RI 7786

Bureau of Mines Report of Investigations/1973

An Algorithm for Calculating Multiphase Chemical Equilibrium

UNITED STATES DEPARTMENT OF THE INTERIOR

Report of Investigations 7786

An Algorithm for Calculating Multiphase Chemical Equilibrium

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UNITED STATES DEPARTMENT OF THE INTERIOR
Rogers C. B. Morton, Secretary

BUREAU OF MINES
Elburt F. Osborn, Director

This publication has been cataloged as follows:

Spencer, Francis E

An algorithm for calculating multiphase chemical equilibrium, by F. E. Spencer, Jr., and A. A. Orning. [Washington] U.S. Bureau of Mines [1973]

42 p. illus., table. (U.S. Bureau of Mines. Report of investigations 7786)

Includes bibliography.

1. Algorithms. 2. Chemical equilibrium. I. Orning, Arthur Alonzo, 1906- , jt. auth. II. U.S. Bureau of Mines. III. Title. (Series)

TN23.U7 no. 7786 622.06173

U.S. Dept. of the Int. Library

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AN ALGORITHM FOR CALCULATING MULTIPHASE CHEMICAL EQUILIBRIUM

by

F. E. Spencer, Jr.,[1] and A. A. Orning[2]

ABSTRACT

This Bureau of Mines report provides a complete mathematical description of the algorithm employed by a general multiphase chemical equilibrium program developed particularly for the purpose of studying problems in coal combustion, although the generality of the program will allow its application to any equilibrium system in which an appreciable gas phase is present. When applied to coal combustion problems, the program predicts composition and quantity of slag and unconsumed carbon phases as well as calculates accurately the composition of the gas phase including trace species such as free electrons and ions which are important for predicting electrical properties.

INTRODUCTION

Among the new coal combustion schemes being considered for power generation are high-temperature systems to produce plasmas for magnetohydrodynamic energy conversion. Most experimental approaches so far have used "clean" fuels, but future large-scale applications will require the use of coal. At combustor temperatures above 2,100 K, some of the combustion products dissociate, and even the mineral matter is partially gasified. Fortunately, at such high temperatures, the combustion products may be assumed to be in a multiphase equilibrium condition.

The present multiphase equilibrium program, while general in scope and efficiency, is particularly well suited to the study of coal combustion and to the prediction of electrical, thermal, and transport properties of the combustion product mixture. The program has also been used in studying combustion of other fuels such as toluene, ethanol, kerosine, and sawdust and in studying certain aspects of sulfur oxide control and coal gasification.

The present program uses the "equilibrium constant" method as contrasted with the currently popular "free energy minimization" method. It is not the purpose of this investigation to weigh the merits of the two approaches, but we do intend to mention features which minimize difficulties encountered in

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[1] Mathematician.

[2] Physical scientist.

the past with the equilibrium constant method of Brinkley (2-3)[3] and Kandiner (9). Zeleznik and Gordon (12) have shown that the two methods lead to equivalent computational systems in considerable generality. We cannot comment on how the free energy method might change if some condensed phases are solutions.

We do believe that our program is unusual in that it can fit into a computer with only 16,000 words of memory while still allowing sufficient core space for the dynamic arrays required by a 17-component, two-phase system with a total of 92 species. Since the program takes every advantage of the features of ALGOL, there is no limitation whatever on the number of components, phases, and species considered, other than those of computer size and user budget. Section 3 of this report shows that the phase rule might impose a restriction under certain conditions.

The program uses the methods of Brinkley (2-3) and Kandiner (9) where we have specialized all phases to be ideal and where the representative phase for every component is the gas phase. Since all the applications we have in mind have an appreciable gas phase, this turns out to be a considerable convenience because we avoid the problem of changing stoichiometric coefficients and equilibrium constants in cases where a condensed component, if so chosen, might disappear. On the other hand, we have had no difficulty in computing composition of systems with more than 40 atom-percent condensed material. Spencer, Orning, and Bienstock (10) give an example of a seed regeneration problem with this characteristic.

Because of various simplifications and the present discussion directly in terms of equilibrium constants rather than in terms of chemical potentials, this report should be useful to engineers and programers who may not be conversant with all aspects of chemical thermodynamics. There are common points between the present paper and that of Feldmann (6), but exposition of the new ideas presented demands re-presentation of the algorithm starting from first principles.

Brinkley (3) and Feldmann (6) have observed that activity coefficients can be introduced at appropriate points to account for nonideality, if the coefficients are available. Our applications are generally at the lower pressures (<17 atm) so that the use of the compressibility factors (for example, Glasstone, 7, p. 28) has not been introduced.

Villars (11) found that the methods of Brinkley were elegant but that they were subject to breaking down in two ways: Oscillations can occur, and the Jacobian matrix can be too close to singular for successful inversion. Both problems are avoided in the present algorithm. The oscillation problem is avoided by limiting the magnitude of the correction that is applied to each iteration to two orders of magnitude (section 3) and by introducing two schemes for intelligent guessing of solutions (section 6). The matrix singularity problem has disappeared owing to the use of a computer with the

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[3] Underlined numbers in parentheses refer to items in the list of references preceding the appendixes.

capability of expressing 10 significant figures and quite large and quite small positive numbers ($10^{\pm 308}$), and since the introduction of the modified Doolittle matrix inversion scheme, which appears to be able to invert matrices that are more nearly singular than most schemes for inverting general (not necessarily symmetric) matrices. (See section 5 and appendix B.) It is possible that the matrix inversion problems encountered by Villars were due to the complications attendant to handling a condensed phase of carbon, which might disappear under some conditions. This problem is also avoided in the present algorithm.

In the span of 2 years and over 1,000 problems of different types solved, we have yet to fail in delivering answers to equilibrium problems as requested by different groups at Pittsburgh Energy Research Center.

SECTION 1. - CONDENSATION CRITERION AND CONSTRAINT

Suppose a container is enclosed and partly filled with a single phase of miscible liquids D', E', F' in equilibrium with a gas phase consisting of gases D, E, F of the same respective chemical species. Let $L_{D'}$, $L_{E'}$, $L_{F'}$, be the vapor pressures measured over the respective pure liquids; let $F_{D'}$, $F_{E'}$, $F_{F'}$ be the molar fractions in the solution of each of the three liquids; and let P_D, P_E, P_F be the partial pressures of the respective gases over the solution. Then the classical Raoult law (4, ch. 8) predicts that

$$P_D = F_{D'} L_{D'} ,$$

$$P_E = F_{E'} L_{E'} ,$$

$$P_F = F_{F'} L_{F'} ,$$

and by the definition of molar fraction, we get the equation $1 = F_{D'} + F_{E'} + F_{F'}$

or

$$1 = \frac{P_D}{L_{D'}} + \frac{P_E}{L_{E'}} + \frac{P_F}{L_{F'}}, \qquad (1)$$

which can be extended to an arbitrary number of liquid-gas pairs and is a constraint for two-phase equilibrium; that is, whenever the ideal solution is present, the partial pressures P_D, P_E, P_F must satisfy the equation 1. Further, liquid will form whenever the right-hand sum of three terms exceeds 1, and the liquid will continue to condense until the right-hand side equals 1. It is also predicted by this theory that a solution of all three liquids appears when any liquid whatever appears in this phase.

Now suppose that the three liquids D', E', F' and the three gases D, E, F are all in equilibrium with gaseous elements A, B, C from which they are formed (for example, suppose the formula for D is $D = A_{V_{AD}} B_{V_{BD}} C_{V_{CD}}$ where some of the V's might be zero), then the gas partial pressures must also meet the requirements (7, ch. 13):

$$P_D = K_D P_A^{V_{AD}} P_B^{V_{BD}} P_C^{V_{CD}} , \qquad (2)$$

$$P_E = K_E P_A^{V_{AE}} P_B^{V_{BE}} P_C^{V_{CE}} , \tag{3}$$

$$P_F = K_F P_A^{V_{AF}} P_B^{V_{BF}} P_C^{V_{CF}} , \tag{4}$$

in addition to the equation 1 (if condensation occurs) and to mass conservation (stoichiometric) requirements.

Let us digress to look at the relations holding among $L_{D'}$, $L_{E'}$, $L_{F'}$, K_D , K_E , K_F and the liquid-phase equilibrium constants $K_{D'}$, $K_{E'}$, $K_{F'}$. Above a pure liquid D' at equilibrium, the partial pressure P_D is equal to the vapor pressure $V_{D'}$. Three equations must hold:

$$1 = K_{D'} P_A^{V_{AD'}} P_B^{V_{BD'}} P_C^{V_{CD'}} , \tag{5}$$

$$P_D = K_D P_A^{V_{AD}} P_B^{V_{BD}} P_C^{V_{CD}} , \tag{6}$$

$$P_D = L_{D'} . \tag{7}$$

Note that equation 6 is different from equation 2 since equations 5-8 apply to a system with pure liquid D'. The left side of equation 5 is 1 since D' is a pure liquid, and hence has unit activity by convention (6, p. 281). Since the stoichiometric coefficients: $V_{AD'}$, V_{AD} ; $V_{BD'}$, V_{BD} ; $V_{CD'}$, V_{CD} are pairwise equal, we can substitute equation 6 into equation 5 and get $1 = K_{D'} P_D / K_D$, or $P_D = K_D / K_{D'}$. But, using equation 7

$$L_D = K_D / K_{D'} . \tag{8}$$

By analogous reasoning for systems over the respective pure liquids E' and F', we get

$$L_{E'} = K_E / K_{E'} \tag{9}$$

$$L_{F'} = K_F / K_{F'} \tag{10}$$

Now we reformulate equation 1: substitute equations 2, 8; 3, 9; 4, 10 into the respective right-hand terms of section 1. Equation 1 becomes

$$\begin{aligned} 1 = {} & K_{D'} P_A^{V_{AD'}} P_B^{V_{BD'}} P_C^{V_{CD'}} + \\ & K_{E'} P_A^{V_{AE'}} P_B^{V_{BE'}} P_C^{V_{CD'}} + \\ & K_{F'} P_A^{V_{AF'}} P_B^{V_{BF'}} P_C^{V_{CF'}} . \end{aligned} \tag{11}$$

This relation is an equational constraint on the partial pressures of the elements A, B, C caused by the presence of the liquid phase D', E', F'. All the remarks following equation 1 apply, mutatis mutandis, to equation 11. In particular, when the right side of equation 11 exceeds 1, condensation must occur, and each term on the right side of equation 11 is a molar fraction. When there is only one species in a condensed phase, the equation 11 reduces to equation 5 as it should. Furthermore, when only one species appears in a condensed phase, equations 1 and 11 reduce to the simple requirement that partial pressure equals vapor pressure at equilibrium.

The following observation is important: This mathematical formulation does not require knowledge of equilibrium constants for the gaseous version of any liquid species or knowledge of vapor pressures[4] for any liquid; for example, gaseous K_2SO_4 and Al_2O_3 may not exist (opinion is divided). We infer, and statistical mechanics concurs, that these vapor pressures and equilibrium constants are quite small but positive. Nevertheless, we can consider liquid or crystal Al_2O_3 or K_2SO_4 in our condensed phases (pure or as ideal solution constituents) without need for vapor pressures or gas phase equilibrium constants. The equation 11 calculates, say K_2SO_4 at mole fraction activity in the phase in which the data bank puts it. If K_2SO_4 is the only species in the phase, it is calculated at unit activity.

This ideal solution model can be and has been applied in situations where considerable nonideality occurs. The results obtained by considering $K_2SO_4(\ell)$, for instance, are quite different from treating a solution of K_2O and SO_3 or of K, S, and O liquids.

Feldmann (<u>6</u>) makes a distinction between liquids produced by condensation and liquids produced by heterogeneous reaction. In light of the algebraic discussion of this section, this is not a valid thermodynamic distinction. It leads to unnecessary complications in the program coding. In his terminology, all our condensed species are produced by "heterogeneous reaction."

Finally, it should be emphasized that nothing whatever changes in this derivation if the representative components are any other gases than the gaseous elements. Components will be discussed in the next section.

SECTION 2. - FORMULATION OF THE ALGEBRAIC PROBLEM

Certain gaseous species are selected as components (<u>2</u>-<u>3</u>, <u>9</u>). For simplicity, one can think of components as elements or as reactants, but the concept of component is not so restrictive. For example, we use CO_2 gas as the representative component for carbon rather than graphite crystal, which is the JANAF reference state (<u>5</u>). In any case, each element considered must have a representative component, and the chemical equation producing end product species must be unique in terms of the selected components.

Example: H_2, O_2, CO_2 would be an acceptable component list since every compound that can be produced from these three reactants can be produced in

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[4] The term "vapor pressure" properly refers to partial pressure of the gas of identical composition to the corresponding liquid, and not to the total pressure of decomposition products.

only one way, whereas H_2, O_2, CO, CO_2 is not acceptable as a component list because there is ambiguity in production of carbon compounds. Either of the reactions $CO-\frac{1}{2}O_2 \rightarrow C(c)$[5] or $CO_2-O_2 \rightarrow C(c)$ could be considered for the production of graphite.

The present algorithm takes all components to be gases because this avoids the complication that would arise if a condensed component were to disappear or if a condensed component were a constituent of a solution at other than unit activity. Programs have been written that change components, equilibrium constants, and stoichiometric coefficients (6) when the phase makeup changes. The approach used in the present algorithm avoids these difficulties since all problems solved have an appreciable gas phase. Furthermore, both theory and experience have shown that appropriate guessing coefficients obviate the need to select components as the most prevalent species containing the given element[6] as advocated by Brinkley (2-3) and Kandiner (9).

Let r be the number of components, and let $\vec{Q}$ be an r-vector whose entries are the stoichiometrically equivalent numbers of gram-moles of the components. If the third component selected is Cl_2, then Q_3 is to be the equivalent number of moles of Cl_2 in all the species present at equilibrium. The r entries in the $\vec{Q}$ vector (or Q list as we call it) are r of the total r+2 independent variables that specify a problem to the program. The other two independent variables are pressure (P) in atmospheres and temperature (T) in kelvins.

Let $\vec{X}$ be another r-vector which, at equilibrium, will be the vector whose entries are the equilibrium quantities of the components in gram-moles.

Let s be the number of gaseous species other than the components, let ph be the number of distinct condensed phases, and let $c_1, \ldots, c_{ph}$ be the numbers of species in the respective condensed phases considered. Let Y be an $(s + \sum c_k)$-vector whose entries will be the number of gram-moles of all these noncomponent species. Following Brinkley (3), all such species will be called constituents. For example, if the 63d constituent is $K_2SO_4(\ell)$, then, at equilibrium, Y_{63} will be the number of gram-moles of liquid potassium sulfate present. Each condensed phase may consist of one constituent only (for example, a phase of solid carbon) or an ideal solution of several species (for example, liquid oxides of Al, Fe, and Si).

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[5] The parenthetical modifiers c, ℓ, and g serve to distinguish species of the same composition as to their phase, crystal, liquid, and ideal gas, respectively.

[6] Component selection might become important if the present algorithm were implemented for a computer representing, say, at most six significant figures. Using 10-figure arithmetic, the precise problem $H_2(g)+\frac{1}{2}O_2(g) \leftrightarrow H_2O(g)$ with components H_2 and O_2 remains tractable down to 700 K. Below this temperature, Jacobian inversion requires more figures unless a component switch is introduced. Higher precision is only required by the inversion scheme, a fact that may be useful with certain machines. An ad hoc solution to the singularity problem might be to perturb either stoichiometric item by 10^{-6}%.

The number N will be, at equilibrium, the total number of moles of gas. The numbers N_k for k = 1, ..., ph will be the total moles in the respective condensed phases.

Each constituent Y_j, gaseous or condensed, has an equilibrium constant K_j (in terms of the gaseous component), which is a function of temperature and is selected from files in advance of working the problem, and a set of stoichiometric coefficients $[V_{ij}]_{i=1}^{r}$, one for each component. An efficient ALGOL procedure for calculating the Y_j's is reproduced in appendix C. Two examples will now serve to explain the relationships of Y_j, X_i, V_{ij}, K_j, N, and N_k to each other.

If there are five components Cl_2, H_2, K, O_2, S_2, then

1. The number of moles of gaseous HCl is computed by

$$Y_{HCl(g)} = \frac{N}{P} K_{HCl(g)} \left(\frac{X_{Cl_2} P}{N} \right)^{\frac{1}{2}} \left(\frac{X_{H_2} P}{N} \right)^{\frac{1}{2}}, \tag{12}$$

where $V_{1,HCl} = V_{2,HCl} = \frac{1}{2}$ and $V_{3,HCl} = V_{4,HCl} = V_{5,HCl} = 0$.

2. The number of moles of liquid potassium sulfate is computed by

$$Y_{K_2SO_4(\ell)} = N_k K_{K_2SO_4(\ell)} \left(\frac{X_K P}{N} \right)^{2} \left(\frac{H_{O_2} P}{N} \right)^{2} \left(\frac{X_{S_2} P}{N} \right)^{\frac{1}{2}}, \tag{13}$$

where $V_{3,K_2SO_4} = V_{4,K_2SO_4} = 2$, $V_{5,K_2SO_4} = \frac{1}{2}$, $V_{1,K_2SO_4} = V_{2,K_2SO_4} = 0$ and where it is assumed that $K_2SO_4(\ell)$ is one of the species in the kth condensed phase. From the discussion in section 1 following equation 11, it can be seen that the right side of equation 13, divided by N_k, is the mole fraction of $K_2SO_4(\ell)$.

