BDOT*XSI)
ALG(I) = DIGG10(G(I))
GO TO 50
30 CONTINUE
GO TO 50

CONTINUE

G(I) = 1.0000

ALG(I) = 0.0000

CONTINUE

K = NDXINC, 1)

CALCULATE GAMMA OF H2O

G(K) = ACT(K) * .01801534D0

ALG(K) = DLOG10(G(K))

RETURN

SUBROUTINE XICALC(C, Z, ELECT, NST, XI)

CALCULATES IONIC STRENGTH AND ELECTRICAL BALANCE

IMPLICIT REAL*8(A - H, O - Z)

DIMENSION C(200), Z(200)

XI = 0.0000

ELECT = 0.

DO 10 I = 1, NST

B = Z(I)

IF (DABS(B) .LT. 1.0D-5) GO TO 10

A = C(I) * B

XI = XI + 5.0D-01 * A * B

ELECT = ELECT + A

CONTINUE

IF (XI .GT. 30) XI = 30

IF (DABS(ELECT) .GT. 30.) ELECT = (DABS(ELECT)/ELECT) * 30.

RETURN

END

SUBROUTINE SOLSP3(GRMTOT, XTPPM)

THIS ROUTINE CALCULATES THE TOTAL MOLALITY, TOTAL GRAMS, AND TOTAL PPM OF THE IONS IN SOLUTION

IMPLICIT REAL*8(A - H, O - Z)

COMMON /PATDAT/ NDX(200, 2), COMPM(20, 200), AZERO(200), GMIN(200),

1 GSOL(200), GNAS(10), COMPS(20, 200), Z(200), RZ(20),

2 COMEG(20, 10), WGHTM(200), WGHTS(200), WNGHTG(10), GNEUT(4),

3 P, T, ADH, BDH, BDCT, AMH2O, ALEN, NAMER(5, 200),

4 NAMES(2, 200), NAMER(5, 10), NAMER(5, 20), MOA(20),

5 IREACT(20), NMT, NXT, NC, NGAS, NET, MAX, NDLINC, INION,

6 NK

COMMON /CONCT/ G(200), ALG(200), ACT(200), AAL(200), C(200),

1 ALC(200), B(20, 200), TOTM(20), XTPPM(200), TN(200),

2 GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXIT

DIMENSION XTPPM(40), GRMTOT(40)

SGSP = 0.0000

DO 10 J = 1, NC

XTPPM(J) = 0.0000

TOTM(J) = 0.0000

CONTINUE

10 DO 30 J = 1, NC

IF (DABS(COMPS(J, I)) .LT. 1.0D-13) GO TO 20

IF (ALC(I) .LT. -99.) GO TO 20

TOTM(J) = TOTM(J) + COMPS(J, I) * C(I)

20 CONTINUE

30 CONTINUE
DO 60 I = 1, NC
   IF (NDX(I,2) .EQ. 0) GO TO 40
   GRMTOT(I) = TOTM(I) * WGHTM(NDX(I,1))
   GO TO 50
40   GRMTOT(I) = TOTM(I) * WGHTS(NDX(I,1))
50   CONTINUE
60 CONTINUE
NSMTOT = NSM + GRMTOT(I)

DO 70 I = 1, NC
   XTEEM(I) = GRMTOT(I) * ARTP
70 CONTINUE
RETURN
END

SUBROUTINE OUTPUT

THIS SUBROUTINE DOES ALL OF THE OUTPUT FOR THE PROGRAM PATH

IMPLICIT REAL*8 (A - H, O - Z)
COMMON /PAT DAT/ NBX(200,2), COMPM(20,200), AZERO(200), GMIN(200),
   GSOL(200), GNAS(10), COMPS(20,200), Z(200), BB(20),
   COM(200), WGHTM(200), WGHTS(200), WGHTG(10), GNEUT(4),
   P, T, ADH, BDH, BDOT, AMH20, ALMH20, NAMEM(5,200),
   NAMES(2,200), NAMEG(5,10), NAMER(5,20), MOA(20),
   IREACT(20), NMT, NST, NC, NGA3, NET, MAXI, NDINLC, INION,
   COMMON /CONCT/ G(200), ALG(200), ACT(200), ALA(200), C(200),
   ALC(200), B(20,200), TOTM(20), XPPM(200), TN(200),
   GSP(200), AGAS(20), XI, ELECT, XIPPT, DELXIT
COMMON /C A R B A Y/ QM(200), OLS(200), BB(20,200), A(20,20), DN(200),
   CC(200,20), X(200,4), CV(200), HCV(20), CSVE(200), DC(200),
   WS(20,20), W(20,200), XD(200,4), ASYS(200), AMADE(200),
   ADEST(200), A10, XI, DELXI, IPBOD, NDELXI, ISAT, NPT,
   NOD, IINF, IPRINT
DIMENSION GRMTOT(40), XTPPM(40)
DATA HDRBOG /'H+ '/'
   IF (NRB .GT. 0) WRITE (6,430)
   IF (NRB .EQ. 0) WRITE (6,440)
   IF (NRB .LT. 0) GO TO 90
WRITE (6,450) DELXI
XDEL = DLOG10 (DELXI)
WRITE (6,460) DELXI, XDEL
IF (NRB .LT. 1) GO TO 20
WRITE (6,470) DELXI, XDEL
WRITE (6,480)
WRITE (6,490)
C
REACTANT SUMMARY
DO 10 I = 1, NRT
   K = IREACT(I)
   GMINRL = ADEST(K) * WGHTM(K)
   XLMNRL = DLOG10 (DABS (GMINRL))
   XLDELS = DLOG10 (DABS (ADEST(K)))
10   WRITE (6,500) (NAMEM(J,K),J=1,5), GMINRL, XLMNRL, ADEST(K), XLDELS,
   1RS(I), GMIN(K), QM(K)
20   IF (NPT) 90, 30
30   WRITE (6,520)
   WRITE (6,540)
C
REACTION PRODUCT SUMMARY
DO 80 I = 1, NPT
K = IPROC(I)
GMNRL = ASYS(K) * WGHLM(K)
IF (GMNRL .LE. 0.) GO TO 40
XLGMNRL = DLOG10(GMNRL)
XLCDEL = DLOG10(A SYS(K))
GO TO 50
40 CONTINUE
GMNRL = 0.0000
XLGMNRL = 0.0000
XLCDEL = 0.0000
50 CONTINUE
NC1 = NC - 1
DO 60 LL = 1, NC1
   IF (K .NE. NDX(LL,1) .OR. NDX(LL,2) .NE. 1) GO TO 60
   NN = LL
   GO TO 70
60 CONTINUE
70 WRITE (6,500) (NAMEM(J,K), J=1,5), GMNRL, XLMNRL, ASYS(K),
               1 XLCDEL, X(NN,1), GMIN(K), QM(K).
80 CONTINUE
90 CONTINUE
WRITE (6,510)
DO 100 NM = 1, NMIT
   WRITE (6,530) (NAMEM(J,NM), J=1,5), GMIN(NM), QM(NM)
100 CONTINUE
110 CONTINUE
IF (NGAS .LT. 1) GO TO 130
WRITE (6,360)
DO 120 J = 1, NGAS
   WRITE (6,370) (NAMEG(JJ,J), JJ=1,5), GGAS(J), AGAS(J), ALGAS(J)
120 CONTINUE
130 IF (NET .LT. 0) GO TO 350
   CALL S0.LSP1(NST, C, GSP, HGHTS, XPPM)
   WRITE (6,540)
   DO 150 I = 1, NST
      IF (XPPM(I) .EQ. 0.0000) XLPPM = -1000.0000
      IF (XPPM(I) .EQ. 0.0000) GO TO 140
      XLPPM = DLOG10(XPPM(I))
140  WRITE (6,550) (NAMES(J,I),J=1,2), C(I), ALC(I), ACT(I), ALA(I),
                          1 G(I), ALG(I), GSP(I), XPPM(I), XLPPM
150 CONTINUE
C SPECIES K AND Q AND CEFF
DO 160 K = 1, NST
   IF (NAMES(1,K) .EQ. NHYDRO) GO TO 170
   CONTINUE
160 CONTINUE
170 IH = K
   WRITE (6,560)
   NC1 = NC - 1
   DO 180 K = 1, NC1
IF (NDX(K, 2) .NE. 0) GO TO 180
I = NDX(K, 1)
CZ = Z(I)
IF (CZ .GT. 9.9) CZ = 0.0
CL2 = ALA(I) - CZ * ALA(IN)
WRITE (6, 570) (NAMES(J, J), J = 1, 2), GSOL(I), QS(I), X(K, 1),
1 XD(K, 1), X(K, 2), XD(K, 2), X(K, 3), XD(K, 3)

180 CONTINUE
NC3 = NC + 3
DO 190 K = NC3, NK
J = K - 2
I = NDX(J, 1)
CZ = Z(I)
IF (CZ .GT. 9.9) CZ = 0.0
CL2 = ALA(I) - CZ * ALA(IN)
WRITE (6, 570) (NAMES(J, J), J = 1, 2), GSOL(I), QS(I), X(K, 1),
1 XD(K, 1), X(K, 2), XD(K, 2), X(K, 3), XD(K, 3)

190 CONTINUE
NC2 = NC + 2
WRITE (6, 690)
K = NDX(NC, 1)
WRITE (6, 570) (NAMES(J, K), J = 1, 2), GSOL(K), QS(K), X(NC, 1),
1 XD(NC, 1), X(NC, 2), XD(NC, 2), X(NC, 3), XD(NC, 3)
WRITE (6, 680)
CALL SOLSP3 (GRMTOT, XTPPM)
DO 250 J = 1, NC
IF (XTPPM(J) .LE. 0.0) GO TO 200
XLTFPM = DLOG10 (XTPPM(J))
GO TO 210

200 XLTFPM = -1000.0
210 IF (TOTM(J) .LE. 0.0) GO TO 220
XLMTOT = DLOG10 (TOTM(J))
GO TO 230

220 XLMTOT = -1000.0
230 IF (NDX(J, 2) .NE. 0) GO TO 240
WRITE (6, 590) (NAMES(JJ, J), JJ = 1, 2), TOTM(J), XLMTOT,
1 GRMTOT(J), XTPPM(J), XLTFPM
GO TO 250

240 WRITE (6, 600) (NAMES(JJ, J), JJ = 1, 5), TOTM(J), XLMTOT,
1 GRMTOT(J), XTPPM(J), XLTFPM

250 CONTINUE
C

MASS TRANSFER SUMMARY
C
WRITE (6, 650)
C
REACTANTS
C
IF (NRT .LT. 1) GO TO 270
DO 260 I = 1, NRT
J = IRED (I)
GMNRL = ADEST(J) * WGHTM(J)
XGMNRL = AMADE(J) * WGMTM(J)
CL = ASYS(J) * WGMTM(J)

260 WRITE (6,660) (NAMEN(JJ,J),JJ=1,5), ADEST(J), GMNRL, AMADE(J),
1XGMNRL, ASYS(J), CL
270 IF (NFT .EQ. 0) GO TO 290
DO 280 I = 1, NFT
J = IPROD(I)

C PRODUCTS BEING DESTROYED
C
GMNRQ = AMADE(J) * WGMTM(J)
GMNRQL = ADEST(J) * WGMTM(J)
GMNRQLB = ASYS(J) * WGMTM(J)
WRITE (6,670) (NAMEN(JJ,J),JJ=1,5), AMADE(J), GMNRQ, ADEST(J),
1GMNRQL, ASYS(J), GMNRQLB

280 CONTINUE
290 CONTINUE

C REACTION PRODUCTS
C
DO 340 I = 1, NMT
IF (NRT .LT. 1) GO TO 310
DO 300 II = 1, NRT
IF (I .EQ. ISEACT (II)) GO TO 340
300 CONTINUE
310 IF (NPT .LT. 1) GO TO 330
DO 320 II = 1, NPT
IF (I .EQ. IPBOD (II)) GO TO 340.
320 CONTINUE
330 CONTINUE

IF (CAES (AMADE(I)) .LT. 1.0D-20 .AND. DABS (ADEST (I)) .LT. 1.0D-20) GO TO 340
GMNRQL = AMADE(I) * WGMTM(I)
GMNRQL = ADEST(I) * WGMTM(I)
GMNRQLB = ASYS(I) * WGMTM(I)

WRITE (6,670) (NAMEN(JJ,I),JJ=1,5), AMADE(I), GMNRQL, ADEST(I),
1GMNRQL, ASYS(I), GMNRQLB

340 CONTINUE
WRITE (6,610) NDELXI
WRITE (6,620) XI, ELECT
WRITE (6,630) NET
IF (NFT .EQ. 0) STOP
RETURN

350 CONTINUE
IF (NFT .EQ. -1) WRITE (6,420)
STOP

360 FORMAT (//, ' GASES', //, ' NAME', 24X,
1 ' LOG K', 9X, ' ACTIVITY', 8X, ' LOG ACTIVITY', //)
370 FORMAT (1X, 5A4, 5X, F12.5, 5X, E12.5, 5X, F12.5)
380 FORMAT (//=, ' TOTAL MOLES **')
390 FORMAT (//=, ' TOTAL MOLES OF WATER IN THE SYSTEM IS ', F12.5,
1 ' MOLES')
400 FORMAT (//=, ' THIS RUN HAS BEEN TERMINATED BECAUSE THE INITIAL'
1 ' SOLUTION IS SUPERSATURATED WITH RESPECT TO ONE OR MOR
2E PHASES, /)

430 FORMAT (*NEW STEP SUMMARY *'/')

440 FORMAT ('/ ', 6X, 'THE ABOVE SOLUTION IS NOW AT EQUILIBRIUM WITH', 1
1 2A4, /, 6X, 'LOG K = ', E13.6, /, 6X, 2
2 'IT WILL BE ADDED TO THE MATRIX')