If we should happen to know in advance the equilibrium values for N, N_k, and for the X_i, then the calculations 12 and 13 would be precise. This generally does not happen except after several iterations; nevertheless, it is convenient for the reader to understand that at any step of iteration the calculation of any Y_j is a straight-forward assignment, and that when the variables N, X_i, and N_k are precise, the values of the Y_j are precise.

One can infer from the two examples above that the primary interest in solving a general equilibrium problem is shifted to the determination of the equilibrium values for N, for the X_i, and for the N_k.

In the present algorithm, it is always assumed that there is a gas phase present. This choice is partly conditioned by our interest in combustion problems, but in more generality, we can take the view that all condensed species have vapor pressures.[7] In concept we must solve the following gas phase problem for the unknowns $\vec{X}$, $\vec{Y}$, N whenever we solve any problem.

$$Y_j = \left(\frac{N}{P}\right) K_j \prod_{i=1}^{r} \left(\frac{X_i P}{N}\right)^{v_{ij}} \qquad 1 \le j \le s \tag{14}$$

$$N = \sum_{i=1}^{r} X_i + \sum_{j=1}^{s} Y_j \tag{15}$$

$$Q_i = X_i + \sum_{j=1}^{s} v_{ij} Y_j \qquad 1 \le i \le r \tag{16}$$

If after solving the preceding problem, we find that

$$\sum_{j=1+d_{k-1}}^{d_k} K_j \prod_{i=1}^{r} \left(\frac{PX_i}{N}\right)^{v_{ij}} \le 1 \tag{17}$$

for each condensed phase k = 1, ..., ph considered, then all the condensed phases are absent and the full solution to the problem is the solution to the gas-phase problem augmented by zeros for every condensed species and phase. The summation limits are defined by $d_o = s$ and, inductively, $d_k = d_{k-1} + c_k$ for k=1, ..., ph.

Now, suppose condensation might occur. Let R_k be the left side of inequality 17, which is similar to the right side of equation 11 of section 1. If after the calculation of the Y_j's in some iteration it turns out that some of the R_k's are greater than 1, or that some of the N_k's are greater than zero, then at the next iteration the following system must be solved:

$$N = \sum_{i=1}^{r} X_i + \sum_{j=1}^{s} \left(\frac{P}{N}\right)^{v_{oj}} K_j \prod_{i=1}^{r} X_i^{\,v_{ij}} \tag{18}$$

$$Q_i = X_i + \sum_{j=1}^{s} v_{ij} \left(\frac{P}{N}\right)^{v_{oj}} K_j \prod_{i=1}^{r} X_i^{\,v_{ij}}$$

$$+ \sum_{k=1}^{ph} \sum_{j=1+d_{k-1}}^{d_k} v_{ij} N_k K_j \left(\frac{P}{N}\right)^{v_{oj}} \prod_{i=1}^{r} X_i^{\,v_{ij}} \tag{19}$$

$$1 = \sum_{j=1+d_{k-1}}^{d_k} K_j \left(\frac{P}{N}\right)^{v_{oj}} \prod_{i=1}^{r} X_i^{\,v_{ij}} \tag{20}$$

for all k with $R_k \ge 1$ or $N_k \ge 0$

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[7] There exist systems with no gas phase. The present algorithm will not solve the problem $H_2(g)+\frac{1}{2}O_2(g)\longleftrightarrow H_2O(\ell)$ at 1 atm and 300 K regardless of what (gaseous) components are chosen because the total pressure of all gases in the system at 300 K is less than 1 atm. Perturbation of either stoichiometric item by $10^{-6}\%$ renders this problem tractable because then a small gas phase is present.

where we have defined $$V_{o\,j} = \begin{cases} \sum\limits_{i=1}^{r} V_{i\,j} - 1 & \text{if } Y_i \text{ is gaseous} \\ \sum\limits_{i=1}^{r} V_{i\,j} & \text{if } Y_j \text{ is condensed.} \end{cases}$$

Some of the last terms in equation 19 may drop out when N_k's are zero. The values of N_k are never negative. The system of equations to be solved can and does change from iteration to iteration, depending on the current values of R_k and of N_k.

This automatic switching of the algebraic form of the problem solved as the iterations progress is an improvement over the method of Feldmann (6), who programed for convergence of the gas-phase problem before a decision was reached as to whether his single condensed phase occurred or not. His approach does not seem to be applicable to systems with more than one condensed phase.

SECTION 3. - FUNCTIONAL REFORMULATION; SYMMETRIC JACOBIANS

First, equations 18-20 of section 2 must be transposed. Values for X_i, N, N_k must be found in such a way that the following functions all have value zero:

$$F_N\ (X_1,\ldots,X_r,N,N_1,\ldots,N_{ph}) = N - \sum_{i=1}^{r} X_i - \sum_{j=1}^{s} \left(\frac{P}{N}\right)^{V_{o\,j}} K_j \prod_{i=1}^{r} X_i^{\ V_{i\,j}} \qquad (21)$$

$$F_i\ (X_1,\ldots,X_r,N,N_1,\ldots,N_{ph}) = Q_i - X_i - \sum_{j=1}^{s} V_{i\,j} \left(\frac{P}{N}\right)^{V_{o\,j}} K_j \prod_{i=1}^{r} X_i^{\ V_{i\,j}}$$

$$- \sum_{k=1}^{ph} \sum_{j=1+d_{k-1}}^{d_k} V_{i\,j}\, N_k\, K_j \left(\frac{P}{N}\right)^{V_{o\,j}} \prod_{i=1}^{r} X_i^{\ V_{i\,j}} \qquad (1 \leq i \leq r) \qquad (22)$$

$$F_{N\,k}\ (X_1,\ldots,X_r,N,N_1,\ldots,N_{ph}) = 1 - \sum_{j=1+d_{k-1}}^{d_k} K_j \left(\frac{P}{N}\right)^{V_{o\,j}} \prod_{i=1}^{r} X_j^{\ V_{i\,j}}$$

$$\text{(for all } k \text{ such that } N_k>0 \text{ or } R_k>1) \qquad (23)$$

Recall that we have the definition

$$R_k = \sum_{j=1+d_{k-1}}^{d_k} K_j \left(\frac{P}{N}\right)^{V_{o\,j}} \prod_{i=1}^{r} XX_i^{\ V_{i\,j}} \qquad (23a)$$

This automatic switching of the algebraic form of the problem solved as the iterations progress is an improvement over the method of Feldmann (6), who programed for convergence of the gas-phase problem before a decision was reached as to whether his single condensed phase occurred or not. His approach does not seem to be applicable to systems with more than one condensed phase.

When the appropriate collection of F's is zero, then the values of X_i $(1\leq i\leq r)$, N, and N_k $(1\leq k\leq ph)$, which make the F's zero, will be the equilibrium values, and the determination of the corresponding Y's will be straightforward (as discussed in section 2).

The decision as to which condensed phases appear is made during each iteration. If at the end of any iteration the value of R_k for some phase k is found to be greater than 1, then the calculation of N_k for that phase is enabled for subsequent iterations. If a subsequent calculation of N_k leads to $N_k\leq 0$, then N_k is set to zero and the calculation of further values for N_k is disabled at least until R_k is again found to exceed 1. It is important that the calculation of N_k is not disabled by the occurrence of $R_k\leq 1$, because it is quite common for R_k to be less than 1 at various steps of iteration, for phases with $N_k\geq 0$.

It has been observed that N, the total moles of gas, does not deviate appreciably from $\sum_{i=1}^{r} Q_i$ in combustion processes. Hence we have found that there is no significant disadvantage to separating the iterative correction to N from the corrections to the other variables X_i and N_k. There is an advantage to separating the correction to N: We have found a way to write the correction equations such that the Jacobian matrix for the corrector functions for the X_i and N_k is a symmetric matrix. We have not found a way to include the function for N and to preserve the symmetry. Inversion of a symmetric nonsingular matrix requires only about one-half of the computer operations required to invert a general nonsingular matrix of the same order.

Let us assume temporarily that the value of N is correct and proceed to calculate the (m+1)st iterates $X_i^{(m+1)}$ and $N_k^{(m+1)}$ from the known mth iterates.

The new values will be found by the corrections

$$X_i^{(m+1)} = (1 + h_i)\, X_i^{(m)},$$

and

$$N_k^{(m+1)} = h_{N_k} + N_k^{(m)}.$$

It is worth noting that the corrections to the X's are multiplicative, whereas the N_k corrections are additive. We want the values for X_i to be always positive, whereas the values for N_k may be zero (but not negative).

We have now to find the values h_i and h_{N_k} that make these functions zero:

$$G_i(\vec{h}) = Q_i - (1+h_i)\, X_i - \sum_{j=1}^{s} V_{ij} \left(\frac{P}{N}\right)^{V_{0j}} K_j \prod_{l=1}^{r} [(1+h_l)X_l]^{V_{lj}}$$

$$- \sum_{k=1}^{ph} \sum_{j=1+d_{k-1}}^{d_k} V_{ij}(h_{N_k}+N_k)\, K_j \left(\frac{P}{N}\right)^{V_{0j}} \prod_{l=1}^{r} [(1+h_l)X_l]^{V_{lj}}$$

$$G_{N_k} = 1 - \sum_{j=1+d_{k-1}}^{d_k} K_j \left(\frac{P}{N}\right)^{V_{0j}} \prod_{i=1}^{r} [(1+h_i)X_i]^{V_{ij}}$$

We shall linearize the G's at $\vec{h} = \vec{0}$. The values for the G's at $\vec{h} = \vec{0}$ are

$$G_i(\vec{0}) = F_i\ (\ldots X_i^{(m)}\ldots,N,\ldots N_k^{(m)}\ldots)$$

and
$$G_{N_k}(\vec{0}) = F_{N_k}(\ldots X_i^{(m)}\ldots,N,\ldots N_k^{(m)}\ldots).$$

We now calculate the Jacobian matrix $J_G(\vec{0})$. Routine differentiation gives

$$\left.\frac{\partial G_a}{\partial h_b}\right|_{\vec{h}=\vec{0}} = -\ \delta_{ab}X_b - \sum_{j=1}^{s} V_{aj}V_{bj}K_j\left(\frac{P}{N}\right)^{V_{oj}}\prod_{i=1}^{r} X_i^{\ V_{ij}}$$

$$-\sum_{N_k>0}\ \sum_{j=1+d_{k-1}}^{d_k} V_{aj}V_{bj}K_j\left(\frac{P}{N}\right)^{V_{oj}}\prod_{i=1}^{r} X_i^{\ V_{ij}}$$

$$= -\ \delta_{ab}X_b - \sum_{j=1}^{s} V_{aj}V_{bj}Y_j - \sum_{N_k>0}\ \sum_{j=1+d_{k-1}}^{d_k} V_{aj}V_{bj}Y_j \qquad (24)$$

where δ_{ab} is the Kronecker delta defined to be zero except $\delta_{ab} = 1$ when a = b.

$$\left.\frac{\partial G_{N_k}}{\partial h_{N_j}}\right|_{\vec{h}=\vec{0}} = 0 \qquad \text{(for all pairs of condensed phases } N_k \text{ and } N_j\text{)} \qquad (25)$$

$$\left.\frac{\partial G_a}{\partial h_{N_b}}\right|_{\vec{h}=\vec{0}} = \left.\frac{\partial G_{N_b}}{\partial h_a}\right|_{\vec{h}=\vec{0}} = \sum_{j=1+d_{b-1}}^{d_b} V_{aj}K_j\left(\frac{P}{N}\right)^{V_{oj}}\prod_{i=1}^{r} X_i^{\ V_{ij}} \qquad (26)$$

By inspection of equations 24-26, the Jacobian matrix

$$J_G\ (\vec{0}) = \begin{pmatrix} \frac{\partial G_1}{\partial h_1} & \cdots & \frac{\partial G_r}{\partial h_1} & \frac{\partial G_{N_1}}{\partial h_1} & \cdots & \frac{\partial G_{N_k}}{\partial h_1} \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial G_1}{\partial h_r} & \cdots & \frac{\partial G_r}{\partial h_r} & \frac{\partial G_{N_1}}{\partial h_r} & \cdots & \frac{\partial G_{N_k}}{\partial h_r} \\ \frac{\partial G_1}{\partial h_{N_1}} & \cdots & \frac{\partial G_r}{\partial h_{N_1}} & 0 & \cdots & 0 \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial G_1}{\partial h_{N_k}} & \cdots & \frac{\partial G_r}{\partial h_{N_k}} & 0 & \cdots & 0 \end{pmatrix}$$

is symmetric. The linear approximations to the values of the components of $\vec{h}$ will be given by the solution to the linear system

$$\vec{0} = \vec{G}(\vec{0}) + [J_G(\vec{0})] (\vec{h}),$$

or

$$\vec{h} = - [J_G(\vec{0})]^{-1} \; . \; \vec{G}(\vec{0}).$$

Brinkley (3) points out that it is a consequence of Gibb's phase rule that $p \leq c+2$, where p is the total number of phases and c is the number of components. In the notation table (appendix A), this translates to $1+ph \leq r+2$ or $ph \leq r+1$. On the other hand, it is obvious that a matrix of the form of $J_G\ (\vec{0})$ is necessarily singular if the square corner of zeros is more than half the width of the whole matrix.[8] It might be hoped that data banks might be prepared with many allowed phases and that the program, when applied, would automatically choose and compute those phases which appear. In practice this has worked, but the preceding remarks show that corrections to more than r condensed phases cannot be computed at any iteration, even though the phase rule allows r+1 condensed phases. (See section 4.)

Experience has shown that the linear approximations to the h_i are sometimes too large or too small. We have had success in avoiding oscillations and negative values for the X_i by "cutting off" the corrections to the X_i in the following way: If h_i is less than -0.99, then we take $X_i^{(m+1)} = 0.01 \cdot X_i^{(m)}$; if h_i is greater than 99.0, we take $X_i^{(m+1)} = 100.0 \cdot X_i^{+(m)}$. Of course, for other values of h_i we take $X_i^{(m+1)} = (1+h_i)\ X_i^{(m)}$.

If the value of h_{N_k} is such that $h_{N_k}+N_k$ is negative at some iteration, then we set $N_k=0$, and, as mentioned earlier, disable the calculation of the phase.

We have yet to derive the (one-dimensional) correction expression for N, the total moles of gas. In order to put this and the other parts of the process into the proper perspective, consider the simplified flow chart[9] of the algorithm:

1° Read P, T, Q_i's

2° Guess X_i's, N_k's, N (section 6)

3° Calculate gas phase Y_j's (example: equation 1, section 2)

4° Correct N (next topic in this section)

5° Calculate Y_j's for condensed phases (example: equation 2, section 2)

6° Check for convergence (section 7); exit if criteria satisfied

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[8] For example, if r = 3 and ph = 4, then the Jacobian, when viewed as a coefficient matrix, has the property that the bottom four rows correspond to 4 equations in 3 unknowns.

[9] A more complete flow chart appears in appendix A.

7° Calculate and invert Jacobian matrix (this section)

8° Correct X_i's and N_k's (this section)

9° Go to 3°.

We now derive the (one-dimensional) correction for N, the total moles of gas. Let $N^{(m)}$ be the current value of N, let $X_i^{(m)}$ be the current values for X_i, and let $Y_j^{(m)}$ be the current values for Y_j given by

$$Y_j^{(m)} = \left(\frac{P}{N^{(m)}}\right)^{V_{oj}} \cdot K_j \cdot \prod_{i=1}^{r} X_i^{V_{ij}} \tag{27}$$

as in equation 1 of section B. We want to find a new value $N^{(m+1)}$ for N so that

$$N^{(m+1)} = \sum_{i=1}^{r} X_i^{(m)} + \sum_{j=1}^{s} K_j \left(\frac{P}{N^{(m+1)}}\right)^{V_{oj}} \prod_{i=1}^{r} \left(X_i^{(m)}\right)^{V_{ij}} \tag{28}$$

It is worth noting that the terms of this second summation are not the same as the $Y_j^{(m)}$ -- they differ in that the denominator is $N^{(m+1)}$ rather then $N^{(m)}$. Let us define h by $N^{(m+1)} = (1+h)\, N^{(m)}$ and

$$F_N(h) \equiv N^{(m)}(1+h) - \sum_{i=1}^{r} X_i^{(m)} - \sum_{j=1}^{s} K_j \left(\frac{P}{N^{(m)}(1+h)}\right)^{V_{oj}} \prod_{i=1}^{r} X_i^{V_{ij}}. \tag{29}$$

Finding h so that function 29 is zero will be equivalent to solving equation 28. Differentiate function 29 with respect to h:

$$\frac{dF_N}{dh} = N^{(m)} - \sum_{j=1}^{s} K_j \left(\prod_{i=1}^{r} X_i^{V_{ij}}\right) V_{oj} \left(\frac{P}{N^{(m)}(1+h)}\right)^{V_{oj}-1} \left(\frac{P}{N^{(m)}}\right)(-1)(1+h)^{-2}$$

so that

$$\left.\frac{dF_N}{dh}\right|_{h=0} = N^{(m)} + \sum_{j=1}^{s} V_{oj}\, Y_j^{(m)}.$$

Now, the linearization of F_N is

$$F_N(h) \sim F_N(0) + h \left.\frac{dF}{dh}\right|_{h=0}.$$

So that h is given approximately as

$$h = -F_N(0) \Big/ \left.\frac{dF}{dh}\right|_{h=0}.$$

So the algorithm for $N^{(m+1)}$ is

$$N^{(m+1)} = \left(1 - \frac{F_N(0)}{F'_N(0)} \right) N^{(m)}$$

$$= \left(1 - \frac{N^{(m)} - \sum X_i{}^{(m)} - \sum Y_i{}^{(m)}}{N^{(m)} + \sum V_{o\,j} Y_j{}^{(m)}} \right) N^{(m)} .$$

The occurrence of the numbers $Y_j{}^{(m)}$ in this equation explains why step 4° of the simplified algorithm fits where it is.

SECTION 4. - PHASE INTERDEPENDENCIES

Correcting all condensed phases at one time does not seem to lead to a Jacobian singularity when the phases are not very interdependent, as for instance in the case that the two phases are graphite on the one hand and a solution of $K_2CO_3(\ell)$ and $K_2SO_4(\ell)$ on the other hand. We have run our program successfully several times under conditions where both these phases occur and are corrected simultaneously (10).

Let us now consider an example that shows in a rather spectacular way that the application of the theory up to this point can lead to a singular Jacobian matrix: Suppose that we consider two only condensed phases, one of which is $K_2SO_4(c)$ only and the other of which is $K_2SO_4(\ell)$ only. Suppose further that, at some iteration, the values of X_K, X_{S_2} and X_{O_2} are so large that both of

$$R_{(c)} \equiv R_{K_2SO_4(c)} = K_{K_2SO_4(c)} \left(\frac{P}{N} \right)^{9/2} X_K{}^2 X_{S_2}{}^{\frac{1}{2}} X_{O_2}{}^2$$

and

$$R_{(\ell)} \equiv R_{K_2SO_4(\ell)} = K_{K_2SO_4(\ell)} \left(\frac{P}{N} \right)^{9/2} X_K{}^2 X_{S_2}{}^{\frac{1}{2}} X_{O_2}{}^2$$

exceed 1. Then, if we proceed to calculate both phase corrections simultaneously, we are led to a singular Jacobian matrix, since the two adjacent columns for the two condensed phases are proportional. More specifically,

$$\frac{\partial G_{(\ell)}}{\partial h_K} = V_{K,(\ell)} R(\ell) \qquad \frac{\partial G_{(c)}}{\partial h_K} = V_{K,(c)} R(c)$$

$$\frac{\partial G_{(\ell)}}{\partial h_{S_2}} = V_{S_2,(\ell)} R(\ell) \qquad \frac{\partial G_{(c)}}{\partial h_{S_2}} = V_{S_2,(c)} R(c)$$

$$\frac{\partial G_{(\ell)}}{\partial h_{O_2}} = V_{O_2,(\ell)} R(\ell) \qquad \frac{\partial G_{(c)}}{\partial h_{O_2}} = V_{O_2,(c)} R(c)$$

All other partials of $G_{(\ell)}$ and $G_{(c)}$ are zero. Since the stoichiometric coefficients for the crystal and liquid are pairwise equal, it is clear that the two columns are proportional.

The simplest solution to this particular problem would be to treat $K_2SO_4(\ell)$ and $K_2SO_4(c)$ as the two constituents in one ideal solution, to zero the equilibrium constant for the crystal above the melting point, and to zero the equilibrium constant for the liquid below the melting point. The effect thus being that only one of the two species is "active" at a given temperature. This zeroing of selected equilibrium constants is accomplished when the data banks are prepared and does not involve any change in the program itself since it works with the data supplied.

A more general solution to the similar problems that can occur in cases of phase interdependencies is to code the program so that only the most out-of-balance phase is corrected at any iteration. More specificially, from among the phases that are candidates either in the sense that $N_K > 0$ or else in the sense that $R_K > 1$, make an iterative correction to only that phase among these candidates for which $|1 - R_K|$ is the largest. In the preceding examples, if the temperature exceeds the melting point, we would have $R_{(\ell)} > R_{(c)}$ so that the only phase corrected at the next iteration would be the liquid phase. When the problem has converged $R_{(\ell)} = 1$ and $R_{(c)} < R_{(\ell)}$ so that the crystal phase would not appear. This procedure seems to be always convergent, but it is slow for two reasons: first, because different condensed phases must be corrected at different iterations, and secondly, because it requires extra coding and storage to omit Jacobian inversion (discussed in section 6).

Finally, it is possible and sometimes economical to steer a middle course between two extremes of correcting all condensed phases at once and correcting only the most out-of-balance phase at each iteration. We have had success in correcting phases one at a time until all the "active" R's are between 0.95 and 1.05 and then switching over to correcting all phases at once. Naturally, the parameter 0.05 in $|1 - R_K| \leq 0.05$ can be adjusted as a data item in the implementation of this last idea if it appears necessary.

In the crystal-liquid example where each is treated as a separate phase, Jacobian singularity occurs no matter what the values of the X's if the specified temperature happens to be the melting temperature, since the two phase rows are not only proportional but, in fact, identical.[10] But under

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[10] Suppose compount SALT has a congruent melting point T_m and that the enthalpy of fusion is ΔH_m. Let ΔS be the change in absolute entropy at formation of 1 mole of SALT(c) at T_m, and let ΔH be the enthalpy of 1 mole of SALT(c) at T_m measured above the elements in their reference states at T_m. Consider two reactions:

$$S + A + L + T \rightarrow \mathrm{SALT}(c) \qquad \Delta G = \Delta H - T_m \Delta S$$

$$S + A + L + T \rightarrow \mathrm{SALT}(\ell) \qquad \Delta G = (\Delta H + \Delta H_m) - T_m \left(\Delta S + \frac{\Delta H_m}{T_m} \right),$$

where the left sides are both the (same) reference states. At this temperature the free energy change is the same for both reactions so that the equilibrium constants $K_p = \Delta G/RT_m$ are equal.

such conditions, the system is thermodynamically indeterminant anyway.[11] Another thermodynamically independent variable such as enthalpy would suffice to resolve the ambiguity as to how much material is in each condensed phase. Our program does not, at present, allow for this occasional variation in identification of independent variables.

SECTION 5. - MATRIX INVERSION AND SKIPPING IT

We reserve a square matrix of words $(r + ph) \times (r + ph)$ so that there is space to calculate the Jacobian even in the unlikely event that all possible condensed phases appear at one time. We then effectively ignore those rows and columns that are not "activated" by one of the criteria $R_k > 1$ or $N_k > 0$. Since activation or inactivation of the various phase rows and columns is controlled by the occurrence of "true" or "false" in the entries of a Boolean array, it is an easy extension to "shut off" the rows and columns corresponding to components when the Q item for a component has been input as zero.

This "shutting off" is in fact necessary since $Q_i = 0$ implies $X_i \equiv 0$, which implies that all Y_j corresponding to constituents j (which require component i in their production) are zero; then by equations 24 and 26 of section 3 the resulting Jacobian has a whole row of zeros, so the Jacobian is singular. Corrections for such X's are not necessary anyway. Therefore, it is very convenient to extend the "ignoring of rows and columns" to rows and columns corresponding to components.

Not only do we avoid the problem of matrix singularity in cases where a Q-item is zero, we in fact get a speedup in the operation of the inversion. The speed improvement runs almost as the square of (r-m), where m is the number of rows and columns omitted by the occurrence of zero items in the Q-list. It seems noteworthy that the program scales down and speeds up when zero Q-items are entered.

The algorithm for inverting the Jacobian matrix is reproduced in ALGOL in the appendix. The algorithm is a modified Doolittle procedure (1, pp. 307-313), which we have modified to ignore rows and columns that correspond to zero phases or to zero components.

An economy was found in a criterion for skipping Jacobian construction and inversion when convergence is near (8, p. 98). Store the diagonal elements of the Jacobian whenever it is inverted and then compare the ratios of the proposed Jacobian diagonal elements divided by the corresponding diagonal elements of the last Jacobian inverted. If it turns out that

$3/4 \leq d_i^{(old)}/d_i^{(new)} \leq 4/3$ for all the diagonal elements d_i, then the construction and inversion of the complete new Jacobian can be skipped. It is estimated that the resulting saving in computer time can be as high as 40 percent. Naturally, it is necessary that a new Jacobian be computed and inverted whenever a new condensed phase appears.

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[11] Assuming the idealization that activities of condensed species are independent of pressure.

We do not understand the precise mathematical reason for this criterion to be effective, but we were motivated to try it by the considerations that the diagonal elements of the Jacobian tend to be the largest entries in the matrix as confirmed by inspection of some test cases and by inspection of equation 24 (section 3). The coefficients V_{aj}, V_{bj} for each off-diagonal summand are not very well correlated, so that many terms in the summation are zero for the off-diagonal entries. A matrix norm might be used if core space is available.

SECTION 6. - SEQUENTIAL AND INITIAL GUESSING

One might say that "nothing improves the speed of an iterative algorithm as well as guessing right the first time." In this spirit, two features were incorporated that serve to improve the first guess on a given problem.

Suppose we have specified a given P and $\vec{Q}$ and wish to calculate composition at several temperatures; Say, T = 2800(-100)2000 K. After the program has calculated composition at 2800 K, it is a triviality to use the resulting answer, $\vec{X}$, as the initial guess for the 2700 K case. For the third and successive temperatures we can use knowledge of the two preceding $\vec{X}$'s to obtain very precise initial guesses.

Specifically, we use the guessing algorithm

$$\ln X_3 = \ln X_2 + \left(\frac{1}{T_3} - \frac{1}{T_2}\right) (\ln X_2 - \ln X_1) \Big/ \left(\frac{1}{T_2} - \frac{1}{T_1}\right),$$

where X_1 and X_2 are the solution numbers of gram-moles of the same component for preceding temperatures T_1 and T_2, and where X_3 is the initial guess to be used for this same component at the temperature T_3. This logarithmic guessing scheme is an application of the generality that "logs of thermodynamic properties are affine in 1/T" (4, p. 3). The success of the scheme (appendix D) can be viewed as a confirmation of the fact that gram-moles of a component in a system is a thermodynamic property. Such a scheme for initial guessing of chained problems will be called a "sequential guessing scheme."

Obviously, one cannot use the formula to obtain guesses for zero components, but this is a minor programing difficulty. On the other hand, one might wish to apply the same algorithm to guessing values for N_k, moles in condensed phases. Doing so has resulted in some problems regarding overestimates of N_k for phases that grow rapidly over a short temperature range after they appear (decreasing temperature order) and then level off. This distinctly nonlinear behavior might not be a problem for short temperature steps (<100 K) between adjacent problems. We have found that using unadjusted answers from the previous problem for the gusses of N_k's while using the logarithmic scheme for the components is just as fast as logarithmic guessing for all N's and X's for typical three-phase, 15-component problems (appendix D).

Our algorithm seems to have more difficulty recovering from overestimates of condensed phases than from underestimates. This means that a distinct advantage obtains from using the scheme advocated in decreasing temperature order, since quantities of material in condensed phases usually increases with decreasing temperature. The initial guesses for N_k will then generally be less than the solution values for a given problem.

Appendix D discusses solution of the same set of 11 problems using 5 different guessing schemes. Two of the schemes are the two different logarithmic schemes previously mentioned, one is the single scheme of using old unadjusted answers, and the other two are schemes we discovered some time ago using the guessing formula $X_3 = X_2/X_1$. It turns out that this old scheme is rather good since it is equivalent to the logarithmic scheme of if one assumes

$$(1/T_3 - 1/T_2)\big/(1/T_2 - 1/T_1) = 1.$$

The older scheme is not well suited to nonuniform temperature spacing.

Next we consider a method useful for obtaining initial guesses for similar problems with different pressures or mildly varying Q-lists.

Initial guesses as to the values of the X_i can be obtained economically by multiplying the respective Q_i by externally supplied or internally generated coefficients which we call "initial guessing coefficients." It should be recalled that equilibrium problems are nonlinear problems which are at best homogeneous in the sense that multiplying the entire Q-list by any positive number serves only to multiply the equilibrium values of the X's and Y's by the same number. This provides a justification for the guessing coefficient idea: Suppose we somehow solve an equilibrium problem, and that we then calculate coefficients X_i^{old}/Q_i^{old} for this solution where the Q_i are the prescribed initial data. Now, if a new problem is prescribed that has a similar Q-list, the initial guesses as to the values of X_i for the new problem will be very good indeed if they are taken to be $Q_i^{new}\ (X_i^{old}/Q_i^{old})$. The remark about homogeneity shows that the guesses will be exactly correct if the new Q-list happens to be a multiple of the old Q-list, and if the pressure and temperature are the same.

The Bureau of Mines program has been coded so that it reads a set of initial guessing coefficients at the beginning of each run. At the conclusion of each problem for which a new Q-list was specified, new values of initial guessing coefficients are calculated. There are at least two common situations where the economy of this procedure will be realized. The first of these situations is the one that occurs where the effect on the equilibrium mixture due to changes in one or a few of the Q-list items is to be studied in successive runs. A second situation where this economy makes itself felt is the calculation of a rectangular array of (P,T)-points for a Mollier chart. Say we are to calculate the points for a Mollier chart for a fixed Q-list and for T = 2800 (-100) 2000 and for P = ½, 1, 2, 4, 8 atmospheres, first, we calculate the (T=2800, P=½) case starting with the externally supplied guessing coefficients. The cases (P= ½, T= 2700 (-100) 2000) are then calculated starting with sequential guessing coefficients as explained at the beginning of this section. When the program works the problem (P = 1, T = 2800), it will start with the coefficients calculated after the (P = ½, T = 2800) case was solved. Since only P will have changed, considerable computer time is saved.

A slight complication arises in the application of the second idea to N_k or to an X_i, the value of which might be affected by Q items other than Q_i. The idea is simply to define the initial guessing coefficient so that, for examples,

$$X_{O_2} = (\text{coef}_{O_2}) \left[Q_{CO_2} + Q_{O_2} + Q_{SiO_2} + Q_{AlO_2} \right]$$

and

$$N_{SiO_2(\ell),Al_2O_3(\ell)} = (\text{coef}_{liq}) \left[Q_{SiO_2} + Q_{AlO_2} \right]$$

Where in the later case N was assumed to be the total gram-moles in a condensed phase of $SiO_2(\ell)$ and $Al_2O_3(\ell)$.

SECTION 7. - CONVERGENCE CRITERIA

It is mentioned in sections 2 and 3 that the values of the Y_j's are always precise relative to the X_i's, N and N_k's. In a sense, the equilibrium constant relations giving Y_j are "always" correct. The requirements that are not necessarily satisfied are 1° stoichiometric balance, 2° that $R_k = 1$ for each phase with $N_k > 0$, and 3° that N is the sum of gaseous moles.

Written out, then, we have to check that

$$|F_{N_k}| \leq 10^{-4} \qquad \text{for k with } N_k > 0. \tag{30}$$

$$|F_i| \leq 10^{-4} Q_i \qquad 1 \leq i \leq r. \tag{31}$$

and

$$\left| \sum_{i=1}^{r} X_i + \sum_{j=1}^{s} Y_j - N \right| \leq 10^{-4} N \tag{32}$$

for four significant figure accuracy. The F's were introduced in section 3.

This statement about accuracy applies to the accuracy of the functional values F_i, F_{N_k}, and F_N--not to the values of the X_i and Y_j. On the other hand, in occasional back checking of the answers obtained, we have never found a case where we could detect any error of the size 10^{-4} X_i (or 10^{-4} Y_j, respectively) or larger.

This convergence criterion is obviously superior to a scheme that checks for stationarity of the components, for example, since component stationarity could lead to large errors in constituents if components are chosen, as we often do, to be species that are not necessarily the most prevalent species containing the given elements.

Three remarks about the inequalities 31 need to be made:

First, for the electron balance inequality, we use

$$| F_{e^-} | \le 10^{-4} (X_{e^-} + \sum_{\text{ions}} Y_j)/2,$$

since the stoichiometric input of electrons is usually zero (electroneutrality), and, because in some cases, the ions may far outnumber the electrons.

Second, we normally choose some components as oxides, so that the inequality 31 in the case of oxygen should be $|F_{O_2}| \le 10^{-4} (Q_{AlO_2}+Q_{CO_2}+Q_{O_2}+Q_{SiO_2})$ for a case where the three oxides shown are components. Note that it is possible for Q_{O_2} to be negative, so we cannot use $| F_{O_2} | \le 10^{-4} Q_{O_2}$. Specification of a Q-list in which $Q_{AlO_2}+Q_{CO_2}+Q_{O_2}+Q_{SiO_2}$ is negative corresponds to a chemically impossible situation. If components should be chosen in some other way, as chlorides say, then other analogous adjustments in the convergence criteria would be necessary.

Third, if any element is absent, then we omit checking the corresponding inequality in the test for convergence.

Obviously, if it can be justified to calculate a different number of significant figures, then the factors 10^{-4} in each of inequalities 30, 31, and 32 can be changed to some other appropriate number.

SECTION 8. - EQUILIBRIUM CONSTANT TABULATION AND INTERPOLATION

Equilibrium constants have been accurately tabulated in the JANAF tables (3) based on the elements in chosen reference states. Since the components chosen may not necessarily be the same as the JANAF reference state elements, it may be necessary to do an algebraic transformation of JANAF equilibrium constants when preparing data for use in this Bureau of Mines program.

The JANAF data are tabulated at 100 K intervals, so this has been a convenient way to prepare a data bank. If it is necessary to compute an equilibrium problem at a temperature other than a multiple of 100 K, a particularly good method for interpolation is to assume that ln K is a linear function of 1/T. The functional form for this interpolation is based on the Van't Hoff equation (7, sec. 33f) and at the end points of the 100 K interval, the fitting function will conform to the supplied data.

Provision must be made to avoid singularity in the interpolating function in case a data bank is used in which zero equilibrium constants have been entered as mentioned in section 4.

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APPENDIX A.--FLOW CHART AND NOTATIONS

Included here is a simplified flow chart (fig. A-1) for the computations for the case that all condensed phases are corrected at each step of iteration. Flow charts for the other options in correcting condensed phases do not differ to a great extent.