450 FORMAT ('//, 6X, 'HAS BEEN USED UP AT THE ABOVE STEP', /, 1
1 29X, 'IT WILL BE REMOVED FROM THE MATRIX')

460 FORMAT (16X, 'DELXI', 22X, '=', E12.6)

470 FORMAT (16X, 'XI', 25X, '=', E13.6, /, 1
1 16X, 'LOG XI', 2X, F7.3)

480 FORMAT ('/ ', 6X, 'REACTANTS', /, 64X, '— — — —', //)

490 FORMAT (25X, 'CUMULATIVE', 3X, 'LOG CUMULAT', 2X, 'CUMULATIVE', 1
1 3X, 'LOG CUMULAT', 2X, 'REACTION', 12X, 'LOG OF', 12X, 2
2 'LOG OF', 4X, 'MINERAL', 14X, 2('GRAM CHANGE', 2X), 2(/ 3
3 'MOLE CHANGE', 2X), 'COEFFICIENT', 4X, 'SOLUBILITY PRODUCT', 4
4 'ION PRODUCT')

500 FORMAT (1X, 5A4, 2X, E13.6, 3X, F7.3, 4X, E13.6, 3X, F7.3, 2X, 1
1 E13.6, 5X, E13.6, 6X, E13.6)

510 FORMAT ('//, 3X, 'MINERALS', 16X, 'LOG K', 12X, 'LOG Q', //)

520 FORMAT ('//, 6X, 'PRODUCTS', //1X, '— — — —', //)

530 FORMAT (1X, 5A4, IX, F10.3, 4X, F15.7) . -

540 FORMAT ('//55X, 'AQUEOUS SPECIES', //1X, 'SPECIES', 8X, 'MOLALITY', 1
1 5X, 'LOG MOL', 4X, 'ACTIVITY', 5X, 'LOG ACT', 3X, 2
2 'ACT COEF', 5X, 'LOG ACT C', 2X, 'GRAMS/KGM H2O', 6X, 'PPM', 3
3 9X, 'LOG FEM')

1 E12.5, 2X, F9.3, 3X, F9.3)

560 FORMAT ('/ ', 1X, 'SPECIES', 5X, 'LOG K', 5X, 'LOG Q', 7X, 'N BAR', 1
1 7X, 'LOG M/DXI', 4X, 'D2 M/DXI', 6X, 'D2LN M/DXI', 6X, 2
2 'D3 M/DXI', 4X, 'D3LN M/DXI')

570 FORMAT (2X, A4, A4, 3X, 2(2X,F8.4), 6(2X,E12.5))

580 FORMAT ('/ ', 3X, 'COMFONENTS', 16X, 'TOTAL', 8X, 'LOG TOTAL', 8X, 1
1 'TOTAL', 10X, 'TOTAL', 11X, 'LOG', 11X, 2X, '/ , 27X, 2
2 'MOLALITY', 6X, 'MOLALITY', 5X, 'GRAMS/KGM H2O', 7X, 'PPM', 3
3 9X, 'TOTAL PPM', 4X, 5X, //)

590 FORMAT ('/', 2A4, 15X, E13.6, 2X, E12.5, 5X, 2(E13.6,3X), E12.5, 1
1 5X, E12.5, 6X, E13.6)

600 FORMAT ('/', 5A4, 3X, E13.6, 4X, E12.5, 5X, 2(E13.6,3X), E12.5, 1
1 5X, E12.5, 6X, E13.6)

610 FORMAT ('//, 6X, 'NUMBER OF DELXI INCREMENTS FORWARD =', 14)

620 FORMAT ('//, 6X, 'IONIC STRENGTH =', E13.6, 15X, 1
1 'ELECTRICAL BAlANCE =', E13.6)

630 FORMAT ('//, 6X, 'TOTAL NUMBER OF PHASE BOUNDARIES PRESENTLY BRING 1
1 CONSIDERED =', 12, '//' )

640 FORMAT (1H1, 30X, 'EQUILIBRIUM HAS BEEN ATTAINED AND SOLUTION CHAR 1
1 ACTERISTICS ARE OUTLINED BELOW', /, 32X, '---------------------' 2
2----------------------------------------'/')

650 FORMAT ('/ ', 50X, 'TOTAL MASS TRANSFER IN THE SYSTEM', /, 50X, 1
1 '----------------------------------------'/')

660 FORMAT ('/ ', 1X, 5A4, 1X, 2E11.4, 1X, 2E11.4, 43X, 2E11.4)
SUBROUTINE ACTIV
IMPLICIT REAL*8(A - H, O - Z)
COMMON /PATRT/ NDX(200,2), COMPS(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GGAS(10), COMPS(20,200), Z(200), RR(20),
2 COMP(20,10), WGHMT(200), WGTG(10), GMEUT(4),
3 G, T, ADH, BDH, BDCT, AMH20, ALAH20, NAMH(5,200),
4 NAMES(2,200), NAMH(5,20), NOA(20),
5 IFRACT(20), NMT, NST, NC, NGAS, NBT, MAXI, NDILNC, INION,
6 NK
COMMON /CONCT/ G(200), ALG(200), ACT(200), ALA(200), C(200),
1 ALC(200), E(20,200), TCTM(20), XPMM(200), TN(200),
2 GSP(200), ALGAS(20), AGAS(20), XL, ELECT, XIFRT, DELXIT

COMPUTE ACTIVITIES OF AQUEOUS SPECIES
DO 10 I = 1, NST
ALA(I) = ALC(I) + ALG(I)
ACT(I) = 10.0E00 ** ALA(I)
10 CONTINUE

COMPUTE ACTIVITY OF SPECIES = 0
DO 30 I = 1, NST
IF (C(I) .NE. 0.0000) GO TO 30
ATEMP = -GSOL(I)
DO 20 J = 1, NC
   IF (NDX(J,2) .NE. 0) GO TO 20
   JJ = NDX(J,1)
   ATEMP = ATEMP + COMPS(J,I) * ALA(JJ)
20 CONTINUE
ALA(I) = ATEMP
ALC(I) = ALA(I) - ALG(I)
C(I) = 10.0D00 ** ALC(I)
ACT(I) = 10.0D00 ** ALA(I)
30 CONTINUE

COMPUTE ACTIVITY OF GASES
DO 70 I = 1, NGAS
ATEMP = -GGAS(I)
DO 60 J = 1, NC
   JJ = NDX(J,1)
   IF (NDX(J,2) .NE. 0) GO TO 60
   ATEMP = ATEMP + COMPG(J,I) * ALA(JJ)
60 CONTINUE
70 CONTINUE

ALGAS(I) = ATEMP
AGAS(I) = 10.0D00 ** ALGAS(I)

COMPUTE LOG q FOR SOLIDS
DO 110 I = 1, NMT

END
\[
\text{CM}(I) = 0.00000
\]
\[
\text{DO } 100 \text{ J} = 1, \text{NC}
\]
\[
\text{JJ} = \text{NDX}(J,1)
\]
\[
\text{IF (NDX(J,2) \cdot NE. 0) GO TO 80}
\]
\[
\text{QM}(I) = \text{CM}(I) + \text{COMPM}(J,I) \cdot \text{ALA}(JJ)
\]
\[
\text{GO TO 100}
\]
\[
\text{IF (NDX(J,2) \cdot NE. 3) GO TO 90}
\]
\[
\text{CM}(I) = \text{CM}(I) + \text{COMPM}(J,I) \cdot \text{ALGAS}(JJ)
\]
\[
\text{GO TO 100}
\]
\[
\text{90 CONTINUE}
\]
\[
\text{100 CONTINUE}
\]
\[
\text{COMPUTE LOG \( Q \) OF AQUEOUS SPECIES}
\]
\[
\text{DO 150 I} = 1, \text{NST}
\]
\[
\text{QS}(I) = -\text{ALA}(I)
\]
\[
\text{GO 140 J} = 1, \text{NC}
\]
\[
\text{JJ} = \text{NDX}(J,1)
\]
\[
\text{IF (NDX(J,2) \cdot NE. 0) GO TO 120}
\]
\[
\text{QS}(I) = \text{CS}(I) + \text{COMPS}(J,I) \cdot \text{ALA}(JJ)
\]
\[
\text{GO TO 140}
\]
\[
\text{IF (NDX(J,2) \cdot NE. 3) GO TO 130}
\]
\[
\text{QS}(I) = \text{CS}(I) + \text{COMPS}(J,I) \cdot \text{ALGAS}(JJ)
\]
\[
\text{GO TO 140}
\]
\[
\text{130 CONTINUE}
\]
\[
\text{140 CONTINUE}
\]
\[
\text{150 CONTINUE}
\]
\[
\text{RETURN}
\]
\[
\text{ENE}
\]
\[
\text{SUBROUTINE FINDC}
\]
\[
\text{FIND A NEW SET OF COMPONENTS.}
\]
\[
\text{FIRST REMOVE GASES FROM COMPONENTS}
\]
\[
\text{THEN SEARCH FOR AQUEOUS SPECIES WITH HIGHEST MOLALITIES}
\]
\[
\text{SOLID PHASES IN EQUILIBRIUM AND WATER ARE LEFT AS COMPONENTS}
\]
\[
\text{IMPLICIT REAL*(A - H, O - Z)}
\]
\[
\text{COMMON /PATDAT/ NDX(200,2), COMPM(20,200), AZERO(200), GMIN(200),}
\]
\[
1 \text{GSOL}(200), \text{GGAS}(10), \text{COMPS(20,200), Z(200), RR(20)},
\]
\[
2 \text{CMPSF}(20,10), \text{WGHIT}(200), \text{WHTS}(200), \text{WHTS}(10), \text{GNEUT(4)},
\]
\[
3 \text{P, T, ADH, BDH, BDCT, AMH2O, ALMH2O, NAMEM(5,200)},
\]
\[
4 \text{NAME(2,200), NAME(5,10), NAME(5,20), ROA(20)},
\]
\[
5 \text{IRFACT(20), NMT, NST, NC, NGAS, NRT, MAXI, HDLINC, INION},
\]
\[
6 \text{NK}
\]
\[
\text{COMMON /CONCI/ QM(200), QS(200), BB(20,200), A(20,20), DN(200)},
\]
\[
1 \text{AGAS(20), ACT(200), ALA(200), C(200),}
\]
\[
2 \text{ALC}(200), \text{E(20,200), TCOTM(20), XPMM(200), TN(200)},
\]
\[
2 \text{GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XPRT, DELXIT}
\]
\[
\text{COMMON /CARRAY/ QM(200), QS(200), BB(20,200), A(20,20), DN(200),}
\]
\[
1 \text{CC(200,20), X(200,4), CV(200), UCV(20), CV(200), DC(200)},
\]
\[
2 \text{WS(20,20), W(20,200), XD(200,4), ASIS(200), AODE(200),}
\]
\[
3 \text{ADES(200), A10, XL, DELXI, IPMOD(20), NDELXI, ISAT, NPT},
\]
\[
4 \text{MOD, IFIN, IPRT}
\]
\[
\text{C}
\]
\[
\text{REMOVE GASES}
\]
\[
\text{NC2} = \text{NC} + 2
\]
\[
\text{NI} = \text{NK} - \text{NC2}
\]
\[
\text{NC1} = \text{NC} - 1
\]
BC = 20
I = 1, NC
IF (NDX(I,1) .LT. 3) GO TO 20
ATEMP = 0.0000
DO 10 J = 1, NX
IF (DABS(E(I,J)) .LT. 1.0D-10) GO TO 10
K = NDX(NC + J,1)
IF (C(K) .LE. ATEMP) GO TO 10
II = K
ATEMP = C(K)
10 CONTINUE
NDX(I,1) = II
NDX(I,2) = 0
IET = -1
CALL TRANS(E, IET)
20 CONTINUE
30 CONTINUE
NOW FIND AQUEOUS SPECIES WITH HIGHEST MOLALITY
DO 50 I = 1, NC
IGNORE SOLID PHASES
IF (NDX(I,2) .NE. 0) GO TO 50
LL = NDX(I,1)
ATEMP = C(II)
II = LL
DO 40 J = 1, NX
IF (DABS(E(I,J)) .LT. 1.0D-10) GO TO 40
K = NDX(NC + J,1)
IF (C(K) .LT. ATEMP) GO TO 40
II = K
ATEMP = C(K)
40 CONTINUE
IF (II .EQ. LL) GO TO 50
NDX(I,1) = II
IET = -1
CALL TRANS(E, IET)
GO TO 30
50 CONTINUE
50 CONTINUE
END
SUBROUTINE MATSOL
IMPLICIT REAL*8 (A - H, O - Z)
COMMON /PAI DAT/ NDX(200,2), COMPM(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GAS(10), COMP(20,200), Z(200), BB(20),
2 COMEG(20,10), WHTS(200), WHTG(10), GMBRT(4),
3 P, T, ADH, BDH, BDCT, AMH2O, ALNH2O, NAMEM(5,200),
4 NAMES(2,200), NAMEG(5,10), NAMEG(5,20), MOA(20),
5 IREAT(20), NRT, NST, NC, NGAS, NET, MAXI, NDLINC, INION,
6 NK
COMMON /CONCT/ G(200), ALG(200), ACT(200), ALA(200), C(200),
1 ALC(200), B(20,200), TOTM(20), XPM(200), TN(200),
2 GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXIT
COMMON /CARRAY/ QM(200), QS(200), BB(20,200), A(20,20), DN(200),
1 CC(200,20), X(200,4), CV(200), UCV(20), CSVE(200), DC(200),
2 WS(20,20), W(20,200), XD(200,4), ASYS(200), AMATE(200),
C DIMENSIONS SHOULD BE A (N, N), B (M, N), C (M, N), X (N+M), Y (N+M)
WE (N, N), W (N, N) WHERE N SHOULD BE LARGER THAN NC+2
AND M SHOULD BE LARGER THAN NK-NC-2