Also included is a list of notations for the convenience of the reader.

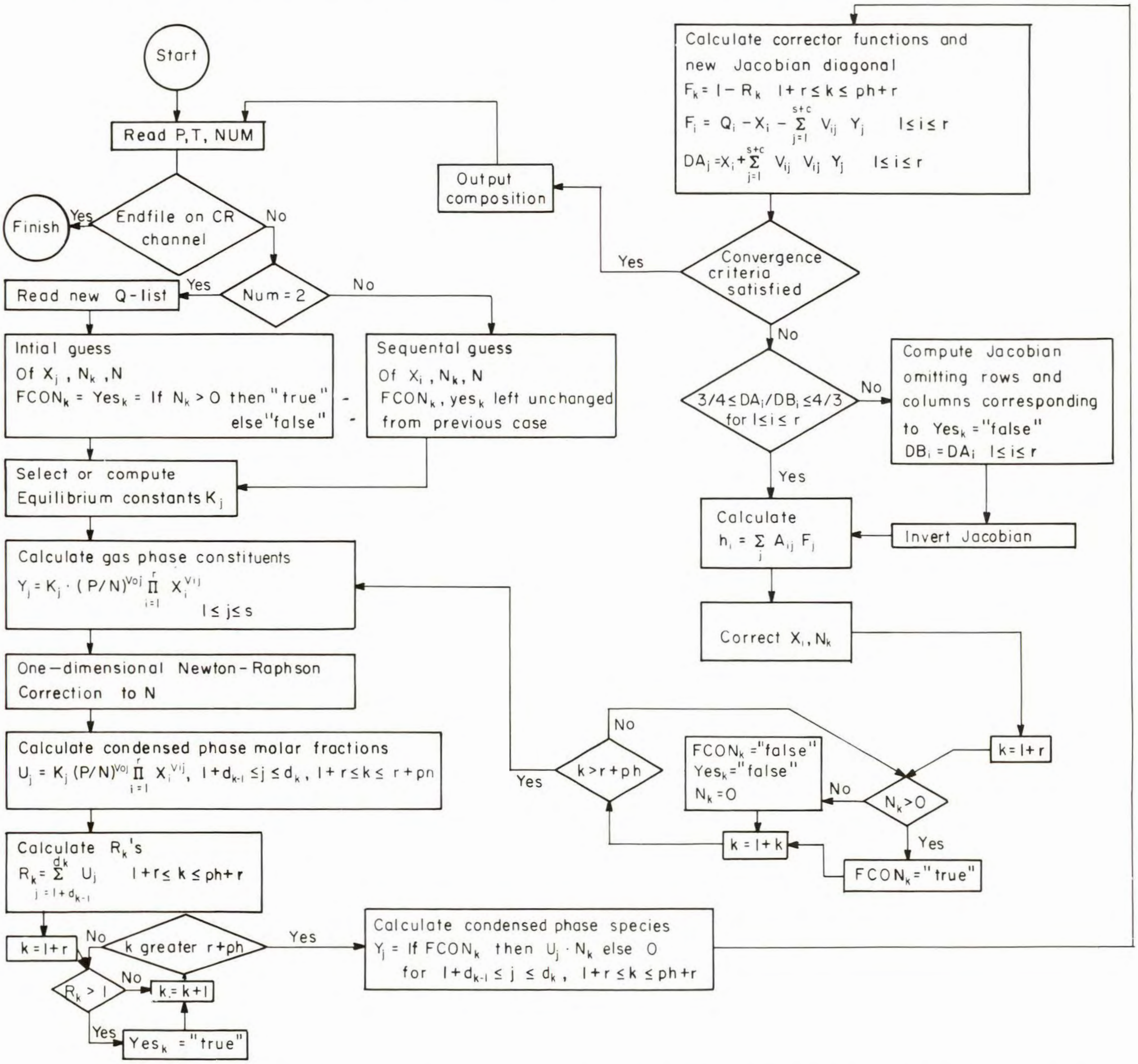

FIGURE A-1. - Flow chart for multiphase chemical equilibrium algorithm—option in which all existent condensed phases are correct at each iteration.

Notations

X	The vector whose entries contain the number of gram-moles of components at each step of iteration.
X_i	One entry of vector X.
Y	The vector whose entries are gram-moles of constituents.
Y_j	One entry of vector Y.
Q	The vector whose entries are gram-moles equivalent of components in the whole system at equilibrium. These numbers are independent variables in specifying a problem and do not change as the iterations proceed.
Q_i	One entry of vector Q.
P	Pressure, atmospheres.
T	Temperature, kelvins.
K_j	The partial pressure equilibrium constant for constituent number j. The equilibrium constants are in the representation of the JANAF tables.
V_{ij}	The stoichiometric coefficient of the ith component in the jth species.
R_k	The current value of the sum of mole fractions in condensed phase k. If $R_k < 1$ at equilibrium then phase k does not appear, while $R_k = 1$ at equilibrium if phase k does appear.
r	The number of components.
s	The number of constituents in the gas phase.
c	The number of constituents in the condensed phases.
c_k	The number of constituents in the kth condensed phase.
d_0	= s.
d_k	$= d_{k-1}+c_k$, for k greater than zero.
$L_{D'}$	= Vapor pressure over liquid D' (used in section 1 only).

APPENDIX B.--THE MATRIX INVERSION SCHEME

We reproduce here, in ALGOL, the matrix inversion scheme for the symmetric matrix $J_G(\vec{0})$ of section 3. In this implementation, the matrix is called A, and it has been assumed to have been loaded with the partial derivatives of section 3. Rows and columns corresponding to zero phases or to zero components have been loaded with zeros. The identifier RPH is equal to the sum of r and ph (section 2) so that both the square matrices $A = J_G(\vec{0})$, and IN have space for partials of all components and all condensed phases. The global Boolean array YES (/ 1..RPH/) controls the ignoring of rows and columns corresponding to zero components and zero phases. If on the reading of the Q-list for a particular problem it is found that, say Q_3 is zero then YES_3 is set equal to false, otherwise true. The logical values true or false have been assigned to YES_{r+1} ... YES_{r+ph} at the last iteration according to the rules: YES_{r+k} = true if $R_k>1$ or if $N_k>0$ and YES_{r+k} = false if both $R_k<1$ and $N_k\leq 0$.

```
≠BEGIN≠≠COMMENT≠  MATRIX INVERSION BLOCK.,
        ≠ARRAY≠IN(/1..RPH,1..RPH/).,
        ≠REAL≠ PIVOT.,
M.=RPH.,

≠FOR≠I.=1≠STEP≠1≠UNTIL≠M≠DO≠
≠BEGIN≠
≠FOR≠J.=1≠STEP≠1≠UNTIL≠M≠DO≠
IN(/I,J/).=0.0.,
IN(/I,I/).=1.0.,
≠END≠ I LOOP AND LOADING ARRAY IN WITH IDENTITY MATRIX.,

  ≠FOR≠ J.=1 ≠STEP≠ 1 ≠UNTIL≠ M ≠DO≠
≠IF≠  YES(/J/) ≠THEN≠
≠BEGIN≠

≠FOR≠ I.=J≠STEP≠ 1 ≠UNTIL≠ M ≠DO≠
≠IF≠ YES(/I/) ≠THEN≠
≠FOR≠L.=1≠STEP≠1≠UNTIL≠J-1≠DO≠
A(/J,I/).=A(/J,I/)-A(/L,I/)*A(/J,L/).,

≠FOR≠I.=1≠STEP≠1≠UNTIL≠ M ≠DO≠
≠IF≠ YES(/I/) ≠THEN≠
≠FOR≠ L.=1≠STEP≠1≠UNTIL≠ J-1≠DO≠
  IN(/J,I/).=IN(/J,I/) - IN(/L,I/) * A(/L,J/).,

  ≠IF≠ ABS(A(/J,J/)) ≠LESS≠≠-150 ≠THEN≠ ≠GOTO≠ SINGULAR.,
PIVOT.=1.0/A(/J,J/).,

≠FOR≠I.=J+1≠STEP≠ 1 ≠UNTIL≠M≠DO≠
A(/I,J/).=A(/J,I/)*PIVOT.,

  ≠FOR≠ I.=1 ≠STEP≠ 1 ≠UNTIL≠ M ≠DO≠
  IN(/J,I/).=IN(/J,I/) * PIVOT.,
≠END≠ J LOOP.,

  ≠FOR≠ I.=1 ≠STEP≠ 1 ≠UNTIL≠ M ≠DO≠
  A(/I,M/).=IN(/M,I/).,

≠FOR≠ I.= M-1 ≠STEP≠ -1 ≠UNTIL≠ 1 ≠DO≠
≠IF≠ YES(/I/) ≠THEN≠
≠FOR≠ J.= 1 ≠STEP≠ 1 ≠UNTIL≠ I ≠DO≠
≠BEGIN≠
     A(/J,I/).=IN(/I,J/).,
≠FOR≠  L.=M≠STEP≠ -1 ≠UNTIL≠ I+1 ≠DO≠
  A(/J,I/).=A(/J,I/) - A(/J,L/) * A(/L,I/).,
≠END≠ I--J DOUBLE LOOP.,

  ≠FOR≠ J.=2 ≠STEP≠ 1 ≠UNTIL≠ M   ≠DO≠ ≠FOR≠I.=J-1≠STEP≠-1 ≠UNTIL≠ 1
  ≠DO≠ A(/J,I/).=A(/I,J/).,

≠END≠ OF MATRIX INVERSION BLOCK.,
```

APPENDIX C.--EFFICIENT CALCULATION OF Y'S

We reproduce the ALGOL procedure (QUILB) for time-optimal calculation of the expressions for Y's, for example, equations 12 and 13 of section 2. When the procedure is called, the formal parameter RAY is replaced with the identifier for the array to be calculated--Y in the case of gaseous constituents and U in the case of condensed constituents. The formal parameters BOTTOM and TOP are replaced with the actual limits within the array between which the calculations are to be performed. The formal parameter SIGMA is replaced with N when gaseous Y's are to be calculated and with RN(K) for the calculation of an expression R_k in the notation of section 3. Two examples serve to explain this more completely:

The coding

```
QUILB(Y,1,S,N0).,

'for' I = 1 'step' 1 'until' R 'do' N0=N0+X(/I/).,
```

serves to calculate the gram moles of each gaseous constituent and to add up the corresponding (intermediate) value of total moles of gas. N0 is then used in the one dimensional Newton-Raphson correction to N, as discussed at the end of section 3.

The coding

```
QUILB(U,1+S,S+C1,RK)

'for' I=S+1 'step' 1 'until' S+C1 'do'

Y(/I/)=NK*U(/I/).,
```

serves to load the array U with the terms of the expression for R_k (section 3, equation 23a) and the identifier RK gets the value of R_k. The values for the Y(/I/) conform to the expression 13 of section 2.

The procedure QUILB is optimal in the senses that the most likely values for the stoichiometric coefficients are taken care of first and that the library procedure "power" is used only as a last resort.

The Boolean array YES, discussed in appendix B and in section 5, the stoichiometric coefficient matrix V, the equilibrium constant array K, and the variables PON($=P/N^{(m)}$) and SQRPN($=\sqrt{PON}$) must all be global to the procedure.

An implementor of this algorithm should check that the computer with which it is to be used is capable of checking the indicated equalities between real variables; if it is not, then the inefficient call of the library procedure "power" R+1 times may be necessary.

```
≠PROCEDURE≠QUILB(RAY,BOTTOM,TOP,SIGMA).,
≠COMMENT≠ AN EXPERIMENT ON 20JAN72 SHOWED THE FOLLOWING RATHER HEAVY-
HANDED APPEARING CALCULATION SCHEME FOR THE  GRAM-MOLES OF GASES AND
 FOR THE MOLE-FRACTIONS OF THE LIQUIDS TO BE AT LEAST 14 PER
CENT FASTER THAN WOULD BE R+1 CALLS OF THE LIBRARY PROC *POWER* AT
EACH EVALUATION OF RAY(J).  BY THIS WE MEAN THAT THE WHOLE PROGRAM
RAN IN 3MIN28SEC VS 3MIN54SEC FOR TWO TEST CASES.  THE RELATIVE
SPEED-UP OF THIS PROCEDURE ITSELF MUST BE ENORMOUS.,
≠VALUE≠BOTTOM,TOP.,
≠INTEGER≠BOTTOM,TOP.,     ≠REAL≠ SIGMA.,    ≠ARRAY≠RAY.,
≠BEGIN≠      ≠REAL≠  PROD,B.,
SIGMA.=0.0.,
≠FOR≠ J.= BOTTOM ≠STEP≠ 1 ≠UNTIL≠ TOP ≠DO≠
≠BEGIN≠          PROD.=K(/J/).,
≠FOR≠ I.=1 ≠STEP≠ 1 ≠UNTIL≠ R    ≠DO≠
≠BEGIN≠
B.=V(/I,J/).,
≠IF≠ B ≠EQUAL≠ 0.0 ≠THEN≠ ≠GOTO≠ QUILB1.,
≠IF≠≠NOT≠YES(/I/)≠THEN≠≠BEGIN≠RAY(/J/).=0.0.,≠GOTO≠QUILB2.,≠END≠.,
≠IF≠B        ≠EQUAL≠0.5≠THEN≠
≠BEGIN≠PROD.=PROD*SQRT(X(/I/)).,             ≠GOTO≠QUILB1.,≠END≠.,
≠IF≠B        ≠EQUAL≠ 1.0 ≠THEN≠
≠BEGIN≠PROD.=PROD*X(/I/).,           ≠GOTO≠QUILB1.,≠END≠.,
≠IF≠B        ≠EQUAL≠-1.0≠THEN≠
≠BEGIN≠PROD.=PROD/X(/I/).,           ≠GOTO≠QUILB1.,≠END≠.,
≠IF≠B        ≠EQUAL≠-0.50≠THEN≠
≠BEGIN≠PROD.=PROD/SQRT(X(/I/)).,   ≠GOTO≠  QUILB1.,  ≠END≠.,
≠IF≠B        ≠EQUAL≠2.0≠THEN≠
≠BEGIN≠PROD.=PROD*X(/I/)*X(/I/).,           ≠GOTO≠QUILB1.,≠END≠.,
≠IF≠B        ≠EQUAL≠1.5≠THEN≠
≠BEGIN≠PROD.=PROD*X(/I/)*SQRT(X(/I/)).,≠GOTO≠QUILB1.,   ≠END≠.,
PROD.=PROD*X(/I/)≠POWER≠B.,
QUILB1.. ≠END≠ I LOOP.,
B.=V(/0,J/).,
≠IF≠B ≠EQUAL≠ 0.5 ≠THEN≠
≠BEGIN≠ RAY(/J         /).=             PROD*SQRPN.,
≠GOTO≠ QUILB2.,  ≠END≠.,
≠IF≠ B ≠EQUAL≠ 1.0 ≠THEN≠ ≠BEGIN≠ RAY(/J          /).=
       PROD*PON.,  ≠GOTO≠ QUILB2.,  ≠END≠.,
≠IF≠ B ≠EQUAL≠ -0.5 ≠THEN≠ ≠BEGIN≠ RAY(/J         /).=
       PROD/SQRPN.,  ≠GOTO≠ QUILB2.,    ≠END≠.,
≠IF≠B        ≠EQUAL≠0.00≠THEN≠
≠BEGIN≠  RAY(/J/).=        PROD.,  ≠GOTO≠  QUILB2.,  ≠END≠  .,
≠IF≠B        ≠EQUAL≠-1.0≠THEN≠
≠BEGIN≠RAY(/J/).=        PROD/PON.,≠GOTO≠QUILB2.,≠END≠.,
≠IF≠B        ≠EQUAL≠1.50≠THEN≠
≠BEGIN≠RAY(/J/).=        PROD*PON*SQRPN.,≠GOTO≠QUILB2.,≠END≠.,
RAY(/J       /).=          PROD*PON≠POWER≠B.,
QUILB2..
SIGMA.=SIGMA+RAY(/J        /).,
≠END≠ J LOOP AND EVALUATING RAY(/J        /).,
≠END≠ OF PROCEDURE QUILB.,
```

APPENDIX D.--COMPARISON OF SEQUENTIAL GUESSING SCHEMES AND EXAMPLE CALCULATIONS

Equilibrium composition for 11 temperatures and P = 1 atm was calculated for the same Q-list using five different sequential guessing schemes. The temperatures were 2500, 2400, 2300, 2000, 1800, 1700, 1600, 1500, 1400, 1200, and 1000 kelvins. The entries of vector Q were

39.8800	Ar	0.3000	AlO_2	1230.0000	CO_2
0.0700	Ca	0.2800	Cl_2	0.0000	Cs
0.9500	Fe	650.2000	H_2	29.0000	K
3396.0000	N_2	0.1500	Na	349.2000	O_2
5.0000	S_2	4.4800	SiO_2		

in gram-moles. The initial guessing coefficients for all four runs were the same so that the effort to calculate the first two (highest temperature) compositions was the same in all five runs.