C NC = NO. OF COMPONENTS
NK = NO. OF UNKNOWNs (TOTAL)
X IS THE NEAR ARRAY TO BE DETERMINED AND RETURNED
MULTIPLY B TIMES CC AND SUBTRACT FROM A
NC2 = NC + 2
NX = NK - NC2
DO 30 I = 1, NC2
DO 20 J = 1, NC2
ATEMP = 0.0000
DO 10 K = 1, NX
ATEMP = ATEMP + BB(I, K) * CC(K, J)
10 CONTINUE
WS(I, J) = A(I, J) - ATEMP
20 CONTINUE
30 CONTINUE
GET INVERSE OF WS
CALL INVRT (WS, NC2)
DO 60 I = 1, NC2
DO 50 J = 1, NX
ATEMP = 0.0000
DO 40 K = 1, NC2
ATEMP = ATEMP + WS(I, K) * BB(K, J)
40 CONTINUE
W(I, J) = -ATEMP
50 CONTINUE
60 CONTINUE
NDS = 1.
CALL CVSOLV (NDS)
RETURN
END
SUBROUTINE MININ
IMPLICIT REAL*8 (A - H, O - Z)
COMMON /PATDAT/ NDX (200, 2), CMPPH (20, 200), AZERO (200), GMIN (200)
1 GSOL (200), GGAS (10), COMP (20, 200), Z (200), RR (20),
2 CMPPH (20, 10), WGMTH (200), WGMTH (20, 200), WMTH (10), GMEUT (4),
3 P, T, ADH, BDH, BDCT, AMH20, ALM20, NAMEM (5, 200),
4 NAMES (2, 200), NAMIN (5, 10), NAMER (5, 20), NOR (20),
5 NAMEA (20), NMT, NST, NC, NGAS, NBT, MAXI, NDLINC, INI, ON,
6 NK
COMMON /CONCT/ GA (200), ALG (200), ACT (200), ALA (200), C (200),
1 ALC (200), B (20, 200), TOTM (20), XPPM (200), TN (200),
2 GSP (200), ALGAS (20), AGAS (20), XI, ELECT, XIPH, DELXI
COMMON /ARRAY/ QM (200), QS (200), BB (20, 200), A (20, 20), DN (200),
1 CC (200, 200), X (200, 4), CV (200), DNC (200), DC (200),
2 WS (20, 20), W (20, 200), XD (200, 4), ASYS (200), AMADE (200),
3 ADEST (200), A10, XL, DELXI, IPHOD (20), NDELXI, ISAT, NPT,
4 NOD, IFIN, IPRT
C FINDS A DELXI CORRESPONDING TO A PHASE BOUNDARY
WSOC = 100
NC2 = NC + 2
NX = NK - NC2
NC1 = NC - 1
LOOPS = 0
DELXI = DELXI * 0.5D00
DIV = DELXI

10 CONTINUE
DIV = DIV * 0.5D00
CALL STEP
CALL XICALC(C, Z, ELECT, NST, XI)
CALL GAMMA(XI, ADH, BDH, BDOT, NST, NC, AZERO, 2, GNEUT, G, C,
ACT, NDX, XI, ALG)
CALL ACTIV
DIFF = GMIN(ISAT) - QM(ISAT)
ES = DAES(1.0D0-9*GMIN(ISAT))
IF (DAES(DIFF) .LT. ES) RETURN
IF (DIFF .LT. 0.0D00) GO TO 20
DELXI = DELXI + DIV
GO TO 30

20 CONTINUE
DELXI = DELXI - DIV

30 CONTINUE
LOOPS = LOOPS + 1
IF (LOOPS .LT. NSOC) WRITE (6,40) NSOC
STOP

C

40 FORMAT (///, 'PHASE BOUNDARY NOT FOUND IN ', I3, 'HALVINGS.')

END

SUBROUTINE MOVE
IMPLICIT REAL*8(A-H,O-Z)

COMMON /PATTER/ NDX(200,2), CGFM(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GNAS(10), COMPS(20,200), Z(200), RR(20),
2 CONFF(20,10), WGHTS(200), WGHTG(10), GNEUT(4),
3 P, T, ADH, BHD, BDCT, AMH20, ALMH20, NAMEV(5,200),
4 NAMES(2,200), NAMEC(5,10), NAME(5,20), NOA(20),
5 IMEACT(20), IMT, NST, NC, GAS, NRT, MAXT, NDLINC, INION,
6 NK

COMMON /CON/ C(200), ACT(200), ALA(200), C(200),
1 ALC(200), B(20,200), TOTM(20), XPPM(200), TN(200),
2 GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XIPT, DELXI

COMMON /CARR/ QM(200), QS(200), BB(20,200), A(20,20), DN(200),
1 CC(200,20), X(200,4), CV(200), UCY(20), CSVE(200), DC(200),
2 WS(20,20), W(20,200), XD(200,4), ASYS(200), AMADS(200),
3 ADEST(200), A10, XL, DELXI, IPROD(20), NDELXI, ISAT, NPT,
4 NOD, IFIN, IPRINT

NC2 = NC + 2
NC1 = NC - 1
NX = NK - NC2
DO 10 I = 1, NST
10 CSVE(I) = C(I)
CSVE(NST + 1) = ACT(NDX(NC, 1))
CSVE(NST + 2) = AMH20

CALL UDMAT
SUBROUTINE REACTN

WHEN SATURATED WITH A SOLID PHASES
ADD IT TO THE COMPONENTS

IMPLICIT REAL*8(A - H, O - Z)

COMMON /PATDAT/ NDX(200,2), CGMPS(20,200), AZERO(200), GMN(200),
1 GSOL(200), GGAS(10), COMPS(20,200), Z(200), BB(20),
2 COMEG(20,10), WGHTM(200), WGHTS(200), WGHT(10), GMEUT(4),
3 P, T, ADH, BDH, BDOT, AMH20, AMH20, NAME(5,200),
4 NAMES(2,200), NAMQ(5,10), NAMER(5,20), MOA(20),
5 IERACT(20), NMT, NST, NC, NGAS, WHT, MAI, NDLINC, INION,
6 NC

COMMON /CONCT/ G(200), ALG(200), ACT(200), ALA(200), C(200),
1 ALC(200), B(20,200), TOTM(20), XPPM(200), TN(200),
2 GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXIT

COMMON /CARRAY/ QM(200), QS(200), BB(20,200), A(20,20), DN(200),
1 CC(200,20), X(200,4), CV(200), UCY(20), CSYE(200), DC(200),
2 WS(20,20), W(20,200), XD(200,4), ASTS(200), AMAD(200),
3 ADEST(200), AI0, XI, DELXI, IPROM(20), NDLXI, ISAT, NPT,
4 NOD, IFIN, IPRINT

NC1 = NC - 1
NC2 = NC + 2
NK = NK - NC2
IPROM(NET + 1) = ISAT
NPT = NPT + 1
K = IPROM(NPT)
DO 10 I = 1, NC1
IF (NDX(I,2) .NE. 0) GO TO 10
IF (NABS(NCOMP(I,K)) .LT. 1.0D-9) GO TO 10
NDX(I,1) = K
NDX(I,2) = 1
GO TO 20
10 CONTINUE
IRET = -1
20 CALL TEAMS(E, IRET)
CALL FINDC
CALL ACTIV
CALL SETCOL
ISAT = 0
IF (IFIN .NE. 0) RETURN
CALL SETMAT
ISIM = 1
RETURN
END

SUBROUTINE SATCHK
SUBROUTINE TO CHECK FOR SUPERSATURATION OF SOLID PHASES

IMPLICIT REAL*8(A - H, O - Z)
COMMON /PATDAT/ NDX(200,2), COMPM(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GNAS(10), COMPS(20,200), Z(200), RR(20),
2 COMEG(20,10), WGHTM(200), WGT(S(200), WGTG(10), GNEUT(4),
3 P, T, ADH, BDH, BDOT, AMH20, ALM20, NAMEM(5,200),
4 NAMES(2,200), NAMEMG(5,10), NAMER(5,20), MOA(20),
5 IREACT(20), NMT, NST, NC, NGAS, NR, MAXI, NDLINC, INION,
6 NK
COMMON /CONC/ G(200), ALG(200), ACT(200), A1A(200), C(200),
1 ALC(200), BL(20,200), TOTM(20), XPM(200), TN(200),
2 GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXIT
COMMON /CASH/ QM(200), QS(200), BB(20,200), A(20,20), D(200),
1 CC(200,20), X(200,4), CV(200), UCY(20), CSV(200), DC(200),
2 WS(20,20), W(20,200), XD(200,4), ASYS(200), AMADE(200),
3 ADEST(200), A10, XL, DELX, IPROD(20), NDELXI, ISAT, NPT,
4 NOB, IFIN, IMPRT
10 ISAT = 0
11 ILL = 0
DO 80 I = 1, NMT
10 IF (NPT) 40, 40, 20
20 DO 30 J = 1, NPT
21 IF (IPROD(J) - I) 30, 80, 30
30 CONTINUE
40 DIFF = GMIN(I) - QM(I)
42 ES = CABS(1.0D-9*GMIN(I))
44 IF (CABS(DIFF) - ES) 70, 70, 50
50 IF (DIFF) 60, 70, 80
60 ISAT = I
62 N = NDELXI
64 WRITE (6,90) NAMEM(1,1), NAMEM(2,1), NAMEM(3,1), NAMEM(4,1),
66 NAMEM(5,1), N, GMIN(I), QM(I)
68 IF (N .EQ. 0) GO TO 70
70 CALL MININ
72 GO TO 10
74 ISAT = I
76 ILL = ILL + 1
80 CONTINUE
RETURN
90 FORMAT(//,6X,'THE LOG K FOR ', 5A4, ' HAS BEEN EXCEEDED',
1    ' AT STEP ', I4, '/', 6X, ' LOG K = ', F14.7, 2X,
2    ' LOG C = ', F14.7, '/
END
SUBROUTINE SETCCCL

UPDATE KNOWN COLUMN VECTOR

IMPLICIT REAL*8(A - H, O - Z)
COMMON /PATDAT/ NDX(200,2), COMPM(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GNAS(10), COMPS(20,200), Z(200), RR(20),
2 COMEG(20,10), WGHTM(200), WGT(S(200), WGTG(10), GNEUT(4),
3 P, T, ADH, BDH, BDOT, AMH20, ALM20, NAMEM(5,200),
4 NAMES(2,200), NAMEMG(5,10), NAMER(5,20), MOA(20),
5 IREACT(20), NMT, NST, NC, NGAS, NR, MAXI, NDLINC, INION,
6 NK
SUBROUTINE SETMAT

SUBROUTINE TO SET UP THE NON-CHANGING PARTS OF A AND B ARRAYS AFTER CHANGE OF COMPONENT BASE.

IMPLICIT REAL*8 (A - H, O - Z)

COMMON /PATCAT/ NDX(200,2), COMP(M(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GGAS(10), COMP(M(20,200), Z(200), RR(20),
2 CONFIG(20,10), WHTM(200), WHTS(200), WHTG(10), GWEUT(4),
3 T, T, ABH, BHH, DHT, AHM20, ALMH20, NAMEM(5,200),
4 NAMES(5,20), NAMEG(5,10), NAMES(5,20), MOA(20),
5 IREACT(20), NMT, NST, NC, NGAS, NST, MAXI, NDLINC, INION,
6 NK

COMMON /CONCI/ G(200), ALG(200), ACT(200), ALA(200), C(200),
1 ALC(200), B(20,200), TOTM(20), XPPM(200), TN(200),
2 GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DEXIT

COMMON /CARRAY/ CM(200), QS(200), BB(20,200), A(20,20), DN(200),
1 CC(200,20), X(200,4), CV(200), UCY(20), CSVE(200), DC(200),
2 WS(20,20), W(20,200), XD(200,4), ASYS(200), AMADE(200),
3 ADEST(200), A10, XL, DELXI, IPROD(20), NDELXI, ISAT, NPT,
4 MOD, IFIN, IPRINT

IF (ISAT .EQ. 0) GO TO 30

NNN = NNT
DO 20 I = 1, NNN
IF (IREACT(I) .NE. ISAT) GO TO 20
NNN = NNN - 1
IF (NNN .EQ. 0) GO TO 60
DO 10 J = I, NNN
IREACT(J) = IREACT(J + 1)
10 CONTINUE
GO TO 30
20 CONTINUE
GO TO 30
30 DO 50 I = 1, NC
UCV(I) = 0.0
DO 40 J = 1, NRT.
K = IREACT(J)
IF (DABS(COMPM(I,K)) .LT. 1.0D-12) GO TO 40
UCV(I) = UCV(I) + COMPM(I,K) * RR(J)
40 CONTINUE
50 CONTINUE
GO TO 70
60 FIN = 1
70 RETURN

END
DC 10 J = 1, NC1
CC (I,J) = 0.0000
IF (NDX(J,2) .NE. 0) GO TO 10
CC (I,J) = - B(J,I)
10 CONTINUE
CC (I,NC) = 0.0
CC (I,NC2) = - B(NC,I)
20 CONTINUE
SET UP A MATRIX
DO 30 I = 1, NC2
DO 30 J = 1, NC2
A(I,J) = 0.0
30 CONTINUE
A(NC + 1,NC + 1) = 1.0
A(NC2,NC2) = 1.0
RETURN
END
SUBROUTINE UEDMAT
IMPLICIT REAL*8 (A - H, O - Z)
COMMON /PATOM/ NDX(200,2), COMPM(200,200), AZERO(200), GMIN(200),
1 GSOI(200), GGAS(10), COMPS(20,200), Z(200), BB(20),
2 CONFIG(20,10), WHT(200), WHTS(200), WHRG(10), MANEXT(4),
3 NEXS(200), NAMEG, NAME(5,20), LDA (20),
4 TMAPX(20), NAME, LST, NC, NGS, NMX, NDX, NDUD, WDX, WDXN,
5 NDX
COMMON /CARSAY/ QM(200), QS(200), BB(20,200), A(20,200), BN(200),
1 GSP(200), AGLA(20), AGAS(20), XI, ELECT, XIPRT, KDL
CCOMMN /CARAAY/ GM(200), QS(200), BB(20,200), A(20,200), BN(200),
1 A(C(200,20), X(200,4), CV(200), UC(200), CSS(200), DC(200),
2 WS(20,20), W(20,200), XD(200,4), ASYS(200), AMAD(200),
3 ADEST, A, KL, CL, DELXI, IPDAX(20), NDELXI, ISAT, NPT,
4 NOD, IFIN, IPRT
SUBROUTINE TO PUT IN CHANGES TO MATRIX DUE TO CHANGES
IN MOLALITIES, BH20, ETC...
NC2 = NC + 2
NC1 = NC - 1
NX = NK - NC2
PUT IN CHANGES TO A MATRIX
DO 20 I = 1, NC1
K = NDX(I,1)
IF (NDX(I,2) .NE. 0) GO TO 10
A(I,I) = C(K)
GO TO 20
10 A(I,I) = 1.0 / (0.1801534D00 * AMH20)
20 CONTINUE
DC 60 I = 1, NC1
K = NDX(I,1)
IF (NDX(I,2) .NE. 0) GO TO 50
IF (Z(K) .GT. 9.99) GO TO 30
A(NC + 1,I) = -0.5D00 * (Z(K)**2) * C(K)
GO TO 40
30 A(NC + 1,I) = 0.0
40 A(NC2,I) = C(K) * .01801534D00
GO TO 60
A(NC + 1,1) = 0.0
A(NC2,1) = 0.0
60 CONTINUE
DO 90 I = 1, NC
ATEMP = 0.0
IF (NDX(I,2) .NE. 0) GO TO 70
ATEMP = ATEMP + C(NDX(I,1))
70 DO 80 J = 1, NX
ATEMP = ATEMP + B(I,J) * C(NDX(NC + J,1))
80 CONTINUE
A(I,NC) = ATEMP
90 CONTINUE
ATEMP = 0.0
DC(I) = 0.0
IF (DAES(Z(I)) .LT. 1.0D-05) GO TO 100
IF (Z(I) .GE. 9.99) GO TO 110
DC(I) = ADD * Z(I) * Z(I) * 0.5 * (XI**(-0.5))
DC(I) = DC(I) / ((1.0 + BDI*AZERO(I))*(XI**-(0.5)))***2
DC(I) = A10 * (BDOT - DC(I))
ATEMP = ATEMP + C(I) * DC(I)
GO TO 110
100 DC(I) = A10 * XL / XI
ATEMP = ATEMP + C(I) * DC(I)
110 CONTINUE
A(NC2,NC + 1) = ATEMP * 0.01801534DDD0
C UPDATE COLUMN VECTOR FOR CHANGE IN MOLES OF H2O IN SOLVENT
DO 120 I = 1, NC
CV(I) = UCV(I) / (0.01801534DDD0*AMH2O)
120 CONTINUE
NI = NC + 1
DO 130 I = NI, NK
CV(I) = 0.0
130 CONTINUE
C LOAD UP CC MATRIX WITH MASS ACTION EQUATIONS
DO 150 I = 1, NX
K = NDX(NC + I,1)
CC(I,NC + 1) = 0.0
DO 140 J = 1, NC
IF (NDX(J,2) .NE. 0) GO TO 140
L = NDX(J,1)
CC(I,NC + 1) = CC(I,NC + 1) - B(J,I) * DC(L)
140 CONTINUE
IP = NDX(NC + I,2) .NE. 0 GO TO 150
CC(I,NC + 1) = CC(I,NC + 1) + DC(K)
150 CONTINUE
C PUT IN CHANGES TO BB MATRIX
DO 190 I = 1, NX
K = NDX(NC + I,1)
DO 160 J = 1, NC
IF (DAES(B(J,I)) .LT. 1.0D-13) GO TO 160
EE(J,I) = 0.0D00
EE(J,I) = B(J,I) * C(K)
160 CONTINUE
IF (Z(K) .GE. 9.99) GO TO 170
EE(NC + 1,1) = -0.5D00 * Z(K) * Z(K) * C(K)
SUBROUTINE FJNMV

IMPLICIT REAL*8 (A - H, O - Z)
COMMON /PAT DAT/ NDX(200, 2), COMPS(200, 200), AZERO(200), GMIN(200),
GSOL(200), GGAS(10), COMPS(20, 200), Z(200), RS(20),
COMPG(20, 10), WGHTM(200), WGHTS(20), WGHTT(10), GNEUT(4),
F, T, ADH, BDH, BDQT, AMH20, ALMH20, NAME1(5, 200),
ADG(5, 200), NAME1(5, 10), NAME1(5, 20), MO(20),
IREFQ(20), MM, MR, NC, MGAS, NRT, MAXI, MDLINC, INION,
NNK
COMMON /CONC/ G(200), ALG(200), ACT(200), ALA(200), C(200),
ALC(200), B(20, 200), TQM(20), XPPM(200), TN(200),
COMMON /CART/ G(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXII
COMMON /CARAY/ QM(200), CS(200), BS(20, 200), A(20, 20), DN(200),
CC(200, 20), X(200, 4), CV(200), NCV(20), CSVE(200), DC(200),
WS(20, 20), W(20, 200), XD(200, 4), ASYS(200), AMADE(200),
ADEST(200), A10, XL, DELXI, IPROD(20), NDELXI, ISAT, NPT,
NO, JPIN, IPRINT
DO 30 I = 1, NC
170 BB(NC + 1, I) = 0.0D00
180 BB(NC2, I) = C(K) * 0.01801534D00
190 CONTINUE
RETURN
END

SUBROUTINE FINMV

IMPLICIT REAL*8 (A - H, O - Z)
COMMON /PAT DAT/ NDX(200, 2), COMPS(200, 200), AZERO(200), GMIN(200),
GSOL(200), GGAS(10), COMPS(20, 200), Z(200), RS(20),
COMPG(20, 10), WGHTM(200), WGHTS(20), WGHTT(10), GNEUT(4),
F, T, ADH, BDH, BDQT, AMH20, ALMH20, NAME1(5, 200),
ADG(5, 200), NAME1(5, 10), NAME1(5, 20), MO(20),
IREFQ(20), MM, MR, NC, MGAS, NRT, MAXI, MDLINC, INION,
NNK
COMMON /CONC/ G(200), ALG(200), ACT(200), ALA(200), C(200),
ALC(200), B(20, 200), TQM(20), XPPM(200), TN(200),
COMMON /CART/ G(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXII
COMMON /CARAY/ QM(200), CS(200), BS(20, 200), A(20, 20), DN(200),
CC(200, 20), X(200, 4), CV(200), NCV(20), CSVE(200), DC(200),
WS(20, 20), W(20, 200), XD(200, 4), ASYS(200), AMADE(200),
ADEST(200), A10, XL, DELXI, IPROD(20), NDELXI, ISAT, NPT,
NO, JPIN, IPRINT
DO 30 I = 1, NC
170 BB(NC + 1, I) = 0.0D00
180 BB(NC2, I) = C(K) * 0.01801534D00
190 CONTINUE
RETURN
END
IF (I .GT. NST) GO TO 100  
GO TO 50  
90 CONTINUE  
100 IF (NNN .EQ. NET) GO TO 120  
CALL SETCOL  
GO TO 120  
110 IF IN = 1  
GO TO 260  
120 IF (NPT) 260, 260, 130  
130 NNN = NPT  
DO 250 I = 1, NNN  
K = IPROD(I)  
DO 140 J = 1, NC1  
JL = J  
IF (NDX(J,2) .EQ. 0) GO TO 140  
IF (NDX(J,1) .EQ. K) GO TO 150  
140 CONTINUE  
150 IF (XD(JI,1) .GT. 0.0D00) GO TO 250  
IF (ASYS(K) .LT. 1.0D-12) GO TO 250  
GO TO 250  
160 NPT = NPT - 1  
IPRINT = 1  
IF (NPT) 200, 200, 170  
170 IF (I .GT. NPT) GO TO 190  
DO 180 J = I, NET  
IEBOD(J) = IPROD(J + 1)  
180 CONTINUE  
190 CONTINUE  
200 ASYS(K) = 0.0D00  
DO 210 J = 1, NC1  
IF (NDX(J,2) .EQ. 0) GO TO 210  
IF (NDX(J,1) .EQ. K) GO TO 210  
L = J  
GO TO 220  
210 CONTINUE  
220 DO 230 J = 1, NX  
IF (DAES(COMPS(L,J)) .LT. 1.0D-10) GO TO 230  
NDX(L,1) = NDX(NC + J,1)  
NDX(L,2) = 0  
GO TO 240  
230 CONTINUE  
240 IEET = -1  
250 CONTINUE  
260 CALL FINDC  
CALL ACTIV  
CALL SETCOL  
CALL SETMAT  
RETURN  
END  
SUBROUTINE SPECLG(K)  
IMPLICIT REAL*8(A - H, O - Z)  
COMMON /PDTDAT/ NDX(200,2), COMPM(20,200), AZERO(200), GMIN(200),  
1 GSCL(200), GCAS(10), COMPS(20,200), Z(200), RR(20),  
2 COMPG(20,10), WGHTM(200), WGHTS(200), WGHTG(10), GNEUT(4),  
3 P, T, ADN, DBN, DDT, AMH20, ALNH20, NAMEM(5,200),  
4 NAMES(2,200), NAMEG(5,10), NAMER(5,20), MOA(20),  

A subroutine reads the data source for "PATH" and puts it in the common block "PATH".

**EXTERNAL CALC**

```fortran
INTEGER*2 DUMMY(100), NCOMP(4,40), INPUT(60,20), DUMMY2(60)
INTEGER*2 TYPE(4,6), WATER(60), NSW, BLANK
DATA WATER /"H", »2*, *0«, 6*» »,  '«H • , » (• ,
DATA STAR /•*•// ELANK /» »/
 DATA F/
DIMENSION ANCOM(40), PHCMF(40), NAMECO(5,20), NDOM(5), B(20,200)
DIMENSION WEIGHT(40), ASYS(200), TEMPER(8), ZCOM(40)
COMMON /OOP/ A IN TU (20), IM(5,20), IS(2,20), IG(5,20), NDOM(2),
 COMMON /PAT DAT/ ND (200,2), COMPS(20,200), AZERO(200), GMIN(200),
 COMMON /GA S(200), GGAS(10), COMPS(20,200), Z(200), R(20),
 COMMON /COMFG(20,10), WAGTS(200), WAGHTS(200), WAGHTG(10), GENTH(4),
 COMMON /P E, T, ADH, BHD, BDOT, ADH20, ALNH20, NAMEH(5,200),
 COMMON /HAMES(2,200), NAMES(5,10), NAMER(5,20), MOA(20),
 COMMON /IRAC(20), I RACTN, NST, NC, NAGAS, NRT, MAXI, NDLINE, INION,
 COMMON /NIOB, IFIN, IPRINT
```

The following call specifies that FORTRAN unit 19 is to be used for memory-to-memory I/O with a buffer length of 30 bytes. This routine is found only at MTS installations and must be removed and unit 19 assigned to a temporary file. The rewind statements in subroutine DECO will have to have the 'C' removed.
CALL FTNCMD('EUFER 19 LENGTH=30', 19)

READ IN THE "A" DEBYE-HUCKEL TERMS

READ (3,920) TEMPER
CALL STRA(TEMPER, T, PAR)
ADH = PAR

READ IN THE E DEBYE-HUCKEL TERMS (X 10E-8)

READ (3,920) TEMPER
CALL STRA(TEMPER, T, PAR)
BDH = PAR

READ IN THE EDOT (DEVIA TION FUNCTION) TERMS

READ (3,920) TEMPER
CALL STRA(TEMPER, T, PAR)
EDOT = PAR

READ IN THE GAMMA OF CO2 IN NACL SOLUTIONS

DO 10 J = 1, 4
    READ (3,920) TEMPER
    CALL STRA(TEMPER, T, PAR)
    GNEUT(J) = PAR
10 CONTINUE

NMI = 0
NST = 0
NGAS = 0
READ (3,930) NCTZ

READ IN THE ELEMENTS OF THE COMPOSITIONAL ARRAY'S TO DUMMY.

READ (3,960) ((NCOMP(J,II), J=1,4),II=1,NCTZ)

READ THE WEIGHT'S OF EACH OF THE COMPONENTS

READ (3,970) (WEIGHT(I), I=1,NCTZ)