The data bank used caused the program to calculate the quantities at equilibrium of each of the following species:

Gas Phase

Ar	AlO_2	CO_2	Ca	Cl_2
Cs	Fe	H_2	K	N_2
Na	O_2	S_2	SiO_2	e^-
Al	AlO	$Al(OH)_2$	Al_2O	CO
COS	CaOH	Cl	CsCl	CsO
CsOH	FeO	$Fe(OH)_2$	H	HCl
H_2O	H_2S	KCl	KO	KOH
N	NH_3	NO	NO_2	NaCl
NaO	NaOH	O	OH	S
SO	SO_2	SO_3	Si	SiO
AlO_2^-	CN^-	CO_2^-	Cl^-	Cs^+
K^+	NO^-	NO_2^-	Na^+	O^-
OH^-	O_2^-	SH^-	SO^-	SO_2^-

Slag Phase

$Al_2O_3(\ell)$	$Al_6Si_2O_{13}(\ell)$	$CaO(\ell)$	$CsOH(\ell)$
$FeAl_2O_4(\ell)$	$FeO(\ell)$	$KAlO_2(\ell)$	$K_2SiO_3(\ell)$
$NaOH(\ell)$	$SiO_2(\ell)$		

Condensed Seed Phase

$K_2CO_3(\ell)$	$K_2CO_3(c)$	$K_2SO_4(\ell)$	$K_2SO_4(c)$

a total of 79 species in three phases.

Compositions for the 11 temperatures were calculated using five different sequential guessing schemes as follows:

Scheme I: Guesses for new temperature are exactly the same as answers obtained for immediately preceding case. No temperature or other adjustment is applied to either component guesses X_i or to total mole guesses N, N_k.

Scheme II: Guesses for second temperature same as answers for first temperature (as in scheme I). For third and successive temperatures, the guesses are taken to be $X_3 = X_2X_2/X_1$ where X_1 and X_2 are answers for the preceding two cases. This estimation scheme applied to N and N_k as well as to X_1.

Scheme III: Like scheme II except old values for N_k used.

Scheme IV: Answers for first temperature serve as guesses for second temperature (as in I and II). For third and succeeding temperatures, the guesses are taken to be given by

$$\ln (X_3) = \ln (X_2) + (1/T_3 - 1/T_2)(\ln X_2 - \ln X_1)/(1/T_2 - 1/T_1)$$

as in section 6. This guessing scheme is applied to both components and to the N_k.

Scheme V: Same as scheme III except that guesses for the N_k are taken to be the answers from preceding (higher temperature) problem; that is, we do not apply the logarithmic guessing to N_k--only to the X_i.

In table D-1, which shows the main results using the five schemes, we give the following information. The subcolumn of numbers subheaded INV is the number of matrix inversions and the subcolumn subheaded ITR is the number of iterations around the main computational loop to obtain convergence using the scheme I, II, III, IV, or V. The total elapsed time to load the program, call in the data bank and compute the 11 cases is shown at the bottom of the respective columns I, II, III, IV, or V. The time shown includes all time necessary for I/O operations so it is only a relative measure of computing speed. The time figures do not include time to run the property calculation satellite program.

TABLE D-1. - Comparison of running time for five distinct sequential guessing schemes used with present algorithm to solve eleven typical problems

Temp K	Scheme I: OLD ANS → NEW GUESS		Scheme II: $X_3=X_2X_2/X_1$ $N_3=N_2N_2/N_1$		Scheme III: $X_3=X_2X_2/X_1$		Scheme IV: $\ln(X_3)$ $\ln(N_3)$		Scheme V: $\ln(X_3)$		N_{gas}	N_{slag}	N_{seed}
	INV	ITR	INV	ITR	INV	ITR	INV	ITR	INV	ITR			
2500	5	10	5	10	5	10	5	10	5	10	$0.5526_{10}+4$	$0.0000_{10}+0$	$0.0000_{10}+0$
2400	8	9	8	9	8	9	8	9	8	9	$.5472_{10}+4$	$.3187_{10}+1$	$.0000_{10}+4$
2300	8	11	3	6	3	6	3	6	3	6	$.5430_{10}+4$	$.4957_{10}+1$	$.0000_{10}+0$
2000	14	18	23	28	22	25	4	9	3	8	$.5365_{10}+4$	$.5671_{10}+1$	$.0000_{10}+0$
1800	25	28	3	8	3	8	4	9	4	9	$.5348_{10}+4$	$.5743_{10}+1$	$.0000_{10}+0$
1700	9	11	5	10	5	10	3	8	3	8	$.5345_{10}+4$	$.5770_{10}+1$	$.0000_{10}+0$
1600	7	10	3	8	3	8	2	7	2	7	$.5344_{10}+4$	$.5788_{10}+1$	$.0000_{10}+0$
1500	12	20	6	11	6	11	6	11	6	11	$.5326_{10}+4$	$.5780_{10}+1$	$.6859_{10}+1$
1400	13	18	5	11	5	11	5	11	5	11	$.5320_{10}+4$	$.5759_{10}+1$	$.9359_{10}+1$
1200	30	36	31	36	28	33	7	16	7	16	$.5318_{10}+4$	$.5756_{10}+1$	$.1003_{10}+2$
1000	68	78	18	27	17	25	5	15	5	17	$.5318_{10}+4$	$.5714_{10}+1$	$.1035_{10}+2$
Elapsed time...	19:16		11:38		11:07		6:44		6:41		-	-	-

Numerous conclusions are to be drawn from table D-1:

1. Scheme V is the fastest both for total time to solve the 11 composition problems and also the fastest for all but one individual problem.

2. Scheme IV is as fast as scheme V except that in temperature ranges where there is sharp curvature in the total number of moles in a condensed phase, the scheme may result in overestimation of the number of moles in a condensed phase. The program takes a long time to recover from such overestimates (compare the schemes III and IV at 1200 K).

3. At temperatures where the overestimate problem does not occur, schemes IV and V are equally efficient (as are II and III, to each other), even though it might seem that the careful guessing of quantities in condensed phases might help scheme IV over scheme V (and scheme II over scheme III).

4. A guess of 0 mole in a condensed phase does not of itself cause an appreciable slowdown in the calculation for a given temperature when the guesses for the components are good. (See schemes IV and V, 1600 K.)

5. Both schemes IV and V are faster than schemes II and III, particularly when temperatures are not uniformly spaced. (Compare total time and schemes II, III, IV, and V at 2000 K.)

6. Scheme I is inferior to other schemes in the large and for particular temperatures, except overestimates of N_k's cannot occur. Scheme V, of course, shares this advantage with scheme I.

Finally, we give the complete calculated compositions for the 11 cases mentioned, as an example of the capability of the program when used with a large data bank.

The fact that the cesium input is zero for each problem demonstrates that the program avoids the implied Jacobian singularity.