DO 20 J = 1, 40
    ANCGM(J) = 0.0
20 CONTINUE

NC = NC + 1
DO 30 J = 1, 60
    INPUT(J,NC) = WATER(J)
30 CONTINUE

NDX(NC,2) = 0
MCA(NC) = 0
DO 40 J = 1, NC
    DUMMY2(J) = INPUT(J,I)
40 CONTINUE

CALL DECODE(PHCMP, NDUM, NCTZ, NCOMP, DUMMY2, 60)
DO 50 J = 1, NCTZ
    ANCGM(J) = PHCMP(J) + ANCGM(J)
50 CONTINUE
   DO 60 J = 1, 5
      NAMECO(J,1) = NDUM(J)
60 CONTINUE
70 CONTINUE
   GO TO 150
80 I = 0
90 I = I + 1
   IF (DUMMY(I) .EQ. STAR) GO TO 90
   I = I - 1
   DO 110 JJ = 1, 6
   DO 100 J = 1, 4
      IF (DBMH3'(I + J)' .NE. TYPE(J, JJ)) GO TO 10
100 CONTINUE
   NPWS = JJ
   GO TO 120
110 CONTINUE
   GO TO 140
120 GO TO (150, 150, 150, 150, 130, 390), NPWS
130 CALL READ(NSW, DUMMY, &390)
   IF (NSW .EQ. Star) GO TO 80
   IF (NSW .NE. BLANK) GO TO 140
   GO TO 130
140 WRITE (6, 880) NSW, DUMMY
   STOP
150 CALL READ(NSW, DUMMY, &390)
   IF (NSW .EQ. STAR) GO TO 80
   IF (NSW .NE. BLANK) GO TO 140
   READ (3, 940) H, S, A, BB, C, V
   IF (H .GT. 99999.) GO TO 150
   H = H / 4.184
   S = S / 4.184
   A = A / 4.184
   BB = BB / 4.184
   C = C / 4.184
   CALL DECODE(FHCMP, NDUM, NCTZ, NCOMP, DUMMY, 100)
   C
DC 160 J = 1, NCTZ
   IF (FHCMP(J') .GT. 1.0D-10 .AND. AMCON(J') .LT. 1.0D-10)
11 GO TO 150
160 CONTINUE
   GO TO (180, 270, 170, 330), NPWS
170 WRITE (6, 890)
   GO TO 130
180 IF (IMX .EQ. 0) GO TO 240
   DO 220 K = 1, IMX
   DO 190 J = 1, 5
      IF (IM(J,K) .NE. NDUM(J)) GO TO 220
190 CONTINUE
   IF (K .EQ. IMX) GO TO 230
   KK = K
   LOOP = IMX - 1
   DO 200 JJ = KK, LOOP
      IM(JJJ, JJ) = IM(JJJ, JJ + 1)
200 CONTINUE
210 CONTINUE
GO TO 230
220 CONTINUE
GO TO 240
230 IMX = IMX - 1
GO TO 150
240 NMT = NMT + 1
DO 250 J = 1, 5
NAME(J,NMT) = NDUM(J)
250 CONTINUE
WGHTM(NMT) = 0.0
LOOP = 0
DO 260 J = 1, NCTZ
WGHTM(NMT) = WGHTM(NMT) + PHCM(J) * WEIGHT(J)
260 CONTINUE
GMIN(NMT) = CALCK(H,S,A,B,C,V,T,P)
GO TO 150
270 AZ = EB * 4.184
ZZ = C * 4.184
V = 0
IF (ISX .EQ. 0) GO TO 300
DO 290 K = 1, ISX
DO 280 J = 1, 2
IF (IS(J,K) .NE. NDUM(J)) GO TO 290
280 CONTINUE
GO TO 150
290 CONTINUE
300 NSI = NST + 1
DO 310 J = 1, 2
NAME(J,NSI) = NDUM(J)
310 CONTINUE
WGHTS(NSI) = 0.0
LOOP = 0
DO 320 J = 1, NCTZ
WGHTS(NSI) = WGHTS(NSI) + PHCM(J) * WEIGHT(J)
320 CONTINUE
AZERC(NSI) = AZ
Z(NSI) = ZZ
Z1 = 0.0
GSOL(NSI) = CALCK(H,S,A,Z1,Z1,Z1,T,P)
GO TO 150
330 V = 0
IF (IGX .EQ. 0) GO TO 360
DO 350 K = 1, IGX
DO 340 J = 1, 5
IF (IG(J,K) .NE. NDUM(J)) GO TO 350
340 CONTINUE
GO TO 150
350 CONTINUE
360 NGAS = NGAS + 1
DO 370 J = 1, 5
NAMEG(J,NGAS) = NDUM(J)
370 CONTINUE
CONTINUE
WGHTG(NGAS) = 0.0
LCOF = 0
DO 380 J = 1, NCTZ
    WGHTG(NGAS) = WGHTG(NGAS) + PHCMP(J) * WEIGHT(J)
    IF (ANCOM(J) .LT. 1.0D-11) GO TO 380
    LOOP = LOOP + 1
    COMPG(LOOP,NGAS) = PHCMP(J)
380 CONTINUE
V = 0.0
GGAS(NGAS) = CALCK(H, S, A, BB, C, V, T, P)
GO TO 150
390 NEEDSW = -1
400 DO 520 I = 1, NC
    ISWIT = NDX(I,2) + 1
    GO TO <410, 440, 440, 470>, ISWIT
410 DO 430 K = 1, NST
    LIP = K
    GO TO 510
420 CONTINUE
430 CONTINUE
    WRITE (6,990) (NAMECO(J,I), J=1,2)
    GO TO 860
440 DO 460 K = 1, NMT
    LIP = K
    GO TO 510
450 CONTINUE
    WRITE (6,980) (NAMECO(J,I), J=1,5)
    GO TO 860
470 IF (NGAS .LT. 1) GO TO 500
    DO 490 K = 1, NGAS
        LIP = K
        GO TO 510
480 CONTINUE
500 WRITE (6,980) (NAMECO(J,I), J=1,5)
510 NDX(I,1) = LIP
520 CONTINUE
    IF (LCOF .EQ. NC) GO TO 560
    NEEDSW = 1
    DO 530 I = 1, NMT
        COMPS(NC,I) = 0.0
    530 CONTINUE
    DO 540 I = 1, NST
        COMPS(NC,I) = -Z(I)
    540 CONTINUE
    IF (Z(I) .GT. 9.9) COMPS(NC,I) = 0.0
    IF (NGAS .LT. 1) GO TO 560
DO 550 I = 1, NGAS
   COMIG (NC, I) = 0.0
CONTINUE

560 CONTINUE
   IRET = -1
   CALL TRANS (E, IRET)
   IF (NEEDSW .GT. 0) GO TO 780
   LIM = NST - 1
   NC1 = NC + 1
   LOOP = 1
   DO 570 J = 1, NC
      IF (NDX (J, 2) .NE. 0) ZCOMP (J) = 0.0D+00
      IF (NDX (J, 2) .NE. 0) GO TO 570
      ZCCKF (J) = Z (NDX (J, 1))
      IF (DABS (ZCOMP (J)) .GT. 9.9) ZCOMP (J) = 0.0D+00
   CONTINUE
   DO 630 I = 1, NST
      ATEMP = -Z (LOOP)
      IF (DABS (Z (LOOP)) .GT. 9.9) ATEMP = 0.0
      DO 580 J = 1, NC
         ATEMP = ATEMP + ZCOMP (J) * COMPS (J, LOOP)
      CONTINUE
      IF (DABS (ATEMP) .LT. 1.0D-05) GO TO 620
      DO 610 K = LOOP, LIM
         Z (K) = Z (K + 1)
         GSOL (K) = GSOL (K + 1)
         AZERO (K) = AZERO (K + 1)
         WGHTS (K) = WGHTS (K + 1)
         DO 590 J = 1, NC
            COMPS (J, K) = COMPS (J, K + 1)
         CONTINUE
         DO 600 J = 1, 2
            NAMES (J, K) = NAMES (J, K + 1)
         CONTINUE
      CONTINUE
      LIM = LIM - 1
      IF (LIM .LT. 1) GO TO 870
      GO TO 630
   CONTINUE
   LOOP = LOOP + 1
630 CONTINUE
   NST = LOOP - 1
   LIM = NMT - 1
   LOOP = 1
   DO 700 I = 1, NMT
      ATEMP = 0.0D+00
      DO 640 J = 1, NC
         ATEMP = ATEMP + ZCOMP (J) * COMPJ (J, LOOP)
      CONTINUE
      IF (DABS (ATEMP) .LT. 1.0D-05) GO TO 690
      DO 650 K = LOOP, LIM
         GMIN (K) = GMIN (K + 1)
         WGHTM (K) = WGHTM (K + 1)
         DO 660 J = 1, NC
            COMPM (J, K) = COMPM (J, K + 1)
         CONTINUE
         DO 670 J = 1, 5
      CONTINUE
   CONTINUE
   GO TO 680
680 CONTINUE
   LIM = LIM - 1
   IF (LIM .LT. 1) GO TO 870
   GO TO 630
690 CONTINUE
   LIM = LIM - 1
   IF (LIM .LT. 1) GO TO 870
   GO TO 630
700 CONTINUE
   LIM = LIM - 1
   IF (LIM .LT. 1) GO TO 870
   GO TO 630
NAMEM(J,K) = NAMEM(J,K + 1)

670 CONTINUE

680 CONTINUE
LIM = LIM - 1
IF (LIM .LT. 1) GO TO 770
GO TO 700

690 LOOP = LOOP + 1

700 CONTINUE
NFT = LOOP - 1
IF (NGAS .LT. 1) GO TO 770
LIM = NGAS - 1
LOOP = 1
DO 760 I = 1, NGAS
ATEMP = 0.0D+00
DO 710 J = 1, NC
ATEMP = ATEMP + ZCOMP(J) * COMPG(J/LOOP)

710 CONTINUE
IF (DABS(ATEMP) .LT. 1.0D-05) GO TO 750
DO 740 K = LOOP, LIM
GGAS(K) = GGAS(K + 1)
WGHTG(K) = WGHTG(K + 1)
DO 720 J = 1, NC
COMPG(J,K) = COMPG(J,K + 1)

720 CONTINUE
DO 730 J = 1, 5
NAMEG(J,K) = NAMEG(J,K + 1)

730 CONTINUE

740 CONTINUE
LIM = LIM - 1
GO TO 760

750 LOOP = LOOP + 1

760 CONTINUE
NGAS = LOOP - 1

770 LOOP = NC
NEEDSW = 1
GO TO 400

780 IF (NET .LT. 1) GO TO 820
DO 810 K = 1, NET

C
DO 800 I = 1, NMT
C
DO 790 J = 1, 5
IF (NAMEG(J,K) .NE. NAMEM(J,K + 1)) GO TO 800

790 CONTINUE
;
;IEEACT(K) = I
;ASYS(I) = AINIT(K)
GC TO 810

800 CONTINUE
WRITE (6,900) (NAMER(J,K),J=1,5)
WRITE (6,1000)
WRITE (6,1010)
STOP
C

800 CONTINUE
820 DO 840 I = 1, NST
C
DO 830 J = 1, 2
   IF (NAMES(J,I) .NE. NION(J)) GO TO 840
C
   INICN = I
   GO TO 850
C
840 CONTINUE
C
WRITE (6,1020) (NION(J),J=1,2)
C
GO TO 850
C
850 RETURN;
C
860 WRITE (6,1000)
C
STOP
C
870 WRITE (6,910)
C
STOP
C
880 FORMAT (1X, 5('******'),//, 'IMPROPERLY FORMATED DATA BANK',
4. 'LINE IN ERROR IS ---',//, 30A1, //)
C
890 FORMAT (///, 5('******'),//, 'SOLID SOLUTION IS NOT WORKING IN THIS VERSION',//, 'ALL SOLID SOLUTION PHASES WILL BE IGNORED',//,
2 5('******'))
C
900 FORMAT (///, 'INITIAL REACTANT ', SA4, ' COULD NOT BE FOUND!')
C
910 FORMAT (///, ' ', 'A CONSTRAINT PHASE ', 'CONTAINS TWO OXIDATION STATES - BUT THERE IS NO REDOX', ' COUPLE. YOU MUST HAVE A 2REDOX COUPLE IF YOU HAVE TWO', ' OXIDATION STATES.')
C
920 FORMAT (8F8.4)
C
930 FORMAT (1X, 26I3)
C
940 FORMAT (5X, 6F12.3)
C
950 FORMAT (1X, 150A1)
C
960 FORMAT (7(4A1,4X))
C
970 FORMAT (7F10.5)
C
980 FORMAT (///, 'COMPONENT ', SA4, ' COULD NOT BE FOUND!')
C
990 FORMAT (///, 'COMPONENT ', 2A4, ' COULD NOT BE FOUND!')
C
1000 FORMAT (' CHECK IF COMPONENT IS PRESENT IN DATA DECK AND THAT',//, 'YOU HAVE SPELLED IT THE SAME AND THAT IT IS LEFT ',//,
2 'JUSTIFIED IN THE INPUT FIELD!!!')
C
1010 FORMAT ('ALSO CHECK THAT THIS PHASE DOES NOT HAVE TWO OXIDATION STATES',//, 'IF THE SOLUTION ONLY CONSTRANS ONE ',
1 'STATED',//, 'CHosen AS THE ION TO BE ',//,
1 'BALANCED', 'ON, COULD NOT BE FOUND')
C
END
C
SUBROUTINE DECODE(PHCM, NNDUM, NCTZ, NCOMP, NOUT, ISIZE)
C
C
THIS ROUTINE IS CALLED BY PREAD
C
AND DECODES THE FORMULAS.
C
ON SOME SYSTEMS, THE CALLS TO WRITE AND READ WILL NOT WORK. COMMENT THESE OUT AND REMOVE THE "C" FROM
C
INFRONT OF THE REWINDS, WRITE AND READS ON UNIT 19.
C
IMPLICIT REAL*8(A - H, O - Z)
C
DIMENSION PHCM(40), INDEX(40), NNDUM(5)
C
INTEGER*2 NCOMP(4,40), NOUT(ISIZE), NNUM(25), NUMBS(10)
C
INTEGER*2 NCMS(5,40), NFORM(2,40), NBRAC(2), PERIOD, BLANK
C
DATA NUMBER /'0', '1', '2', '3', '4', '5', '6', '7', '8', '9', '0'/
C

DO 10 I = 1, 25
   M.D0M(I) = EIAKK
10 CONTINUE

DO 40 I = 1, NCTZ
   PHCMF(I) = 0.0
40 CONTINUE

DO 20 J = 1, 2
   NFORM(J, I) = BLANK
20 CONTINUE

DO 30 J = 1, 5
   NNCOM(J, I) = BLANK
30 CONTINUE

DO 50 I = 1, ISIZE
   IF (I .EQ. BLANK .AND. NOUT(I + 1) .EQ. BLANK .AND. NOUT(I + 2) .EQ. BLANK) GO TO 60
   IF (I .GT. 25) GO TO 50
   NDUM(I) = MOUT(I)
50 CONTINUE

C REWIND 19
C WRITE (19, 1) NDUM
CALL WRITE (NDUM, 25)
C REWIND 19
C READ (19, 2) NNDUM
CALL READ (NNDUM, 5)

NN = 1
I = 0
70 NN = NN + 1
   IF (NOUT(NN) .EQ. BLANK) GO TO 70
80 J = 0
   I = I + 1
90 IF (NOUT(NN) .EQ. BLANK .AND. NOUT(NN + 1) .EQ. BLANK .AND. NOUT(NN + 2) .EQ. BLANK) GO TO 120
   IF (NOUT(NN) .EQ. NBRAC(1)) GO TO 100
   J = J + 1
   NFORM(J, I) = NOUT(NN)
   NN = NN + 1
   GO TO 90
100 J = 0
110 NN = NN + 1
   NSWIT = -1
   IF (NOUT(NN) .EQ. NBRAC(2)) NSWIT = 1
   IF (NSWIT .EQ. 1) NN = NN + 1
   IF (NSWIT .EQ. 1) GO TO 80
   IF (NOUT(NN) .EQ. BLANK) GO TO 110
   J = J + 1
   NNCOM(J, I) = NOUT(NN)
   GO TO 110
C
C 120 LI = 0
C
EC 150 K = 1, 40
IF (NFORM(1,K) .EQ. BLANK) GO TO 160
DO 140 I = 1, NCTZ
DO 130 J = 1, 2
IF (NFORM(J,K) .NE. NCOMP(J,I)) GO TO 140
CONTINUE
INDEX(K) = I
LI = LI + 1
GO TO 150
CONTINUE
DO 160 I = 1, LI
JJ = 1
COUNT = 10.0D00
IF (NNCCM(2,I) .EQ. PERIOD OR NNCOM(2,I) .EQ. BLANK)
1 COUNT = 1.0D00
170 IF (NNCOM(JJ,I) .EQ. BLANK) GO TO 210,
IF (NNCOM(JJ,I) .EQ. PERIOD) GOTO 200
180 JJ = JJ + 1
IF (JJ .LT. 6) GO TO 170
210 CONTINUE
RETURN
220 FORMAT (1X, 25A1)
230 FORMAT (1X, 5A4)
END
FUNCTION CALCK(H, S, A, B, C, V, T, P)
CALCULATE LCG K FROM H, S, A, B, C, V
IMPLICIT REAL*8 (A - H, 0 - Z).
X = 10.
A10 = DLOG(X)
TB = 298.15
R = 1.98726
X1 = A * (T - TB) + B / 2 * (T**2 - TR**2) - C * (1/T - 1/TR)
X2 = A * (DLOG(T/TR)) + B * (T - TB) - C / 2 * (T**(-2) - TR**(-2))
X3 = (H - (T*S)) + V * .02390064 * (P - 1)
X4 = X3 + X1 - T * X2
CALCK = -X4 / ((-A10)*R*T)
RETURN
END
SUBROUTINE IATAIN (TOTM)
READ DATA INPUT FOR UNIT 5, DO LIMITED ERROR CHECKING
ECHO ON OUTPUT DEVICE.

IMPLICIT REAL*8(A - H, O - Z)
INTEGER*2 INPUT(60,20)
COMMON /DUP/ AINIT(20), IM(5,20), IS(2,20), IG(5,20), NION(2),
1 IMF, ISX, IGX, INPUT
DIMENSION TITLE(40), TOTM(20)
COMMON /PATM/ NDX(200,2), COMPM(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GGAS(10), COMPS(20,200), Z(200), BR(20),
2 COMG(20,10), WGHTM(200), WGTG(10), GNEUT(4),
3 P, T, ADH, BDH, BDOT, AMH20, ALMH20, NAMEM(5,200),
4 NAMES(2,200), NAMG(5,10), NAME(5,20), MOA(20),
5 IREAT(20), NMT, NST, NC, NGAS, NRT, MAXI, NDLINC, INION,
6 NK
READ (5,240) (TITLE(I),I=1,40)
READ (5,200) T, P, NRT, AMH20, NDLINC, MAXI, IMX, ISX, IGX
IF (AMH20 .LT. 1.0) AMH20 = 1.0D0 / .01801534D00
ALMH20 = DLOG10 (AMH20)
IF (MAXI .LT. 1) MAXI = 100000
READ (5,210) (NION(I),I=1,2)
IF (NBT .LT. 1) MAXI = 1
IF (NBT .LT. 1) NDLINC = 0
IF (NBT .LT. 1) GO TO 10
READ (5,220) (BR(I),AMIT(I),(NAME(I,J),J=1,5),I=1,NRT)
10 IF (IMX .EQ. 0) GO TO 20
READ (5,230) ((IM(J,1),J=1,5),I=1,IMX)
20 IF (ISX .EQ. 0) GO TO 30
READ (5,250) ((IS(J,1),J=1,2),I=1,ISX)
30 CONTINUE
IF (IGX .LT. 1) GO TO 40
READ (5,230) ((IG(J,1),J=1,5),I=1,IGX)
40 IF (IMX .LT. 1) GO TO 70
READ (5,230) ((IM(J,1),J=1,5),I=1,IMX)
50 IF (IMX .LT. 1) GO TO 70
READ (5,260,END=60) MOA(I), NDX(I,2), TOTM(I), (INPUT(J,1),J=1,60)
LIM = LIM + 1
READ (5,260,END=60) MOA(I), NDX(I,2), TOTM(I), (INPUT(J,1),J=1,60)
LIM = LIM + 1
GO TO 50
60 CONTINUE
NC = LIM

DATA ECHO HERE

WRITE (6,270)
WRITE (6,240) (TITLE(I),I=1,40)
WRITE (6,280) T, P, MAXI, NDLINC, (NION(I),I=1,2), AMH20
IF (NBT .LT. 1) GO TO 70
WRITE (6,290)
WRITE (6,300) ((NAME(I,J),J=1,5),BR(I),AMIT(I),I=1,NRT)
70 IF (IMX .LT. 1) GO TO 80
WRITE (6,320)
WRITE (6,330)
WRITE (6,340) ((IM(J,1),J=1,5),I=1,IMX)
80 IF (ISX .LT. 1) GO TO 90
WRITE (6,360)
WRITE (6,350)
WRITE (6,150)
WRITE (6, 250) ((IS(J,I), J=1,2), I=1,ISX)
90 IF (IGX .LT. 1) GO TO 100
WRITE (6, 320)
WRITE (6, 130)
WRITE (6, 230) ((IG(J,I), J=1,5), I=1,IGX)
100 WRITE (6, 310)
C
DO 110 I = 1, NC
   IF (MOA(I) .EQ. 1 .AND. NDX(I,2) .EQ. 0) WRITE (6, 160) TOTM(I),
      1 (INPUT(J,I), J=1,60)
   IF (MOA(I) .EQ. 0 .AND. NDX(I,2) .EQ. 0) WRITE (6, 170) TOTM(I),
      1 (INPUT(J,I), J=1,60)
   IF (NDX(I,2) .EQ. 1) WRITE (6, 180) TOTM(I),
      1 (INPUT(J,I), J=1,60)
   IF (NDX(I,2) .EQ. 3) WRITE (6, 190) TOTM(I),
      1 (INPUT(J,I), J=1,60)
CONTINUE
C
WRITE (6, 320)
WRITE (6, 140) TITLE(I), I=1,400
RETURN
130 FORMAT (/,' THE FOLLOWING GAS(ES) HAVE BEEN SUPPRESSED',/)
140 FORMAT (' ', 20A4, ' ', 20A4, '/)
150 FORMAT (/,' THE FOLLOWING AQUEOUS SPECIES HAVE BEEN SUPPRESSED',/)
160 FORMAT (' ', D15.8, ' LOG ACT.', ' 5X, 60A1, ' AQUEOUS SPECIES', '/)
170 FORMAT (' ', D15.8, ' MOALITY', ' 5X, 60A1, ' AQUEOUS SPECIES', '/)
180 FORMAT (' ', D15.8, ' GRAMS ', ' 5X, 60A1, ' SOLID', '/)
190 FORMAT (' ', D15.8, ' LOG ACT.', ' 5X, 60A1, ' GAS', '/)
200 FORMAT (2F10.3, 15, F10.3, 5X)
210 FORMAT (2A4)
220 FORMAT (F5.3, 5X, F10.5, 5X, F10.5)
230 FORMAT (3 (5A4,5X))
240 FORMAT (F5.3, 5X, F10.5, 5X, 5A4)
250 FORMAT (F5.3, 5X, F10.5, 5X, 5A4)
260 FORMAT (F5.3, 5X, F10.5, 5X, 5A4)
270 FORMAT (F5.3, 5X, F10.5, 5X, 5A4)
280 FORMAT (F5.3, 5X, F10.5, 5X, 5A4)
290 FORMAT (F5.3, 5X, F10.5, 5X, 5A4)
300 FORMAT (F5.3, 5X, F10.5, 5X, 5A4)
310 FORMAT (F5.3, 5X, F10.5, 5X, 5A4)
320 FORMAT (F5.3, 5X, F10.5, 5X, 5A4)
330 FORMAT (F5.3, 5X, F10.5, 5X, 5A4)
END
SUBROUTINE BREAD(NNWI, DIF,*
INTEGER N(25)
INTEGER*2 LIP(100), OU(100), NNWI
LOGICAL*1 LIPY(200), LLNN(100), ELANK
EQUIVALENCE (LLNN(1), N(1)), (LIPY(1), OU(1))
DATA ELANK /'/
READ (3,40,END=30) NNWI, N
DO 10 I = 1, 100
   J = I * 2 - 1
   K = I * 2
   LIPP(Y(J)) = LLNN(I)
   LIPP(Y(K)) = ELANK
  10 CONTINUE

DO 20 I = 1, 100
   DIF(I) = OU(I)
  20 CONTINUE

RETURN

30 FORMAT 1)
40 FORMAT (A1, 40A4)
END

SUBROUTINE BWITE (NDUM, ISIZE)
  INTEGER*2 NDUM, ISIZE
  WRITE (19, 10) NDUM
  RETURN
10 FORMAT (50A1)
END

SUBROUTINE REEAE (NNDUM, ISIZE)
  INTEGER NNDUM(ISIZE)
  READ (19,10) NNDUM
  RETURN
10 FORMAT (20A4)
END

SUBROUTINE STRA (TEMPER, TK, PAR)
  IMPLICIT REAL*8 (A - H, O - Z)
  C THIS ROUTINE ASSUMES A LINEAR RELATION BETWEEN TWO POINTS AND
  C FINDS
  DIMENSION TEMPER(8), TE(8)
  DATA TE /0.0000, 25.0000, 60.0000, 100.0000, 150.0000, 200.0000,
   250.0000, 300.0000/  
  T = TK - 2.73150D+02
  IAA = 0
  IBB = 1000
  IF (T .GT. TE(8)) J = 8
  IF (T .GT. TE(8)) GO TO 20
  IF (T .LT. TE(1)) J = 1
  IF (T .LT. TE(1)) GO TO 20
  10 CONTINUE
  SLOPE = (TEMPER(IAA) - TEMPER(IBB)) / (TE(IAA) - TE(IBB))
  AINTE = TEMPER(IAA) - SLOPE * TE(IAA)
  PAR = T * SLOPE + AINTE
  RETURN
  20 PAR = TEMPER(J)
  RETURN
END

SUBROUTINE TRANS(E, IBET, *)
  IMPLICIT REAL*8 (A - H, O - Z)
DIMENSION B(20,200), BASIS(20,20), TEMP(20)

COMMON /PATEAT/ NDX(200,2), COMPS(20,200), AZERO(200), GHIN(200),
1 GSOL(200), GGAS(10), COMPS(20,200), Z(200), RR(20),
2 COMT(20,10), WGHITM(200), WGHITG(10), GNEUT(4),
3 P, T, ADH, BHB, BDCT, AMH20, ALM20, NAMEM(5,200),
4 NAMIS(2,200), NAMEG(5,10), NAMER(5,20), MOA(20),
5 IREACT(20), NMT, NST, NC, NGAS, NRT, MAXI, NDLINC, INION,
6 NK
NCZ = NC + 1
C DG 80 I = 1, NC
ISW = NDX(I,2) + 1
C DO 80 J = 1, NC
   GO TO (10, 20, 20, 30), ISW
10 EASIS(J,I) = COMPS(J,NDX(I,1))
   GO TO 40
20 EASIS(J,I) = COMPM(J,NDX(I,1))
   GO TO 40
30 EASIS(J,I) = COMPG(J,NDX(I,1))
40 CONTINUE
C DO TO (50, 60, 60, 70), ISW
50 BASIS(NCZ,I) = GSOL(NDX(I,1))
   GO TO 80
60 BASIS(NCZ,I) = GMIN(NDX(I,1))
   GO TO 80
70 BASIS(NCZ,I) = GGAS(NDX(I,1))
80 CONTINUE
C DG 90 J = 1, NC
   BASIS(J,NCZ) = 0.0
90 CONTINUE
C EASIS(NCZ,NCZ) = 1.
CALL INVBT(EASIS, NCZ, 6330)
C DC 100 I = 1, NCZ
C DO 100 J = 1, NCZ
   IF (DABS(EASIS(I,J)) .LT. 1.0D-13) BASIS(I,J) = 0.0D00
100 CONTINUE
C DO 110 J = 1, NST
   COMPS(NCZ,J) = GSOL(J)
110 CONTINUE
C DC 120 K = 1, NST
C DO 120 I = 1, NCZ
   TEMP(I) = 0.0
120 CONTINUE
C DO 140 I = 1, NCZ
C DO 130 J = 1, NCZ
   TEMP(J) = TEMP(J) + BASIS(J,I) * COMPS(I,K)
130 CONTINUE
DO 150 I = 1, NCZ
   IF (DAES(TMP(I)) .LT. 1.0D-13) TMP(I) = 0.0D00
150  CONTINUE

DO 170 J = 1, NMT
   COMP(NCZ,J) = GMIN(J)
170  CONTINUE

DO 220 K = 1, NMT
   DO 180 I = 1, NCZ
   180  TMP(I) = 0.0
   DO 200 I = 1, NCZ
      DO 190 J = 1, NCZ
         TMP(J) = TMP(J) + BASIS(J,I) * COMP(I,K)
      190   CONTINUE
   200  CONTINUE
   DO 210 I = 1, NCZ
      IF (DAES(TMP(I)) .LT. 1.0D-13) TMP(I) = 0.0D00
   210  CONTINUE

IF (DAES(TMP(NCZ)) .LT. 1.0D-13) TEMP(NCZ) = 0.0D00

GO TO 290

DO 230 J = 1, NGAS
   COMP(NCZ,J) = GGAS(J)
230  CONTINUE

DO 280 K = 1, NGAS
   DO 240 I = 1, NCZ
      TMP(I) = 0.0
   240  DO 260 I = 1, NCZ
      DO 250 J = 1, NCZ
         TMP(J) = TMP(J) + BASIS(J,I) * COMP(I,K)
      250   CONTINUE
   260  CONTINUE