The reader concerned with the long elapsed times shown in D-1 should note that the larger current machines (6600, 360-75, etc.) have cycle times which are easily 20 times less than the cycle time of the machine on which these calculations were made. Another consideration is that the time for an equilibrium calculation is virtually proportional to the cube of the matrix size. On this basis, the problems demonstrated here are necessarily 11.94 times slower than would be simple 7-element gas phase problems ($16^3/7^3 = 11.94$), run on the same machine with the same program.

```
U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                         5 10

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION   22%ASH
     .3988≠+02 AR      .3000≠ 00 ALO2     .1230≠+04 CO2     .7000≠-01 CA      .2800≠ 00 CL2     .0000≠+00 CS      .9500≠ 00 FE
     .6502≠+03 H2      .2900≠+02 K        .3396≠+04 N2      .1500≠ 00 NA      .3492≠+03 O2      .5000≠+01 S2      .4480≠+01 SIO2

PRESSURE =  1.00 ATM.  TEMPERATURE = 2500 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......     .3988≠+02  AR     .2127≠-02  ALO2   .9827≠+03  CO2    .8162≠-03  CA     .4668≠-08  CL2    .0000≠+00  CS
    .3478≠ 00  FE      .2445≠+02  H2     .1452≠+02  K      .3378≠+04  N2     .1078≠ 00  NA     .1151≠+03  O2     .1110≠-05  S2
    .6468≠ 00  SIO2    .1113≠ 00  E-     .4220≠-05 AL      .1569≠-03 ALO     .2923≠ 00 AL(OH)2 .3448≠-08 AL2O   .2473≠+03 CO
    .2894≠-04 C O S    .6918≠-01 CAOH    .1721≠-01 CL      .0000≠+00 CSCL    .0000≠+00 CS O    .0000≠+00 CSOH    .4577≠ 00 FEO
    .1445≠ 00 FE(OH)2 .9212≠+01 H        .6514≠-01 HCL     .5910≠+03 H2O     .7238≠-04 H2S     .4701≠ 00 KCL     .2673≠ 00 KO
    .1362≠+02 KOH      .1260≠-02 N       .1353≠-04 NH3     .3696≠+02 NO      .9445≠-02 NO2     .1200≠-02 NACL    .1909≠-02 NAO
    .3907≠-01 NAOH     .1147≠+02 O       .4556≠+02 OH      .3481≠-02 S       .3698≠ 00 SO      .9622≠+01 SO2     .2585≠-02 SO3
    .1800≠-06 SI       .3833≠+01 SIO     .5431≠-02 ALO2-   .5260≠-07 CN-     .0000≠+00 CO2-    .6320≠-02 CL-     .0000≠+00 CS+
    .1315≠ 00 K+       .2976≠-05 NO-     .4655≠-04 NO2-    .2402≠-04 NA+     .6755≠-03 O-      .5528≠-02 OH-     .1659≠-03 O2-
    .1011≠-05 SH-      .8688≠-05 SO-     .2066≠-02 SO2-
  GLASS ..........     .0000≠+00 AL2O3 L .0000≠+00 MULLITE .0000≠+00 CAO   L .0000≠+00 CSOH  L .0000≠+00 FEAL2O4L.0000≠+00 FEO   L
    .0000≠+00 KALO2 L .0000≠+00 K2SIO3 L.0000≠+00 NAOH  L .0000≠+00 SIO2  L
  SULF. AND CARB..     .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......     .7216≠-02  AR     .3849≠-06  ALO2   .1778≠ 00  CO2    .1477≠-06  CA     .8447≠-12  CL2    .0000≠+00  CS
    .6294≠-04  FE      .4425≠-02  H2     .2627≠-02  K      .6112≠ 00  N2     .1951≠-04  NA     .2082≠-01  O2     .2008≠-09  S2
    .1170≠-03  SIO2    .2014≠-04  E-     .7636≠-09 AL      .2839≠-07 ALO     .5289≠-04 AL(OH)2 .6239≠-12 AL2O   .4475≠-01 CO
    .5237≠-08 C O S    .1252≠-04 CAOH    .3114≠-05 CL      .0000≠+00 CSCL    .0000≠+00 CS O    .0000≠+00 CSOH    .8282≠-04 FEO
    .2614≠-04 FE(OH)2 .1667≠-02 H        .1179≠-04 HCL     .1069≠ 00 H2O     .1310≠-07 H2S     .8507≠-04 KCL     .4836≠-04 KO
    .2464≠-02 KOH      .2280≠-06 N       .2448≠-08 NH3     .6688≠-02 NO      .1709≠-05 NO2     .2171≠-06 NACL    .3453≠-06 NAO
    .7070≠-05 NAOH     .2076≠-02 O       .8245≠-02 OH      .6300≠-06 S       .6692≠-04 SO      .1741≠-02 SO2     .4678≠-06 SO3
    .3257≠-10 SI       .6936≠-03 SIO     .9828≠-06 ALO2-   .9517≠-11 CN-     .0000≠+00 CO2-    .1144≠-05 CL-     .0000≠+00 CS+
    .2379≠-04 K+       .5385≠-09 NO-     .8423≠-08 NO2-    .4347≠-08 NA+     .1222≠-06 O-      .1000≠-05 OH-     .3002≠-07 O2-
    .1829≠-09 SH-      .1572≠-08 SO-     .3739≠-06 SO2-
  GLASS ..........     .0000≠+00 AL2O3 L .0000≠+00 MULLITE .0000≠+00 CAO   L .0000≠+00 CSOH  L .0000≠+00 FEAL2O4L.0000≠+00 FEO   L
    .0000≠+00 KALO2 L .0000≠+00 K2SIO3 L.0000≠+00 NAOH  L .0000≠+00 SIO2  L
  SULF. AND CARB..     .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C


                                                  IDEALGAS    GLASS ..    SULF. AN    MIXTURE
MOLAR QUANTITY                    (GRAM-MOLES)    .5526≠+04   .0000≠+00   .0000≠+00   .5526≠+04
AVERAGE MOLECULAR WEIGHT                 (AMU)    .2989≠+02   .0000≠+00   .0000≠+00   .2989≠+02
MASS                               (KILOGRAMS)    .1652≠+03   .0000≠+00   .0000≠+00   .1652≠+03
VOLUME                          (CUBIC-METERS)    .1134≠+04   .0000≠+00   .0000≠+00   .1134≠+04
DENSITY             (KILOGRAMS/CUBIC METER)       .1457≠ 00   .0000≠+00   .0000≠+00   .1457≠ 00
ENTROPY                 (GRAMCALORIES/DEGK)       .3746≠+06   .0000≠+00   .0000≠+00   .3746≠+06
REACTION ENTHALPY            (KILOCALORIES)      -.1927≠+05   .0000≠+00   .0000≠+00  -.1927≠+05
HEAT OF FORMATION            (KILOCALORIES)      -.1320≠+06   .0000≠+00   .0000≠+00  -.1320≠+06
SENSIBLE HEAT                (KILOCALORIES)       .1127≠+06   .0000≠+00   .0000≠+00   .1127≠+06
FROZEN CP                (GMCAL/GMMOL-DEGK)       .1024≠+02   .0000≠+00   .0000≠+00   .1024≠+02
ADIABATIC EXPANSION COEFFICIENT                   .1241≠ +1    SONIC SPEED (METERS/SECOND)          .9289≠ +3

DEBYE LENGTH            (METERS).38428≠-06    ELECTRON DENSITY      (PER M↑3).59113≠+20   COLLISION FREQUENCY  (PER SEC).24220≠+12
COEFFICIENTS FOR OHM,S LAW..   SIGMA = SCALAR COND  (MHO/METER)    .6880≠+01     BETA1     (SQM-VOLT/NEWTON)          -.1056≠ 00
BETA2  (ASSUMING ZERO ION SLIP)          (SQM-VOLT/TESLA-NEWTON)   .0000≠+00     THETA1      (VOLT/DEGK)              -.2318≠-05
MAGNETIC INDUCTION (ABS B)        (TESLA)  .0000≠+00   .2000≠+01   .4000≠+01   .6000≠+01   .8000≠+01   .1000≠+02   .1200≠+02
CHI                      (METER-OHM/TESLA)  .1056≠ 00   .1056≠ 00   .1056≠ 00   .1056≠ 00   .1056≠ 00   .1056≠ 00   .1056≠ 00
HALL PARAMETER                              .0000≠+00   .1453≠+01   .2906≠+01   .4359≠+01   .5812≠+01   .7264≠+01   .8717≠+01
PSI                 (METER-OHM/SQ TESLA)  .1750≠-04   .7573≠-05   .2803≠-05   .1368≠-05   .7965≠-06   .5183≠-06   .3632≠-06
THETA2                (VOLT/TESLA-DEGK)  .1327≠-05   .5743≠-06   .2126≠-06   .1037≠-06   .6040≠-07   .3930≠-07   .2754≠-07
THETA3              (VOLT/SQ TESLA-DEGK) -.7595≠-06  -.3287≠-06  -.1217≠-06  -.5936≠-07  -.3457≠-07  -.2250≠-07  -.1576≠-07
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U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                       8  9

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION   22%ASH
    .3988≠+02 AR       .3000≠ 00 ALO2      .1230≠+04 CO2       .7000≠-01 CA       .2800≠ 00 CL2      .0000≠+00 CS       .9500≠ 00 FE
    .6502≠+03 H2       .2900≠+02 K         .3396≠+04 N2        .1500≠ 00 NA       .3492≠+03 O2       .5000≠+01 S2       .4480≠+01 SIO2

PRESSURE =  1.00 ATM,  TEMPERATURE = 2400 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......     .3988≠+02  AR      .3772≠-03  ALO2    .1053≠+04  CO2     .1434≠-03  CA      .2161≠-08  CL2     .0000≠+00  CS
    .1445≠ 00  FE      .1754≠+02  H2      .1221≠+02  K       .3383≠+04  N2      .9887≠-01  NA      .8505≠+02  O2      .4894≠-06  S2
    .3337≠ 00  SIO2    .6359≠-01  E-      .3664≠-06 AL       .1900≠-04 ALO      .1006≠ 00 AL(OH)2 .1124≠-09 AL2O    .1769≠+03 CO
    .1627≠-04 C O S    .1992≠-01 CAOH     .9024≠-02 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .2330≠ 00 FEO
    .1397≠ 00 FE(OH)2  .4911≠+01 H        .4543≠-01 HCL      .6065≠+03 H2O      .4140≠-04 H2S      .4999≠ 00 KCL      .2015≠ 00 KO
    .1593≠+02 KOH      .4784≠-03 N        .9240≠-05 NH3      .2658≠+02 NO       .6565≠-02 NO2      .1350≠-02 NACL     .1591≠-02 NAO
    .4818≠-01 NAOH     .5874≠+01 O        .3083≠+02 OH       .1482≠-02 S        .2375≠ 00 SO       .9757≠+01 SO2      .2724≠-02 SO3
    .2740≠-07 SI       .1544≠+01 SIO      .1358≠-02 ALO2-    .1953≠-07 CN-      .0000≠+00 CO2-     .4284≠-02 CL-      .0000≠+00 CS+
    .7470≠-01 K+       .1373≠-05 NO-      .3263≠-04 NO2-     .1276≠-04 NA+      .2932≠-03 O-       .3413≠-02 OH-      .8510≠-04 O2-
    .4842≠-06 SH-      .4344≠-05 SO-      .1655≠-02 SO2-
  GLASS ..........     .8118≠-01 AL2O3 L .1957≠-02 MULLITE .4994≠-01 CAO    L .0000≠+00 CSOH   L .5558≠-03 FEAL2O4L.4322≠ 00 FEO    L
    .2245≠-01 KALO2 L .3065≠-01 K2SIO3 L.1945≠-05 NAOH   L .2568≠+01 SIO2   L
  SULF. AND CARB..     .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......     .7289≠-02  AR      .6894≠-07  ALO2    .1925≠ 00  CO2     .2620≠-07  CA      .3950≠-12  CL2     .0000≠+00  CS
    .2640≠-04  FE      .3206≠-02  H2      .2231≠-02  K       .6182≠ 00  N2      .1807≠-04  NA      .1554≠-01  O2      .8944≠-10  S2
    .6100≠-04  SIO2    .1162≠-04  E-      .6697≠-10 AL       .3473≠-08 ALO      .1839≠-04 AL(OH)2 .2054≠-13 AL2O    .3233≠-01 CO
    .2974≠-08 C O S    .3641≠-05 CAOH     .1649≠-05 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .4259≠-04 FEO
    .2554≠-04 FE(OH)2  .8975≠-03 H        .8303≠-05 HCL      .1109≠ 00 H2O      .7566≠-08 H2S      .9137≠-04 KCL      .3683≠-04 KO
    .2912≠-02 KOH      .8743≠-07 N        .1689≠-08 NH3      .4857≠-02 NO       .1200≠-05 NO2      .2468≠-06 NACL     .2908≠-06 NAO
    .8805≠-05 NAOH     .1073≠-02 O        .5634≠-02 OH       .2709≠-06 S        .4340≠-04 SO       .1783≠-02 SO2      .4978≠-06 SO3
    .5007≠-11 SI       .2822≠-03 SIO      .2481≠-06 ALO2-    .3570≠-11 CN-      .0000≠+00 CO2-     .7830≠-06 CL-      .0000≠+00 CS+
    .1365≠-04 K+       .2510≠-09 NO-      .5963≠-08 NO2-     .2332≠-08 NA+      .5358≠-07 O-       .6238≠-06 OH-      .1555≠-07 O2-
    .8850≠-10 SH-      .7940≠-09 SO-      .3024≠-06 SO2-
  GLASS ..........     .2548≠-01 AL2O3 L .6140≠-03 MULLITE .1567≠-01 CAO    L .0000≠+00 CSOH   L .1744≠-03 FEAL2O4L.1356≠ 00 FEO    L
    .7046≠-02 KALO2 L .9617≠-02 K2SIO3 L.6105≠-06 NAOH   L .8058≠ 00 SIO2   L
  SULF. AND CARB..     .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

                                                   IDEALGAS     GLASS ..     SULF. AN     MIXTURE
MOLAR QUANTITY                      (GRAM-MOLES)   .5472≠+04    .3187≠+01    .0000≠+00    .5475≠+04
AVERAGE MOLECULAR WEIGHT                   (AMU)   .3015≠+02    .6410≠+02    .0000≠+00    .3017≠+02
MASS                                 (KILOGRAMS)   .1650≠+03    .2043≠ 00    .0000≠+00    .1652≠+03
VOLUME                            (CUBIC-METERS)   .1078≠+04    .8166≠-04    .0000≠+00    .1078≠+04
DENSITY                (KILOGRAMS/CUBIC METER)     .1531≠ 00    .2502≠+04    .0000≠+00    .1533≠ 00
ENTROPY                   (GRAMCALORIES/DEGK)      .3691≠+06    .1557≠+03    .0000≠+00    .3693≠+06
REACTION ENTHALPY                (KILOCALORIES)   -.3164≠+05   -.5162≠+03    .0000≠+00   -.3216≠+05
HEAT OF FORMATION                (KILOCALORIES)   -.1387≠+06   -.6370≠+03    .0000≠+00   -.1393≠+06
SENSIBLE HEAT                    (KILOCALORIES)    .1071≠+06    .1208≠+03    .0000≠+00    .1072≠+06
FROZEN CP                     (GMCAL/GMMOL-DEGK)   .1031≠+02    .2074≠+02    .0000≠+00    .1031≠+02
ADIABATIC EXPANSION COEFFICIENT                    .1239≠ +1     SONIC SPEED (METERS/SECOND)            .9055≠ +3

DEBYE LENGTH               (METERS).48809≠-06   ELECTRON DENSITY      (PER M↑3).35541≠+20   COLLISION FREQUENCY  (PER SEC).25042≠+12
COEFFICIENTS FOR OHM,S LAW..    SIGMA = SCALAR COND   (MHO/METER)    .4002≠+01     BETA1      (SQM-VOLT/NEWTON)              -.1756≠ 00
BETA2  (ASSUMING ZERO ION SLIP)             (SQM-VOLT/TESLA-NEWTON)  .0000≠+00      THETA1      (VOLT/DEGK)                 -.3215≠-05
MAGNETIC INDUCTION (ABS B)          (TESLA)  .0000≠+00    .2000≠+01    .4000≠+01    .6000≠+01    .8000≠+01    .1000≠+02    .1200≠+02
CHI                       (METER-OHM/TESLA)  .1757≠ 00    .1757≠ 00    .1756≠ 00    .1756≠ 00    .1756≠ 00    .1756≠ 00    .1756≠ 00
HALL PARAMETER                               .0000≠+00    .1406≠+01    .2812≠+01    .4217≠+01    .5623≠+01    .7028≠+01    .8434≠+01
PSI                    (METER-OHM/SQ TESLA)  .5578≠-04    .2423≠-04    .8986≠-05    .4387≠-05    .2555≠-05    .1663≠-05    .1165≠-05
THETA2                    (VOLT/TESLA-DEGK)  .1834≠-05    .7968≠-06    .2955≠-06    .1442≠-06    .8402≠-07    .5467≠-07    .3832≠-07
THETA3                 (VOLT/SQ TESLA-DEGK) -.1046≠-05   -.4545≠-06   -.1686≠-06   -.8228≠-07   -.4793≠-07   -.3119≠-07   -.2186≠-07
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U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                              3  6

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION   22%ASH
    .3988≠+02 AR       .3000≠ 00 ALO2     .1230≠+04 CO2      .7000≠-01 CA       .2800≠ 00 CL2      .0000≠+00 CS       .9500≠ 00 FE
    .6502≠+03 H2       .2900≠+02 K        .3396≠+04 N2       .1500≠ 00 NA       .3492≠+03 O2       .5000≠+01 S2       .4480≠+01 SIO2

PRESSURE =  1.00 ATM,  TEMPERATURE = 2300 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......     .3988≠+02  AR      .8802≠-04  ALO2    .1109≠+04  CO2     .2953≠-04  CA      .9442≠-09  CL2     .0000≠+00  CS
    .4575≠-01  FE      .1216≠+02  H2      .9820≠+01  K       .3387≠+04  N2      .8824≠-01  NA      .6060≠+02  O2      .2025≠-06  S2
    .9476≠-01  SIO2    .3389≠-01  E-      .3971≠-07 AL       .2950≠-05 ALO      .4804≠-01 AL(OH)2 .6439≠-11 AL2O     .1206≠+03 CO
    .8556≠-05 C O S    .6952≠-02 CAOH     .4497≠-02 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .9126≠-01 FEO
    .1084≠ 00 FE(OH)2 .2476≠+01 H        .3082≠-01 HCL      .6175≠+03 H2O      .2253≠-04 H2S      .5204≠ 00 KCL      .1428≠ 00 KO
    .1820≠+02 KOH      .1672≠-03 N        .6060≠-05 NH3      .1841≠+02 NO       .4365≠-02 NO2      .1513≠-02 NACL     .1269≠-02 NAO
    .5897≠-01 NAOH     .2829≠+01 O        .1998≠+02 OH       .5897≠-03 S        .1467≠ 00 SO       .9849≠+01 SO2      .2846≠-02 SO3
    .2103≠-08 SI       .3387≠ 00 SIO      .4454≠-03 ALO2-    .6384≠-08 CN-      .0000≠+00 CO2-     .2736≠-02 CL-      .0000≠+00 CS+
    .4044≠-01 K+       .5705≠-06 NO-      .2134≠-04 NO2-     .6478≠-05 NA+      .1148≠-03 O-       .1945≠-02 OH-      .3971≠-04 O2-
    .2123≠-06 SH-      .1994≠-05 SO-      .1258≠-02 SO2-
  GLASS ..........     .9884≠-01 AL2O3 L  .1253≠-02 MULLITE .6302≠-01 CAO    L .0000≠+00 CSOH  L .3592≠-03 FEAL2O4L.7042≠ 00 FEO     L
    .4552≠-01 KALO2 L .1179≠ 00 K2SIO3 L.5343≠-05 NAOH   L .3926≠+01 SIO2   L
  SULF. AND CARB..     .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......     .7344≠-02  AR      .1621≠-07  ALO2    .2043≠ 00  CO2     .5438≠-08  CA      .1739≠-12  CL2     .0000≠+00  CS
    .8426≠-05  FE      .2239≠-02  H2      .1808≠-02  K       .6237≠ 00  N2      .1625≠-04  NA      .1116≠-01  O2      .3730≠-10  S2
    .1745≠-04  SIO2    .6240≠-05  E-      .7313≠-11 AL       .5432≠-09 ALO      .8847≠-05 AL(OH)2 .1186≠-14 AL2O     .2220≠-01 CO
    .1576≠-08 C O S    .1280≠-05 CAOH     .8281≠-06 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .1681≠-04 FEO
    .1997≠-04 FE(OH)2 .4560≠-03 H        .5676≠-05 HCL      .1137≠ 00 H2O      .4148≠-08 H2S      .9584≠-04 KCL      .2630≠-04 KO
    .3351≠-02 KOH      .3079≠-07 N        .1116≠-08 NH3      .3391≠-02 NO       .8038≠-06 NO2      .2785≠-06 NACL     .2336≠-06 NAO