IF (DAES(TMP(I)) .LT. 1.0D-13) TEMP(I) = 0.0D00
**Find maximum element in kth column**

```
C**********************************************************************
C DO 110 K = 1, N
C**********************************************************************
C This routine finds the proper column number needed in the matrix.
C For the inverse of A, the inverse is written over A and returned.
C To find the multiplicative of the inverse of A and to solve
C A and use the unit lower and upper triangular matrices (LU).
C Inversion of matrix A with order N by LU decomposition (Gauss)
C**********************************************************************

C DIMENSION A(20,20), I(20)
C INTEGER B(10,10), N, K, M, I, J, N
C SUBROUTINE INVRAT(A, N)
C
C 2 THE COMPONENTS ARE NOT INDEPENDENT. THESE COMPONENTS ARE:
C
C 1 THE COMPONENTS PASS TO IF FOR THE NEW BASIS MIST
C
C 20 FORMAT (6,1X, 10E6)
C 30 FORMAT (20X, 10E6)
C
C WHERE (I', J') = 1, 2, ..., N
C
C IF (N(I') > N) AND (N(I') > E0, 0) GO TO 200
C
C 20 CONTINUE
C
C IF (N(I) = 1, 1) N
C GO TO 0
C
C 30 CONTINUE
C
C IF (I = 1, 1) N
C GO TO 0
C
C 30 CONTINUE
C
C IF (N(I) = 1, 1) N
C GO TO 0
C```
```c
50 I = I + 1
50 IF (K' = 0) (DON = 40) (I'T. XIM) ETERN 1
50 DO 20 MAX = DAS(V,A)(I',K)
20 IF (K' = 0) (DON = 40) (I'T. XIM) ETERN 1
DO 20 I = 1, N
50 CONTINUE
```
DO 10 X = 1, N
  ATMP = 0.0
  DO 20 I = 1, N
    N = K - NC + 2

  90 CONTINUE
  100 CONTINUE
  150 CONTINUE

DO 10 X = 1, N
  ATMP = 0.0
  DO 20 I = 1, N
    N = K - NC + 2

  90 CONTINUE
  100 CONTINUE
  150 CONTINUE

------------------------------------------------------------------------------------------
ATEMP = ATEMP + WS(I,K) * CV(K)
CONTINUE
DO 20 K = 1, NX
ATEMP = ATEMP + W(I,K) * CV(NC2 + K)
CONTINUE
XD(I,NDS) = ATEMP
CONTINUE
C
SOLVE FOR REMAINING unknowns
DO 50 J = 1, NX
ATEMP = 0.0
DO 40 I = 1, NC2
ATEMP = ATEMP + CC(J,I) * XD(I,NDS)
CONTINUE
XD(NC2 + J,NDS) = CV(NC2 + J) - ATEMP
CONTINUE
RETURN
END
SUBROUTINE STEP
C
TAKES DELXI STEP FOR AQUEOUS SPECIES
IMPLICIT REAL*8(A - H, O - Z)
COMMON /PAT DAT/ NDX(200,2), CONPM(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GGA(10), COMPS(20,200), Z(200), RR(20),
2 CONFG(20,10), WHTM(200), WHTS(200), WHGTG(10), GNEUT(10),
3 P, T, AHD, SDH, BDOT, AMX20, ALMH20, NAMEM(5,200),
4 NAMES(2,200), NAMEG(5,10), NAME(5,20),
5 IEACT(20), NRT, NST, NC, NGA, NRT, MAXI, DEDINC, IMM,
6 N
COMMON /CONC/ G(200), ALG(200), ACT(200), ALA(200), C(200),
1 ALG(200), B(20,200), TOTM(20), XPM(200), TW(200),
2 GSP(20), AGS(20), AGS(20), XI, EXM, XIPRT, DELXI
COMMON /CARSAY/ QM(200), QS(200), BB(20,200), A(20,20), DN(200),
1 CC(200,20), X(200,4), CV(200), UCV(20), CSVE(200), DC(200),
2 WS(20,20), W(20,200), XD(200,4), ASYS(200), AMDE(200),
3 ADEST(200), ATC, XL, DELXI, IPROD(20), NDDEII, ISAT, NPT,
4 NOD, IFIN, IPRINT
NC2 = NC + 2
NC1 = NC - 1
NX = NK - NC2
10 DO 20 I = 1, NC1
K = NDX(I,1)
IF (NDX(I,2) .NE. 0) GO TO 20
CALL MOVST(ATEMP, I)
C(K) = CSVE(K) + ATEMP
IF (C(K) .LT. 0.0000) GO TO 40
ALC(K) = DLOG10(C(K))
CONTINUE
DO 30 II = 1, NX
K = NDX(II + NC,1)
I = NC2 + II
CALL MOVST(ATEMP, I)
C(K) = CSVE(K) + ATEMP
IF (C(K) .LT. 0.0000) GO TO 40
IF (C(K) .GT. 0.0000) CALL SPECLG(K)
IF (C(K) .GT. 0.0000) ALC(K) = DLOG10(C(K))
CONTINUE
CALL MOVST(ATEMP, NC2)
ACT(NDX(NC,1)) = CSVE(NST + 1) + ATEMP
IF (ACT(NDX(NC,1)) .LT. 0.0000) GO TO 40
ALA(NDX(NC,1)) = DLOG10(ACT(NDX(NC,1)))
CALL MOVST(ATEMP, NC)
AMH20 = CSVE(NST + 2) + ATEMP
IF (AMH20 .LT. 0.0000) GO TO 40
ALMH20 = DLOG10(AMH20)
RETURN
40 DELXI = DELXI / 10.0000
GO TO 10
END

SUBROUTINE DEBIV

ROUTINE TO CONVERT LOG DERIV. TO DERIV.

IMPLICIT REAL*8(A - H, O - Z)

COMMON /PAT DAT/ NCX{200,2), COMPM (20, 200) , AZERO (200) , GMIN(200), GSOL(200), GGAS(10), COMPS(20,200), Z(200), RR(20), AMH20, ALMH20, NAFLM(5, 200), NAMES(2, 200), NAMEG(5, 10), NAMEG(5, 20), NAMES(2, 200), NAMEG(5, 10), NAMEG(5, 20), NOA(20), IREACT(20), NMT, NST, NC, NGAS, MRT, MAXI, MRRMC, INION, N.

COMMON /CONCT/ G (200), ALG (200), ACT (200), ALA (200), C (200), ALC(200), B(20, 200), TOTM(20), XPPM(200), TN(200), GSP(200), AGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXI.

COMMON /CARRAY/ QM(200), QS (200), B{20,200), A (20,20), DN(20), CC(200, 20), X(200,4), CV(200), UCV(20), CSVE(200), DC(200), W(20,20), W(20,20), W(20,20), XD(200,4), ASYS(200), AMAD(200), ADESTE (200), A10, XL, DELXI, IPBD(20), NDELE, ISAT, NPT, NOD, IFIN, IPRINT

NC2 = NC + 2
NC1 = NC - 1
NX = NK - NC2

DO 50 J = 1, NOD
AJ = J
DO 20 I = 1, NC1
K = NDX(I,1)
IF (NDX(I,2) .NE. 0) GO TO 10
CALL DTLGD(C(K), I, J)
GO TO 20
10 X(I,J) = XD(I,J)
20 CONTINUE

DO 30 II = 1, NX
K = NDX(NC + II, 1)
I = NC2 + II
CALL DTLGD(C(K), I, J)
30 CONTINUE

X(NC + 1,J) = XD(NC + 1,J)
I = NC
CALL DTLGE(AMH20, I, J)
I = NC2
CALL DTLGE(ACT(NDX(NC,1)), I, J)
50 CONTINUE
RETURN

END

SUBROUTINE MOVST(ATEMP, NC)

IMPLICIT REAL*8(A - H, O - Z)

COMMON /PAT DAT/ NDX(200,2), COMPM(20, 200), AZERO(200), GMIN(200), GSOL(200), GGAS(10), COMPS(20,200), Z(200), RR(20),
ATEMP = XXX * XD(I,1)
AJ = J
IF (J .LE. 1) .AND. XD(I,1) .EQ. 0.0 GO TO 10
ATEMP = ATEMP * (XD(I,1)**(J - 1))
10 X(I,J) = ATEMP
IF (J .LE. 1) GO TO 50
ATEMP = XXX * XD(I,2)
BTEMP = AJ * (AJ - 1.0D0) / 2.0D0
IF (J .LE. 1) .AND. XD(I,1) .EQ. 0.0 GO TO 20
IF (J .LE. 2) GO TO 50
GO TO 30
20 ATEMP = ATEMP + BTEMP
30 X(I,J) = X(I,J) + ATEMP
IF (J .LE. 2) GO TO 50
ATEMP = XXX XE (J,3)

IF ((J = 3) .EQ. 0.0 .AND. XD(I,1) .EQ. 0.0) GO TO 40

ATEMP = ATEMP * (XD(I,1)**(J - 3))

40 ETEMP = AJ * (AJ - 1.0D00) * (AJ - 2.0D00) / 6.0D00

X(I,J) = X(I,J) + BTEMP * ATEMP.

ETEMP = AJ * (AJ - 1.0D00) * (AJ - 2.0D00) / 6.0D00

X(I,J) = X(I,J) + ATEMP * XD(I,2)

ATEMP = ATEMP * XD(I,2)

BTEMP = AJ * (AJ - 1.0D00)

50 CONTINUE

END

SUBROUTINE JUMP

IMPLICIT REAL*8 (A - H, O - Z)

COMMON /P-ATEAT/ NDX(200,2), COMPS(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GGAS(10), COMPS(20,200), Z(200), BS(20),
2 COMG(20,10), WSHM(200), WSHS(200), WSHST(10), GNEUT(4),
3 F, T, ADH, BDH, BDOT, AMH20, ALMH20, NAME(5,200),
4 NAMES(2,200), NAME(5,10) NAME(5,20), MDA(20),
5 IREACT(20), NST, NC, NGAS, RBT, MAXI, WDLINC, INION,
6 N COMMON /CONCT/ G(200), ALG(200), ACT(200), ALA(200), C(200),
1 ALC(200), B(20,200), TOTM(200), XPPM(200), TN(200),
2 GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXI

COMMON /C ARRAY/ QM(200), QS(200), BB(20,200), A(20,200), DN(200),
1 GC(200,20), X(200,4), CV(200), DCY(20), CSV(200), DC(200),
2 MB(20,20), W(20,20), XD(200,4), ASYS(200), ARA(200),
3 ADE(200), A10, X, DELXI, IP(20), NDELA, ISAT, NPT,
4 MOD, IFIN, IPINT

DIMENSION SK(200)
NC2 = NC + 2
NC1 = NC - 1
NX = NK - NC2
DO 10 I = 1, NST
SK(I) = QS(I)
10 CONTINUE

20 CALL STEP

CALL XICNLC(C, Z, ELECT, NST, XI)
CALL GAMMA(XI, ADH, BDH, BDOT, NST, NC, AZERO, NAME, G, C,
1 ACT, NDX, XI, ALG)

CALL ACT\n
II = 0

DO 30 I = 1, NST
ATEMP = EATEQS(QS(I) - SK(I))

30 CONTINUE

GO TO 50

40 DELXI = DELXI / 10.0D00

GO TO 20

50 CONTINUE

IF (II .NE. NST) GO TO 60
DELXI = DELXI * 2.0D00
GO TO 20
60 CONTINUE
70 DC 80 I = 1, NC1
   IF (NDX(I,2) .EQ. 0 .OR. NDX(I,3) .EQ. 3) GO TO 80
   K = NDX(I,1)
   IK = I
   CALL MOVST(ATEMP, IK)
   IF ((ASYS(K) + ATEMP) .LT. 0.0D00) GO TO 90
80 CONTINUE
GO TO 110
90 DELXI = DELXI / 2.0D00
DIV = DELXI
100 DIV = DIV / 2.0D00
CALL STEP
   CALL XICALC(C, Z, ELECT, NST, XI)
   CALL GAMMA(XI, ADH, BDOT, NST, NC, AZEEO, Z, GNEUT, G, C, ACT, NDX, X, ALG)
   CALL ACTIV
   CALL MOVST(ATEMP, IK)
   BTEMP = ASYS(K) * ATEMP
   IF (LABS(BTEMP) .LT. 1.0D-12 .AND. BTEMP .GT. 0.0D00) GO TO 70
   IF (ETEMP .LT. 0.0D00) IF (BTEMP .GT. 0.0D00) GO TO 100
   110 CONTINUE
   DO 130 I = 1, NET.
   K = IEEACT(I)
   BTEMP = ASYS(K) - BS(I) * DELXI
   IF (BTEMP .LT. 0.0D00) GO TO 120
   130 CONTINUE
   BTEMP = DLGL10(DELXI + DELXI)
   IF (BTEMP .GT. XIPRT) IPRINT = 1
   IF (BTEMP .GT. XIPRT) DELXI = (10.0D00**XIPRT) - DELXI
   CALL STEP
   CALL XICALC(C, Z, ELECT, NST, XI)
   CALL GAMMA(XI, ADH, BDOT, NST, NC, AZEEO, Z, GNEUT, G, C, ACT, NDX, X, ALG)
   CALL ACTIV
RETURN
END
SUBROUTINE DI(ATEMP, NDT)
IMPLICIT REAL*8(A - H, O - Z)
COMMON /PATDAT/ NDX(200, 2), COMPM(20, 200), AZEEO(200), GSOL(200),
1 COMPS(20, 200), GNAS(10), P(20),
2 WGTNS(200), WGH(TS(10), GNEUT(4),
3 P, T, ADH, BDOT, AMH20, ALMH20, NAMES(5, 200),
4 NAMES(2, 200), NAM(5, 10), NAM(5, 20), NOA(20),
5 IEEACT(20), NMT, NST, NC, NGAS, NRT, MAXI, NDLINC, INION,
6 NK
COMMON /CONC/ G(200), ALG(200), ACT(200), ALA(200), C(200),