    .1086≠-04 NAOH     .5210≠-03 O        .3680≠-02 OH       .1086≠-06 S        .2702≠-04 SO       .1814≠-02 SO2      .5240≠-06 SO3
    .3873≠-12 SI       .6237≠-04 SIO      .9203≠-07 ALO2-    .1176≠-11 CN-      .0000≠+00 CO2-     .5038≠-06 CL-      .0000≠+00 CS+
    .7447≠-05 K+       .1051≠-09 NO-      .3930≠-08 NO2-     .1193≠-08 NA+      .2113≠-07 O-       .3581≠-06 OH-      .7312≠-08 O2-
    .3909≠-10 SH-      .3672≠-09 SO-      .2316≠-06 SO2-
  GLASS ..........     .1994≠-01 AL2O3 L  .2527≠-03 MULLITE .1271≠-01 CAO    L .0000≠+00 CSOH  L .7245≠-04 FEAL2O4L.1421≠ 00 FEO     L
    .9183≠-02 KALO2 L .2378≠-01 K2SIO3 L.1078≠-05 NAOH   L .7920≠ 00 SIO2   L
  SULF. AND CARB..     .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

                                                  IDEALGAS     GLASS ..     SULF. AN      MIXTURE
MOLAR QUANTITY                    (GRAM-MOLES)    .5430≠+04    .4957≠+01    .0000≠+00    .5435≠+04
AVERAGE MOLECULAR WEIGHT                 (AMU)    .3036≠+02    .6523≠+02    .0000≠+00    .3039≠+02
MASS                               (KILOGRAMS)    .1649≠+03    .3234≠ 00    .0000≠+00    .1652≠+03
VOLUME                          (CUBIC-METERS)    .1025≠+04    .1279≠-03    .0000≠+00    .1025≠+04
DENSITY             (KILOGRAMS/CUBIC METER)       .1608≠ 00    .2527≠+04    .0000≠+00    .1612≠ 00
ENTROPY                (GRAMCALORIES/DEGK)        .3643≠+06    .2428≠+03    .0000≠+00    .3646≠+06
REACTION ENTHALPY             (KILOCALORIES)     -.4244≠+05   -.8108≠+03    .0000≠+00   -.4325≠+05
HEAT OF FORMATION             (KILOCALORIES)     -.1439≠+06   -.9907≠+03    .0000≠+00   -.1449≠+06
SENSIBLE HEAT                 (KILOCALORIES)      .1014≠+06    .1799≠+03    .0000≠+00    .1016≠+06
FROZEN CP                (GMCAL/GMMOL-DEGK)       .1035≠+02    .2091≠+02    .0000≠+00    .1036≠+02
ADIABATIC EXPANSION COEFFICIENT                   .1238≠ +1     SONIC SPEED (METERS/SECOND)          .8829≠ +3

DEBYE LENGTH             (METERS).62968≠-06   ELECTRON DENSITY      (PER M↑3).19913≠+20   COLLISION FREQUENCY  (PER SEC).26065≠+12
COEFFICIENTS FOR OHM,S LAW..   SIGMA = SCALAR COND  (MHO/METER)    .2155≠+01      BETA1     (SQM-VOLT/NEWTON)               -.3134≠ 00
BETA2  (ASSUMING ZERO ION SLIP)           (SQM-VOLT/TESLA-NEWTON)   .0000≠+00      THETA1       (VOLT/DEGK)                  -.4456≠-05
MAGNETIC INDUCTION (ABS B)           (TESLA)  .0000≠+00    .2000≠+01    .4000≠+01    .6000≠+01    .8000≠+01    .1000≠+02    .1200≠+02
CHI                       (METER-OHM/TESLA)  .3138≠ 00    .3136≠ 00    .3135≠ 00    .3135≠ 00    .3135≠ 00    .3135≠ 00    .3135≠ 00
HALL PARAMETER                               .0000≠+00    .1352≠+01    .2703≠+01    .4054≠+01    .5405≠+01    .6757≠+01    .8108≠+01
PSI                    (METER-OHM/SQ TESLA)  .1890≠-03    .8324≠-04    .3107≠-04    .1520≠-04    .8859≠-05    .5767≠-05    .4043≠-05
THETA2                    (VOLT/TESLA-DEGK)  .2512≠-05    .1106≠-05    .4129≠-06    .2019≠-06    .1177≠-06    .7664≠-07    .5372≠-07
THETA3                 (VOLT/SQ TESLA-DEGK) -.1416≠-05   -.6236≠-06   -.2328≠-06   -.1138≠-06   -.6637≠-07   -.4321≠-07   -.3029≠-07
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U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                                   3  8

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION   22%ASH
    .3988≠+02 AR       .3000≠ 00 ALO2      .1230≠+04 CO2      .7000≠-01 CA       .2800≠ 00 CL2      .0000≠+00 CS       .9500≠ 00 FE
    .6502≠+03 H2       .2900≠+02 K         .3396≠+04 N2       .1500≠ 00 NA       .3492≠+03 O2       .5000≠+01 S2       .4480≠+01 SIO2

PRESSURE =  1.00 ATM,  TEMPERATURE = 2000 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......    .3988≠+02  AR      .5878≠-06  ALO2     .1203≠+04  CO2     .1970≠-06  CA      .7036≠-10  CL2     .0000≠+00  CS
    .6683≠-03  FE     .3101≠+01  H2      .3409≠+01  K        .3393≠+04  N2      .4844≠-01  NA      .1865≠+02  O2      .7581≠-08  S2
    .7127≠-03  SIO2   .2995≠-02  E-      .1637≠-10 AL        .4505≠-08 ALO      .3873≠-02 AL(OH)2 .3246≠-15 AL2O    .2666≠+02 CO
    .7094≠-06 C O S   .3047≠-03 CAOH     .4492≠-03 CL        .0000≠+00 CSCL     .0000≠+00 CS O    .0000≠+00 CSOH    .2894≠-02 FEO
    .3926≠-01 FE(OH)2 .2092≠ 00 H        .9003≠-02 HCL       .6339≠+03 H2O      .2263≠-05 H2S     .5477≠ 00 KCL     .3186≠-01 KO
    .2189≠+02 KOH     .3838≠-05 N        .1213≠-05 NH3       .5031≠+01 NO       .1045≠-02 NO2     .2249≠-02 NACL    .4718≠-03 NAO
    .9880≠-01 NAOH    .2099≠ 00 O        .4189≠+01 OH        .2036≠-04 S        .2501≠-01 SO      .9971≠+01 SO2     .3321≠-02 SO3
    .1374≠-12 SI      .9758≠-03 SIO      .8320≠-05 ALO2-     .7957≠-10 CN-      .0000≠+00 CO2-    .5461≠-03 CL-     .0000≠+00 CS+
    .4137≠-02 K+      .2011≠-07 NO-      .3856≠-05 NO2-      .5718≠-06 NA+      .3281≠-05 O-      .2080≠-03 OH-     .2141≠-05 O2-
    .8157≠-08 SH-     .9399≠-07 SO-      .3703≠-03 SO2-
  GLASS ..........    .7916≠-01 AL2O3 L .1412≠-03 MULLITE .6970≠-01 CAO    L .0000≠+00 CSOH   L .2664≠-04 FEAL2O4L.9072≠ 00 FEO    L
    .1369≠ 00 KALO2 L .1492≠+01 K2SIO3 L.3916≠-04 NAOH   L .2986≠+01 SIO2   L
  SULF. AND CARB..    .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......    .7434≠-02  AR      .1096≠-09  ALO2     .2243≠ 00  CO2     .3673≠-10  CA      .1312≠-13  CL2     .0000≠+00  CS
    .1246≠-06  FE     .5780≠-03  H2      .6355≠-03  K        .6326≠ 00  N2      .9029≠-05  NA      .3476≠-02  O2      .1413≠-11  S2
    .1329≠-06  SIO2   .5584≠-06  E-      .3052≠-14 AL        .8398≠-12 ALO      .7220≠-06 AL(OH)2 .6051≠-19 AL2O    .4969≠-02 CO
    .1322≠-09 C O S   .5680≠-07 CAOH     .8373≠-07 CL        .0000≠+00 CSCL     .0000≠+00 CS O    .0000≠+00 CSOH    .5394≠-06 FEO
    .7318≠-05 FE(OH)2 .3900≠-04 H        .1678≠-05 HCL       .1182≠ 00 H2O      .4217≠-09 H2S     .1021≠-03 KCL     .5938≠-05 KO
    .4080≠-02 KOH     .7154≠-09 N        .2261≠-09 NH3       .9378≠-03 NO       .1948≠-06 NO2     .4193≠-06 NACL    .8794≠-07 NAO
    .1842≠-04 NAOH    .3913≠-04 O        .7808≠-03 OH        .3794≠-08 S        .4663≠-05 SO      .1859≠-02 SO2     .6191≠-06 SO3
    .2560≠-16 SI      .1819≠-06 SIO      .1551≠-08 ALO2-     .1483≠-13 CN-      .0000≠+00 CO2-    .1018≠-06 CL-     .0000≠+00 CS+
    .7712≠-06 K+      .3749≠-11 NO-      .7188≠-09 NO2-      .1066≠-09 NA+      .6117≠-09 O-      .3877≠-07 OH-     .3991≠-09 O2-
    .1520≠-11 SH-     .1752≠-10 SO-      .6903≠-07 SO2-
  GLASS ..........    .1396≠-01 AL2O3 L .2490≠-04 MULLITE .1229≠-01 CAO    L .0000≠+00 CSOH   L .4697≠-05 FEAL2O4L.1600≠ 00 FEO    L
    .2414≠-01 KALO2 L .2631≠ 00 K2SIO3 L.6905≠-05 NAOH   L .5265≠ 00 SIO2   L
  SULF. AND CARB..    .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

                                                     IDEALGAS     GLASS ..     SULF. AN     MIXTURE
MOLAR QUANTITY                       (GRAM-MOLES)    .5365≠+04    .5671≠+01    .0000≠+00    .5370≠+04
AVERAGE MOLECULAR WEIGHT                    (AMU)    .3070≠+02    .8822≠+02    .0000≠+00    .3076≠+02
MASS                                  (KILOGRAMS)    .1647≠+03    .5003≠ 00    .0000≠+00    .1652≠+03
VOLUME                            (CUBIC-METERS)     .8805≠+03    .1717≠-03    .0000≠+00    .8805≠+03
DENSITY                (KILOGRAMS/CUBIC METER)       .1870≠ 00    .2914≠+04    .0000≠+00    .1876≠ 00
ENTROPY                    (GRAMCALORIES/DEGK)       .3525≠+06    .3727≠+03    .0000≠+00    .3528≠+06
REACTION ENTHALPY                (KILOCALORIES)     -.6751≠+05   -.1081≠+04    .0000≠+00   -.6859≠+05
HEAT OF FORMATION                (KILOCALORIES)     -.1522≠+06   -.1307≠+04    .0000≠+00   -.1535≠+06
SENSIBLE HEAT                    (KILOCALORIES)      .8473≠+05    .2260≠+03    .0000≠+00    .8495≠+05
FROZEN CP                  (GMCAL/GMMOL-DEGK)        .1034≠+02    .2624≠+02    .0000≠+00    .1036≠+02
ADIABATIC EXPANSION COEFFICIENT                      .1238≠ +1    SONIC SPEED (METERS/SECOND)         .8189≠ +3

DEBYE LENGTH            (METERS).16239≠-05   ELECTRON DENSITY      (PER M+3).20491≠+19   COLLISION FREQUENCY   (PER SEC).29806≠+12
COEFFICIENTS FOR OHM,S LAW..   SIGMA = SCALAR COND   (MHO/METER)    .1947≠ 00     BETA1      (SQM-VOLT/NEWTON)              -.3046≠+01
BETA2  (ASSUMING ZERO ION SLIP)           (SQM-VOLT/TESLA-NEWTON)   .0000≠+00     THETA1       (VOLT/DEGK)                  -.9329≠-05
MAGNETIC INDUCTION (ABS B)         (TESLA)  .0000≠+00    .2000≠+01    .4000≠+01    .6000≠+01    .8000≠+01    .1000≠+02    .1200≠+02
CHI                      (METER-OHM/TESLA)  .3060≠+01    .3053≠+01    .3049≠+01    .3047≠+01    .3047≠+01    .3047≠+01    .3047≠+01
HALL PARAMETER                              .0000≠+00    .1189≠+01    .2375≠+01    .3561≠+01    .4747≠+01    .5933≠+01    .7119≠+01
PSI                   (METER-OHM/SQ TESLA)  .7571≠-02    .3564≠-02    .1377≠-02    .6809≠-03    .3987≠-03    .2601≠-03    .1825≠-03
THETA2                 (VOLT/TESLA-DEGK)    .4946≠-05    .2328≠-05    .8997≠-06    .4448≠-06    .2604≠-06    .1699≠-06    .1192≠-06
THETA3              (VOLT/SQ TESLA-DEGK)   -.2622≠-05   -.1234≠-05   -.4770≠-06   -.2358≠-06   -.1381≠-06   -.9008≠-07   -.6322≠-07
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U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                    4  9

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION   22%ASH
    .3988≠+02 AR      .3000≠ 00 ALO2     .1230≠+04 CO2      .7000≠-01 CA       .2800≠ 00 CL2      .0000≠+00 CS       .9500≠ 00 FE
    .6502≠+03 H2      .2900≠+02 K        .3396≠+04 N2       .1500≠ 00 NA       .3492≠+03 O2       .5000≠+01 S2       .4480≠+01 SIO2

PRESSURE =  1.00 ATM,  TEMPERATURE = 1800 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......    .3988≠+02  AR      .7089≠-08  ALO2    .1224≠+04  CO2     .2403≠-08  CA      .1310≠-10  CL2     .0000≠+00  CS
    .1424≠-04  FE     .8373≠ 00  H2      .1029≠+01  K       .3395≠+04  N2      .2223≠-01  NA      .8974≠+01  O2      .2652≠-09  S2
    .4880≠-05  SIO2   .3054≠-03  E-      .1406≠-13 AL       .1359≠-10 ALO      .3298≠-03 AL(OH)2 .3426≠-19 AL2O    .6060≠+01 CO
    .5334≠-07 C O S   .1960≠-04 CAOH     .8292≠-04 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .1349≠-03 FEO
    .1472≠-01 FE(OH)2 .2386≠-01 H        .3818≠-02 HCL      .6386≠+03 H2O      .2092≠-06 H2S      .5528≠ 00 KCL      .7525≠-02 KO
    .2018≠+02 KOH     .1558≠-06 N        .2475≠-06 NH3      .1904≠+01 NO       .4039≠-03 NO2      .3136≠-02 NACL     .1771≠-03 NAO
    .1243≠ 00 NAOH    .2646≠-01 O        .1175≠+01 OH       .8828≠-06 S        .4833≠-02 SO       .9991≠+01 SO2      .4335≠-02 SO3
    .1261≠-16 SI      .2565≠-05 SIO      .1854≠-06 ALO2-    .1052≠-11 CN-      .0000≠+00 CO2-     .1401≠-03 CL-      .0000≠+00 CS+
    .5723≠-03 K+      .1027≠-08 NO-      .9096≠-06 NO2-     .7182≠-07 NA+      .1414≠-06 O-       .2539≠-04 OH-      .1810≠-06 O2-
    .2766≠-09 SH-     .4699≠-08 SO-      .1001≠-03 SO2-
  GLASS ..........    .4156≠-01 AL2O3 L .1424≠-05 MULLITE .6998≠-01 CAO    L .0000≠+00 CSOH   L .1615≠-05 FEAL2O4L.9351≠ 00 FEO     L
    .2165≠ 00 KALO2 L .3506≠+01 K2SIO3 L.1601≠-03 NAOH   L .9736≠ 00 SIO2   L
  SULF. AND CARB..    .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......    .7456≠-02  AR      .1325≠-11  ALO2    .2288≠ 00  CO2     .4492≠-12  CA      .2449≠-14  CL2     .0000≠+00  CS
    .2662≠-08  FE     .1565≠-03  H2      .1923≠-03  K       .6348≠ 00  N2      .4156≠-05  NA      .1678≠-02  O2      .4958≠-13  S2
    .9124≠-09  SIO2   .5710≠-07  E-      .2628≠-17 AL       .2541≠-14 ALO      .6167≠-07 AL(OH)2 .6406≠-23 AL2O    .1133≠-02 CO
    .9973≠-11 C O S   .3665≠-08 CAOH     .1550≠-07 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .2521≠-07 FEO
    .2752≠-05 FE(OH)2 .4460≠-05 H        .7139≠-06 HCL      .1194≠ 00 H2O      .3911≠-10 H2S      .1034≠-03 KCL      .1407≠-05 KO
    .3773≠-02 KOH     .2913≠-10 N        .4627≠-10 NH3      .3561≠-03 NO       .7552≠-07 NO2      .5864≠-06 NACL     .3311≠-07 NAO
    .2324≠-04 NAOH    .4948≠-05 O        .2196≠-03 OH       .1651≠-09 S        .9037≠-06 SO       .1868≠-02 SO2      .8106≠-06 SO3
    .2357≠-20 SI      .4796≠-09 SIO      .3467≠-10 ALO2-    .1967≠-15 CN-      .0000≠+00 CO2-     .2619≠-07 CL-      .0000≠+00 CS+
    .1070≠-06 K+      .1920≠-12 NO-      .1701≠-09 NO2-     .1343≠-10 NA+      .2643≠-10 O-       .4747≠-08 OH-      .3384≠-10 O2-
    .5172≠-13 SH-     .8786≠-12 SO-      .1871≠-07 SO2-
  GLASS ..........    .7235≠-02 AL2O3 L .2480≠-06 MULLITE .1218≠-01 CAO    L .0000≠+00 CSOH   L .2812≠-06 FEAL2O4L.1628≠ 00 FEO     L
    .3770≠-01 KALO2 L .6105≠ 00 K2SIO3 L.2788≠-04 NAOH   L .1695≠ 00 SIO2   L
  SULF. AND CARB..    .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C


                                                             IDEALGAS     GLASS ..     SULF. AN     MIXTURE
MOLAR QUANTITY                          (GRAM-MOLES)         .5348≠+04    .5743≠+01    .0000≠+00    .5354≠+04
AVERAGE MOLECULAR WEIGHT                       (AMU)         .3075≠+02    .1212≠+03    .0000≠+00    .3085≠+02
MASS                                     (KILOGRAMS)         .1645≠+03    .6961≠ 00    .0000≠+00    .1652≠+03
VOLUME                                (CUBIC-METERS)         .7900≠+03    .2126≠-03    .0000≠+00    .7900≠+03
DENSITY                   (KILOGRAMS/CUBIC METER)            .2082≠ 00    .3274≠+04    .0000≠+00    .2091≠ 00
ENTROPY                      (GRAMCALORIES/DEGK)             .3455≠+06    .5110≠+03    .0000≠+00    .3460≠+06
REACTION ENTHALPY                  (KILOCALORIES)           -.8030≠+05   -.1330≠+04    .0000≠+00   -.8163≠+05
HEAT OF FORMATION                  (KILOCALORIES)           -.1540≠+06   -.1602≠+04    .0000≠+00   -.1556≠+06
SENSIBLE HEAT                      (KILOCALORIES)            .7367≠+05    .2719≠+03    .0000≠+00    .7394≠+05
FROZEN CP                      (GMCAL/GMMOL-DEGK)            .1023≠+02    .3406≠+02    .0000≠+00    .1026≠+02
ADIABATIC EXPANSION COEFFICIENT                              .1241≠ +1     SONIC SPEED (METERS/SECOND)          .7771≠ +3

DEBYE LENGTH                (METERS).36601≠-05    ELECTRON DENSITY      (PER M↑3).23284≠+18   COLLISION FREQUENCY  (PER SEC).33768≠+12
COEFFICIENTS FOR OHM,S LAW..   SIGMA = SCALAR COND  (MHO/METER)     .1962≠-01      BETA1     (SQM-VOLT/NEWTON)              -.2681≠+02
BETA2  (ASSUMING ZERO ION SLIP)              (SQM-VOLT/TESLA-NEWTON)     .0000≠+00       THETA1       (VOLT/DEGK)                  -.1310≠-04
MAGNETIC INDUCTION (ABS B)          (TESLA)  .0000≠+00    .2000≠+01    .4000≠+01    .6000≠+01    .8000≠+01    .1000≠+02    .1200≠+02
CHI                         (METER-OHM/TESLA)  .2705≠+02    .2693≠+02    .2686≠+02    .2683≠+02    .2682≠+02    .2682≠+02    .2681≠+02
HALL PARAMETER                               .0000≠+00    .1057≠+01    .2108≠+01    .3159≠+01    .4211≠+01    .5263≠+01    .6314≠+01
PSI                     (METER-OHM/SQ TESLA)  .1203≠ 00    .6191≠-01    .2521≠-01    .1268≠-01    .7477≠-02    .4895≠-02    .3442≠-02
THETA2                    (VOLT/TESLA-DEGK)  .6359≠-05    .3273≠-05    .1333≠-05    .6703≠-06    .3953≠-06    .2588≠-06    .1820≠-06