1 ALC(200), E(20, 200), TC(20), XPM(200), TM(200),
2 GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XIPRT, DELXI
COMMON /CARRAY/ QM(200), QS(200), BB(20, 200), A(20, 20), DN(200),
NC2 = NC + 2
NX = NK - NC2
NC1 = NC - 1
AJ = NDT
AJ1 = AJ * (AJ - 1.0D00) / 4.0D00
ATEMP = 0.0D00
DO 40 I = 1, NC1
   IF (NDX(I,2) .NE. 0) GO TO 40
   K = NDX(I,1)
   IF (ABS(Z(K)) .LT. 1.0D-5 .OR. Z(K) .GT. 9.99D00)
      GO TO 40
   Z2 = Z(K) * Z(K) * C(K)
   BTEMP = Z2 * XD(I,1)
   BTEMP = BTEMP * XD(I,1)
   IF (NDT - 2) .EQ. 0.0 .AND. XD(I,1) .EQ. 0.0 .GO TO 10
   BTEMP = BTEMP * (XD(I,1)**(NDT - 2))
10   ATEMP = ATEMP + BTEMP / 2.0D00
   IF (NDT .LE. 2) GO TO 40
   BTEMP = AJ1 * Z2 * XD(I,2)
   IF ((NDT - 2) .EQ. 0.0 .AND. XD(I,1) .EQ. 0.0) GO TO 20
   BTEMP = BTEMP * (XD(I,1)**(NDT - 2))
20   ATEMP = ATEMP + BTEMP
   IF (NDT .LE. 3) GO TO 40
   BTEMP = 2.0D00 * Z2 * XD(I,3)
   IF (NDT - 3) .EQ. 0.0 .AND. XD(I,1) .EQ. 0.0 .GO TO 30
   BTEMP = BTEMP * (XD(I,1)**(NDT - 3))
30   ATEMP = ATEMP + BTEMP
   CONTINUE
   DO 80 II = 1, NX
      K = NDX(II + NC,1)
      I = II + NC2
      IF (ABS(Z(K)) .LT. 1.0D-5 .OR. Z(K) .GT. 9.99D00)
         GO TO 80
      Z2 = Z(K) * Z(K) * C(K)
      BTEMP = Z2 * XD(I,1)
      BTEMP = BTEMP * XD(I,1)
      IF (NDT - 2) .EQ. 0.0 .AND. XD(I,1) .EQ. 0.0 .GO TO 50
      BTEMP = BTEMP * (XD(I,1)**(NDT - 2))
50   ATEMP = ATEMP + BTEMP
      IF (NDT .LE. 2) GO TO 80
      BTEMP = AJ1 * Z2 * XD(I,2)
      IF ((NDT - 2) .EQ. 0.0 .AND. XD(I,1) .EQ. 0.0) GO TO 60
      BTEMP = BTEMP * (XD(I,1)**(NDT - 2))
60   ATEMP = ATEMP + BTEMP
      IF (NDT .LE. 3) GO TO 80
      BTEMP = 2.0D00 * Z2 * XD(I,3)
      IF (NDT - 3) .EQ. 0.0 .AND. XD(I,1) .EQ. 0.0 .GO TO 70
      BTEMP = BTEMP * (XD(I,1)**(NDT - 3))
70   ATEMP = ATEMP + BTEMP
   CONTINUE
   DO 80 II = 1, NX
SECOND DERIVATIVE

IMPLICIT REAL*8(A - H, O - Z)
COMMON /PATDAT/ NDX(200,2), COMP(20,200), AZERO(200), GMIN(200),
1 GSOL(200), GGA(10), COMPS(20,200), Z(200), RR(20),
2 COMPG(20,10), WGH(SO0), WGHTS(200), WGHTG(10), GNUT(4),
3 P, T, ADH, BDH, BDCT, AMH2G, ALNH2G, NAME(5,200),
4 NAMER(2,200), NAMER(5,10), NAME(5,20), NAME(20),
5 IREACT(20), NMT, NST, NC, NGAS, NRT, MAXI, NDLINC, INION,
6 NK
COMMON /CONC1/ G(200), ALG(200), ACT(200), ALA(200), C(200),
1 ALC(200), (20,200), TOTM(20), XPMN(200), TN(200),
2 GSP(200), ALGAS(20), AGAS(20), XI, ELECT, XPMNT, DELXIT
COMMON /CARB1/ QM(200), Q(200), BB(20,200), A(20,20), D(200),
1 CV(200), XI(200,4), CV(200), UCV(20), CSVE(200), DC(200),
2 WS(20,20), XW(20,20), XD(200,4), ASYS(200), ANAME(200),
3 ADER(200), A10, XI, DELXIT, IPROD(20), NDDELXIT, ISAT, NPT,
4 NOB, IFIN, IPRF
NC2 = NC + 2
NX = NK - NC2
NC1 = NC - 1
NDT = 2
CALL DI (ATEM, NDT)
CTEEM = 0.0000
SECOND DERIV. MASS BALANCE
DO 40 J = 1, NC
ATEM = 0.0000
ETEEM = 0.0000
CTEEM = 0.0000
ETEEM = 0.0000
IF (J = EQ. NC) GO TO 20
K = NDX(J, 1)
IF (NDX(J, 2) .NE. 0) GO TO 10
ATEM = -(C(K)*XD(J, 1)) * XD(J, 1)
BTERM = -C(K)*XD(J, 1)
GO TO 20
CTEEM = XD(J, 1)
10 CONTINUE
DO 30 II = 1, NX
I = II + NC2
K = NDX(NC + II, 1)
IF (DABS(B(J,II)) .LT. 1.0D-13) GO TO 30
ATEM = ATERM - B(J,II) * (C(K)*XD(I, 1)) * XD(I, 1)
ETEEM = BTERM - B(J,II) * C(K)*XD(I, 1)
30 CONTINUE
BTERM = BTERM * XD(NC, 1)
CTEEM = CTEEM + XD(NC, 1) / (401801536000*AMH2G)
DTERM = UCV(J) * XD(NC, 1) / (401801536000*AMH2G)
CV(J) = ATERM + BTERM + CTEEM + DTERM
CONTINUE
DO 50 I = 1, NST
B.N(I) = O.DO0

IF (ABS(Z(I)) .LT. 1.D-5 .OR. Z(I) .GT. 9.99D00)
1 GO TO 50

XID = XI ** (1.0D00/2.0DO0)

DN(I) = ADH * Z(I) * (1.0D00+1.0D00*AZERO(I)*BDH*XID)

DN(I) = DN(I) / (4.0D00*(XI**3.0D00/2.0D00))

DN(I) = A10 * DN(I)

50 CONTINUE

ATEM = O.DO00

BTERM = O.DO00

CTEM = O.DO00

DC 60 I = 1, NC1

IF (NDX(I,2) .NE. 0) GO TO 60

K = NDX(I,1)

ATEM = ATEM - C(K) * DN(K)

ETEM = ETEM - (C(K)*XD(I,1)) * XD(I,1)

CTEM = CTEM - (C(K)*XD(I,1)) * DC(K)

159 CONTINUE

DC 70 II = 1, NX

K = NDX(NC + II,1)

I = NC2 + II

ATEM = ATEM - C(K) * DN(K)

ETEM = ETEM - (C(K)*XD(I,1)) * XD(I,1)

CTEM = CTEM - (C(K)*XD(I,1)) * DC(K)

70 CONTINUE

ATEM = (ATEM + 0.1801534D00*XD(NC + 1,1)) * XD(NC + 1,1)

ETEM = ETEM * 0.1801534D00

CTEM = CTEM * 0.1801534D00 * XD(NC + 1,1)

CV(NC2) = ATEM + BTERM + CTEM

DC 90 II = 1, NX

K = NDX(NC + II,1)

I = NC2 + II

ATEM = -DN(K)

DO 80 J = 1, NC1

IF (NDX(J,2) .NE. 0) GO TO 80

L = NDX(J,1)

IF (ABS(B(J,II)) .LT. 1.0D-13) GO TO 80

ATEM = ATEM + B(J,II) * DN(L)

80 CONTINUE

ATEM = ATEM * XD(NC + 1,1) * XD(NC + 1,1)

CV(I) = ATEM

90 CONTINUE

NDS = 2

CALL CVSOLV(NDS)

RETURN

END

SUEROUTINE THIRD

C

C THIRD DERIVATIVE

C

IMPLICIT REAL*8(A - H, O - Z)

COMMON /PA Rehab/ NDX(200,2), CCAMEM(20,200), AZERO(200), GMIN(200),

1 GSOL(200), GNAS(10), COMPS(20,200), Z(200), RN(20),

2 COMPG(20,10), WGHTM(200), WGHTS(200), WGHTG(10), GNEUT(4),

3 P, T, ADH, BDH, BDOT, AMH2O, ALMH2O, NAMEM(5,200),

4 NAMES(2,200), NAMEG(5,10), NAMER(5,20), MOA(20),
COMMON /GNCT/ G(200), ALG(200), ACT(200), ALA(200), C(200),
  ALC(200), B(20,200), TOTM(20), XPFM(200), Th(200),
COMMON /CAREAY/ QM(200), QS(200), BB(20,200), L(20,20), DN(200),
  CC(200,20), X(200,4), CV(200), UCV(20), CSVE(200), NC(200),
  WS(20,20), X(200,4), XPS(200), NDE(200),
  ADESTR(200), A10, XI, DELXI, IPROD(20), NDELI, ISAT, NPT,
  NOD, IFIN, IPRINT
NC2 = NC + 2
NC1 = NC - 1
NX = NK - NC2
MNT = 3
CALL DI(ATEMP, NDT)
CV(NC + 1) = ATEMP
DO 40 J = 1, NC
  E1 = 0.0D0
  B2 = 0.0D0
  B3 = 0.0D0
  B4 = 0.0D0
  B5 = 0.0D0
  B6 = 0.0D0
  B7 = 0.0D0
  B8 = 0.0D0
  IF (J .EQ. NC) GO TO 20
  K = NDX(J,1)
  IF (NDX(J,2) .NE. 0) GO TO 10
  B1 = -(C(K) * XD(J,1)) * XD(J,1) * XD(J,1)
  E2 = -(C(K) * XD(J,1)) * XD(J,2)
  B3 = -(C(K) * XD(J,1))
  B4 = -(C(K) * XD(J,1)) * XD(J,1)
  E5 = -(C(K) * XD(J,2)
  GO TO 20
10  B6 = 2.0D0 * XD(J,2)
  E7 = XD(J,1) - UCV(J)
  B8 = B7
  CONTINUE
DO 30 II = 1, NX
  I = II + NC2
  K = NDX(NC + II,1)
  IF (DABS(B(J,II)) .LT. 1.0D-13) GO TO 30
  B1 = B1 - E(J,II) * (C(K) * XD(I,1)) * XD(I,1) * XD(I,1)
  E2 = E2 - E(J,II) * (C(K) * XD(I,1)) * XD(I,2)
  B3 = B3 - E(J,II) * (C(K) * XD(I,1))
  B4 = B4 - E(J,II) * (C(K) * XD(I,1)) * XD(I,1)
  E5 = E5 - B(J,II) * C(K) * XD(J,2)
  CONTINUE
ATEMP = E1 + B2 * 3.0D0
ATEMP = ATEMP + B3 * 2.0D0 * XD(NC,2)
ATEMP = ATEMP + B4 * XD(NC,1)
ATEMP = ATEMP + B5 * XD(NC,1)
BTERM = 1.0D0 / (.01801534D00*AMH20)
ATEMP = ATEMP + B6 * XD(NC,1) * BTERM
ATEMP = ATEMP + B7 * XD(NC,2) * BTERM
ATEMP = ATEMP + B8 * XD(NC,1) * XD(NC,1) * BTERM
CV(J) = ATEMP
40 CONTINUE
DO 50 I = 1, NST
   TN(I) = 0.0D00
   IF (DABS(Z(I)) .LT. 1.0D-5 .OR. Z(I) .GT. 9.99D00) GO TO 50
   XI = XI ** (1.0D00/2.0D00)
   TN(I) = TN(I) * (1.0D00+4.0D00*AZERO(I)*BDH*XID + 5.0D00*(XI**2)*XI)
   XI = XI ** (-1.0D00)
   TN(I) = TN(I) * XI
50 CONTINUE

E1 = 0.0D00
E2 = 0.0D00
E3 = 0.0D00
E4 = 0.0D00
E5 = 0.0D00
E6 = 0.0D00
E7 = 0.0D00
E8 = 0.0D00
E9 = 0.0D00
DO 60 I = 1, NC1
   IF (NDX(I,2) .NE. 0) GO TO 60
   K = NDX(I,1)
   E1 = B1 - C(K) * DN(K)
   E2 = E2 + C(K) * TN(K)
   E3 = B3 - (C(K)*XD(I,1)) * XD(I,2)
   E4 = E4 - (C(K)* XD(I,1)) * XD(I,1) * XD(I,1)
   E5 = E5 - (C(K)* XD(I,1)) * DC(K)
   E6 = E6 - (C(K)* XD(I,1)) * DN(K)
   E7 = E7 - (C(K)* XD(I,2)) * DC(K)
   E8 = E8 - (C(K)* XD(I,1)) * XD(I,1) * DC(K)
60 CONTINUE

DO 70 II = 1, NX
   K = NDX(NC1+II,1)
   I = NC2 + II
   B1 = B1 - C(K) * DN(K)
   E2 = E2 + C(K) * TN(K)
   E3 = B3 - (C(K)*XD(I,1)) * XD(I,2)
   E4 = E4 - (C(K)* XD(I,1)) * XD(I,1) * XD(I,1)
   E5 = E5 - (C(K)* XD(I,1)) * DC(K)
   E6 = E6 - (C(K)* XD(I,1)) * DN(K)
   E7 = E7 - (C(K)* XD(I,2)) * DC(K)
   E8 = E8 - (C(K)* XD(I,1)) * XD(I,1) * DC(K)
70 CONTINUE

AH = 0.01801534D00
E1 = B1 + 3.0D00 * AH * XD(NC1+1,1) * XD(NC1+1,2)
E2 = (B2*AH*XD(NC1+1,1) * XD(NC1+1,1) ** 2
E3 = B3 + 3.0D00 * AH
E4 = E4 * AH
E5 = B5 + 2.0D00 * AH * XD(NC1+1,2)
E6 = B6 + 2.0D00 * AH * XD(NC1+1,1) * XD(NC1+1,1)
E7 = B7 * AH * XD(NC1+1,1)
E8 = B8 * AH * XD(NC1+1,1)
ATERM = B1 + B2 + B3 + B4 + B5 + E6 + B7 + B8
CV(NC2) = ATERM
DO 90 II = 1, NX
    K = NDX(NC + II,1)
    I = NC2 + II
    ATERM = -DK(K)
    ETERM = TN(K)
    DO 80 J = 1, NC1
        IF (NDX(J,2) .NE. 0) GO TO 80
        L = NDX(J,1)
        IF (DABS(B(J,II)) .LT. 1.0D-13) GO TO 80
        ATERM = ATERM + B(J,II) * DN(L)
        ETERM = ETERM - B(J,II) * TN(L)
    80 CONTINUE
    ATERM = ATERM * 3.0D00 * XD(NC + 1,1) * XD(NC + 1,2)
    ETERM = ETERM * (XD(NC + 1,1)**3)
    CV(I) = ATERM + ETERM
90 CONTINUE
NDS = 3
CALL CVSOLVE(NDS)
RETURN
END