THETA3                 (VOLT/SQ TESLA-DEGK) -.3088≠-05   -.15[illegible]≠-05   -.6471≠-06   -.3255≠-06   -.1919≠-06   -.1256≠-06   -.8835≠-07
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U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                                    3  8

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION   22%ASH
    .3988≠+02 AR      .3000≠ 00 ALO2    .1230≠+04 CO2     .7000≠-01 CA      .2800≠ 00 CL2     .0000≠+00 CS      .9500≠ 00 FE
    .6502≠+03 H2      .2900≠+02 K       .3396≠+04 N2      .1500≠ 00 NA      .3492≠+03 O2      .5000≠+01 S2      .4480≠+01 SIO2

PRESSURE =  1.00 ATM,  TEMPERATURE = 1700 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......   .3988≠+02  AR     .4826≠-09  ALO2   .1228≠+04  CO2    .1608≠-09  CA     .5295≠-11  CL2    .0000≠+00  CS
    .1301≠-05  FE    .3486≠ 00  H2     .4871≠ 00  K      .3395≠+04  N2     .1252≠-01  NA     .7200≠+01  O2     .2415≠-10  S2
    .1770≠-06  SIO2  .7451≠-04  E-     .1634≠-15 AL      .3698≠-12 ALO     .6268≠-04 AL(OH)2 .9556≠-22 AL2O   .2267≠+01 CO
    .8432≠-08 C O S  .3673≠-05 CAOH    .3205≠-04 CL      .0000≠+00 CSCL    .0000≠+00 CS O    .0000≠+00 CSOH    .2162≠-04 FEO
    .8070≠-02 FE(OH)2 .6341≠-02 H      .2281≠-02 HCL     .6398≠+03 H2O     .3749≠-07 H2S     .5541≠ 00 KCL     .3431≠-02 KO
    .1943≠+02 KOH    .2363≠-07 N       .8281≠-07 NH3     .1197≠+01 NO      .2850≠-03 NO2     .3529≠-02 NACL    .9825≠-04 NAO
    .1335≠ 00 NAOH   .8702≠-02 O       .5846≠ 00 OH      .1131≠-06 S       .1648≠-02 SO      .9993≠+01 SO2     .5642≠-02 SO3
    .2942≠-19 SI     .4757≠-07 SIO     .1675≠-07 ALO2-   .6130≠-13 CN-     .0000≠+00 CO2-    .6056≠-04 CL-     .0000≠+00 CS+
    .1855≠-03 K+     .1830≠-09 NO-     .4427≠-06 NO2-    .2048≠-07 NA+     .2285≠-07 O-      .7147≠-05 OH-     .4815≠-07 O2-
    .2666≠-10 SH-    .6658≠-09 SO-     .4276≠-04 SO2-
  GLASS ..........   .2218≠-01 AL2O3 L .2154≠-07 MULLITE .7000≠-01 CAO   L .0000≠+00 CSOH  L .2222≠-06 FEAL2O4L.9419≠ 00 FEO    L
    .2556≠ 00 KALO2 L .4133≠+01 K2SIO3 L.3466≠-03 NAOH  L .3470≠ 00 SIO2  L
  SULF. AND CARB..   .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......   .7461≠-02  AR     .9030≠-13  ALO2   .2297≠ 00  CO2    .3008≠-13  CA     .9907≠-15  CL2    .0000≠+00  CS
    .2433≠-09  FE    .6523≠-04  H2     .9113≠-04  K      .6352≠ 00  N2     .2343≠-05  NA     .1347≠-02  O2     .4518≠-14  S2
    .3312≠-10  SIO2  .1394≠-07  E-     .3057≠-19 AL      .6918≠-16 ALO     .1173≠-07 AL(OH)2 .1788≠-25 AL2O   .4241≠-03 CO
    .1577≠-11 C O S  .6872≠-09 CAOH    .5996≠-08 CL      .0000≠+00 CSCL    .0000≠+00 CS O    .0000≠+00 CSOH    .4044≠-08 FEO
    .1510≠-05 FE(OH)2 .1186≠-05 H      .4268≠-06 HCL     .1197≠ 00 H2O     .7014≠-11 H2S     .1037≠-03 KCL     .6418≠-06 KO
    .3636≠-02 KOH    .4420≠-11 N       .1549≠-10 NH3     .2239≠-03 NO      .5331≠-07 NO2     .6603≠-06 NACL    .1838≠-07 NAO
    .2498≠-04 NAOH   .1628≠-05 O       .1094≠-03 OH      .2116≠-10 S       .3083≠-06 SO      .1870≠-02 SO2     .1056≠-05 SO3
    .5505≠-23 SI     .8900≠-11 SIO     .3133≠-11 ALO2-   .1147≠-16 CN-     .0000≠+00 CO2-    .1133≠-07 CL-     .0000≠+00 CS+
    .3470≠-07 K+     .3423≠-13 NO-     .8282≠-10 NO2-    .3831≠-11 NA+     .4275≠-11 O-      .1337≠-08 OH-     .9008≠-11 O2-
    .4989≠-14 SH-    .1246≠-12 SO-     .8001≠-08 SO2-
  GLASS ..........   .3843≠-02 AL2O3 L .3734≠-08 MULLITE .1213≠-01 CAO   L .0000≠+00 CSOH  L .3851≠-07 FEAL2O4L.1632≠ 00 FEO    L
    .4430≠-01 KALO2 L .7163≠ 00 K2SIO3 L.6006≠-04 NAOH  L .6014≠-01 SIO2  L
  SULF. AND CARB..   .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

                                                 IDEALGAS    GLASS ..    SULF. AN     MIXTURE
MOLAR QUANTITY                   (GRAM-MOLES)   .5345≠+04   .5770≠+01   .0000≠+00   .5351≠+04
AVERAGE MOLECULAR WEIGHT                (AMU)   .3076≠+02   .1313≠+03   .0000≠+00   .3087≠+02
MASS                              (KILOGRAMS)   .1644≠+03   .7575≠ 00   .0000≠+00   .1652≠+03
VOLUME                         (CUBIC-METERS)   .7456≠+03   .2257≠-03   .0000≠+00   .7456≠+03
DENSITY            (KILOGRAMS/CUBIC METER)      .2205≠ 00   .3355≠+04   .0000≠+00   .2215≠ 00
ENTROPY                (GRAMCALORIES/DEGK)      .3421≠+06   .5454≠+03   .0000≠+00   .3426≠+06
REACTION ENTHALPY              (KILOCALORIES)  -.8609≠+05  -.1420≠+04   .0000≠+00  -.8751≠+05
HEAT OF FORMATION              (KILOCALORIES)  -.1543≠+06  -.1695≠+04   .0000≠+00  -.1560≠+06
SENSIBLE HEAT                  (KILOCALORIES)   .6821≠+05   .2746≠+03   .0000≠+00   .6848≠+05
FROZEN CP                  (GMCAL/GMMOL-DEGK)   .1016≠+02   .3645≠+02   .0000≠+00   .1019≠+02
ADIABATIC EXPANSION COEFFICIENT                 .1243≠ +1    SONIC SPEED (METERS/SECOND)          .7558≠ +3

DEBYE LENGTH            (METERS).58140≠-05   ELECTRON DENSITY      (PER M↑3).60188≠+17   COLLISION FREQUENCY  (PER SEC).36032≠+12
COEFFICIENTS FOR OHM,S LAW..   SIGMA = SCALAR COND  (MHO/METER)    .4766≠-02    BETA1     (SQM-VOLT/NEWTON)             -.1037≠+03
BETA2  (ASSUMING ZERO ION SLIP)          (SQM-VOLT/TESLA-NEWTON)   .0000≠+00    THETA1      (VOLT/DEGK)                 -.1478≠-04
MAGNETIC INDUCTION (ABS B)        (TESLA)  .0000≠+00   .2000≠+01   .4000≠+01   .6000≠+01   .8000≠+01   .1000≠+02   .1200≠+02
CHI                    (METER-OHM/TESLA)  .1049≠+03   .1044≠+03   .1040≠+03   .1038≠+03   .1038≠+03   .1038≠+03   .1037≠+03
HALL PARAMETER                            .0000≠+00   .9948≠ 00   .1982≠+01   .2970≠+01   .3957≠+01   .4945≠+01   .5933≠+01
PSI                 (METER-OHM/SQ TESLA)  .5649≠ 00   .3043≠ 00   .1277≠ 00   .6488≠-01   .3843≠-01   .2521≠-01   .1775≠-01
THETA2                 (VOLT/TESLA-DEGK)  .6840≠-05   .3685≠-05   .1546≠-05   .7856≠-06   .4653≠-06   .3053≠-06   .2149≠-06
THETA3              (VOLT/SQ TESLA-DEGK) -.3164≠-05  -.1705≠-05  -.7152≠-06  -.3635≠-06  -.2153≠-06  -.1412≠-06  -.9944≠-07
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U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                  2  7

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION    22%ASH
    .3988≠+02 AR       .3000≠ 00 ALO2     .1230≠+04 CO2      .7000≠-01 CA       .2800≠ 00 CL2      .0000≠+00 CS       .9500≠ 00 FE
    .6502≠+03 H2       .2900≠+02 K        .3396≠+04 N2       .1500≠ 00 NA       .3492≠+03 02       .5000≠+01 S2       .4480≠+01 SI02

PRESSURE =  1.00 ATM,  TEMPERATURE = 1600 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......     .3988≠+02  AR     .2136≠-10  ALO2    .1229≠+04  CO2     .7066≠-11  CA      .1954≠-11  CL2     .0000≠+00  CS
    .8089≠-07  FE      .1211≠ 00  H2     .2079≠ 00  K       .3396≠+04  N2      .6071≠-02  NA      .6521≠+01  02      .1203≠-11  S2
    .3464≠-08  SIO2    .1457≠-04  E-     .8553≠-18 AL       .5400≠-14 ALO      .8125≠-05 AL(OH)2 .8425≠-25 AL20    .6925≠ 00 CO
    .8449≠-09 C O S    .5346≠-06 CAOH    .1115≠-04 CL       .0000≠+00 CSCL     .0000≠+00 CS O    .0000≠+00 CSOH    .2724≠-05 FEO
    .4109≠-02 FE(OH)2  .1379≠-02 H       .1245≠-02 HCL      .6403≠+03 H20      .4338≠-08 H2S     .5549≠ 00 KCL     .1507≠-02 KO
    .1917≠+02 KOH      .2847≠-08 N       .2173≠-07 NH3      .7632≠ 00 NO       .2233≠-03 NO2     .3774≠-02 NACL    .5052≠-04 NAO
    .1393≠ 00 NAOH     .2686≠-02 O       .2771≠ 00 OH       .9638≠-08 S        .4563≠-03 SO      .9991≠+01 SO2     .8143≠-02 SO3
    .2260≠-22 SI       .4067≠-09 SIO     .9620≠-09 ALO2-    .2038≠-14 CN-      .0000≠+00 CO2-    .2259≠-04 CL-     .0000≠+00 CS+
    .5461≠-04 K+       .2674≠-10 NO-     .2166≠-06 NO2-     .4872≠-08 NA+      .3004≠-08 O-      .1691≠-05 OH-     .1191≠-07 O2-
    .1514≠-11 SH-      .6515≠-10 SO-     .1553≠-04 SO2-
  GLASS ..........     .8625≠-02 AL203 L .6409≠-10 MULLITE .7000≠-01 CAO   L .0000≠+00 CSOH  L .1850≠-07 FEAL204L.9459≠ 00 FEO    L
    .2827≠ 00 KALO2 L .4391≠+01 K2SIO3 L.8013≠-03 NAOH  L .8937≠-01 SIO2  L
  SULF. AND CARB..     .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......     .7463≠-02  AR     .3997≠-14  ALO2    .2301≠ 00  CO2     .1322≠-14  CA      .3656≠-15  CL2     .0000≠+00  CS
    .1514≠-10  FE      .2265≠-04  H2     .3891≠-04  K       .6355≠ 00  N2      .1136≠-05  NA      .1220≠-02  02      .2252≠-15  S2
    .6482≠-12  SIO2    .2726≠-08  E-     .1601≠-21 AL       .1010≠-17 ALO      .1520≠-08 AL(OH)2 .1577≠-28 AL20    .1296≠-03 CO
    .1581≠-12 C O S    .1000≠-09 CAOH    .2086≠-08 CL       .0000≠+00 CSCL     .0000≠+00 CS O    .0000≠+00 CSOH    .5097≠-09 FEO
    .7689≠-06 FE(OH)2  .2580≠-06 H       .2329≠-06 HCL      .1198≠ 00 H20      .8118≠-12 H2S     .1039≠-03 KCL     .2820≠-06 KO
    .3588≠-02 KOH      .5327≠-12 N       .4067≠-11 NH3      .1428≠-03 NO       .4179≠-07 NO2     .7063≠-06 NACL    .9454≠-08 NAO
    .2607≠-04 NAOH     .5027≠-06 O       .5186≠-04 OH       .1804≠-11 S        .8540≠-07 SO      .1870≠-02 SO2     .1524≠-05 SO3
    .4229≠-26 SI       .7611≠-13 SIO     .1800≠-12 ALO2-    .3814≠-18 CN-      .0000≠+00 CO2-    .4228≠-08 CL-     .0000≠+00 CS+
    .1022≠-07 K+       .5005≠-14 NO-     .4053≠-10 NO2-     .9118≠-12 NA+      .5621≠-12 O-      .3165≠-09 OH-     .2229≠-11 O2-
    .2833≠-15 SH-      .1219≠-13 SO-     .2906≠-08 SO2-
  GLASS ..........     .1490≠-02 AL203 L .1107≠-10 MULLITE .1209≠-01 CAO   L .0000≠+00 CSOH  L .3195≠-08 FEAL204L.1634≠ 00 FEO    L
    .4885≠-01 KALO2 L .7586≠ 00 K2SIO3 L.1384≠-03 NAOH  L .1544≠-01 SIO2  L
  SULF. AND CARB..     .0000≠+00 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .0000≠+00 K2SO4 C

                                                         IDEALGAS     GLASS ..     SULF. AN     MIXTURE
MOLAR QUANTITY                        (GRAM-MOLES)      .5344≠+04    .5788≠+01    .0000≠+00    .5349≠+04
AVERAGE MOLECULAR WEIGHT                     (AMU)      .3076≠+02    .1353≠+03    .0000≠+00    .3088≠+02
MASS                                   (KILOGRAMS)      .1644≠+03    .7833≠ 00    .0000≠+00    .1652≠+03
VOLUME                              (CUBIC-METERS)      .7016≠+03    .2315≠-03    .0000≠+00    .7016≠+03
DENSITY                (KILOGRAMS/CUBIC METER)          .2343≠ 00    .3384≠+04    .0000≠+00    .2354≠ 00
ENTROPY                   (GRAMCALORIES/DEGK)           .3387≠+06    .5508≠+03    .0000≠+00    .3392≠+06
REACTION ENTHALPY                (KILOCALORIES)        -.9164≠+05   -.1471≠+04    .0000≠+00   -.9311≠+05
HEAT OF FORMATION                (KILOCALORIES)        -.1544≠+06   -.1734≠+04    .0000≠+00   -.1562≠+06
SENSIBLE HEAT                    (KILOCALORIES)         .6279≠+05    .2623≠+03    .0000≠+00    .6305≠+05
FROZEN CP                  (GMCAL/GMMOL-DEGK)           .1008≠+02    .3738≠+02    .0000≠+00    .1010≠+02
ADIABATIC EXPANSION COEFFICIENT                         .1246≠ +1     SONIC SPEED (METERS/SECOND)          .7339≠ +3

DEBYE LENGTH            (METERS).96835≠-05    ELECTRON DENSITY       (PER M↑3).12506≠+17    COLLISION FREQUENCY   (PER SEC).38528≠+12
COEFFICIENTS FOR OHM,S LAW..    SIGMA = SCALAR COND   (MHO/METER)       .9284≠-03      BETA1      (SQM-VOLT/NEWTON)            -.4991≠+03
BETA2  (ASSUMING ZERO ION SLIP)              (SQM-VOLT/TESLA-NEWTON)    .0000≠+00      THETA1       (VOLT/DEGK)                -.1628≠-04
MAGNETIC INDUCTION (ABS B)          (TESLA)  .0000≠+00     .2000≠+01     .4000≠+01     .6000≠+01     .8000≠+01     .1000≠+02     .1200≠+02
CHI                          (METER-OHM/TESLA)  .5062≠+03     .5031≠+03     .5009≠+03     .5000≠+03     .4996≠+03     .4995≠+03     .4994≠+03
HALL PARAMETER                               .0000≠+00     .9342≠ 00     .1860≠+01     .2785≠+01     .3711≠+01     .4637≠+01     ,5563≠+01
PSI                      (METER-OHM/SQ TESLA)  .3133≠+01     .1768≠+01     .7660≠ 00     .3940≠ 00     .2345≠ 00     .1542≠ 00     .1087≠ 00
THETA2                       (VOLT/TESLA-DEGK)  .7156≠-05     .4037≠-05     .1750≠-05     .8999≠-06     .5356≠-06     .3523≠-06     .2484≠-06
THETA3                    (VOLT/SQ TESLA-DEGK) -.3145≠-05    -.1774≠-05    -.7689≠-06    -.3954≠-06    -.2354≠-06    -.1548≠-06    -.1092≠-06
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U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                          6 11

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION   22%ASH
    .3988≠+02 AR       .3000≠ 00 ALO2     .1230≠+04 CO2     .7000≠-01 CA      .2800≠ 00 CL2      .0000≠+00 CS      .9500≠ 00 FE
    .6502≠+03 H2       .2900≠+02 K        .3396≠+04 N2      .1500≠ 00 NA      .3492≠+03 O2       .5000≠+01 S2      .4480≠+01 SIO2

PRESSURE =  1.00 ATM,  TEMPERATURE = 1500 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......      .3988≠+02  AR      .1373≠-11  ALO2    .1230≠+04  CO2     .2808≠-12  CA      .4654≠-11  CL2     .0000≠+00  CS
    .4722≠-08  FE       .5090≠-01  H2      .2862≠-01  K       .3396≠+04  N2      .2845≠-02  NA      .3054≠+01  O2      .1449≠-13  S2
    .3760≠-09  SIO2     .1040≠-05  E-      .9270≠-20 AL       .1362≠-15 ALO      .2454≠-05 AL(OH)2 .3689≠-27 AL2O     .2481≠ 00 CO
    .5162≠-10 C O S     .7075≠-07 CAOH     .9145≠-05 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .2561≠-06 FEO
    .1909≠-02 FE(OH)2 .2888≠-03 H          .2006≠-02 HCL      .6471≠+03 H2O      .3155≠-09 H2S      .5462≠ 00 KCL      .1556≠-03 KO
    .5849≠+01 KOH       .2580≠-09 N        .7855≠-08 NH3      .3318≠ 00 NO       .8896≠-04 NO2      .1174≠-01 NACL     .1829≠-04 NAO
    .1335≠ 00 NAOH      .5136≠-03 O        .1016≠ 00 OH       .3554≠-09 S        .4613≠-04 SO       .3142≠+01 SO2      .2835≠-02 SO3
    .1187≠-24 SI        .2366≠-10 SIO      .3741≠-10 ALO2-    .3675≠-16 CN-      .0000≠+00 CO2-     .9051≠-05 CL-      .0000≠+00 CS+
    .1094≠-04 K+        .9897≠-12 NO-      .2274≠-07 NO2-     .2257≠-08 NA+      .9802≠-10 O-       .1272≠-06 OH-      .5775≠-09 O2-
    .1864≠-13 SH-       .9131≠-12 SO-      .6995≠-06 SO2-
  GLASS ..........      .2023≠-01 AL2O3 L .2651≠-08 MULLITE .7000≠-01 CAO    L .0000≠+00 CSOH   L .7565≠-08 FEAL2O4L.9481≠ 00 FEO    L
    .2595≠ 00 KALO2 L .4299≠+01 K2SIO3 L.1905≠-02 NAOH   L .1814≠ 00 SIO2   L
  SULF. AND CARB..      .4211≠-02 K2CO3 L .0000≠+00 K2CO3 C .6855≠+01 K2SO4 L .0000≠+00 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......      .7488≠-02  AR      .2577≠-15  ALO2    .2309≠ 00  CO2     .5272≠-16  CA      .8739≠-15  CL2     .0000≠+00  CS
    .8865≠-12  FE       .9557≠-05  H2      .5373≠-05  K       .6376≠ 00  N2      .5341≠-06  NA      .5734≠-03  O2      .2720≠-17  S2
    .7059≠-13  SIO2     .1953≠-09  E-      .1741≠-23 AL       .2558≠-19 ALO      .4608≠-09 AL(OH)2 .6926≠-31 AL2O     .4658≠-04 CO
    .9693≠-14 C O S     .1328≠-10 CAOH     .1717≠-08 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .4808≠-10 FEO
    .3585≠-06 FE(OH)2 .5422≠-07 H          .3766≠-06 HCL      .1215≠ 00 H2O      .5923≠-13 H2S      .1026≠-03 KCL      .2921≠-07 KO
    .1098≠-02 KOH       .4844≠-13 N        .1475≠-11 NH3      .6230≠-04 NO       .1670≠-07 NO2      .2204≠-05 NACL     .3434≠-08 NAO
    .2506≠-04 NAOH      .9643≠-07 O        .1907≠-04 OH       .6673≠-13 S        .8661≠-08 SO       .5899≠-03 SO2      .5322≠-06 SO3
    .2229≠-28 SI        .4442≠-14 SIO      .7025≠-14 ALO2-    .6899≠-20 CN-      .0000≠+00 CO2-     .1699≠-08 CL-      .0000≠+00 CS+
    .2054≠-08 K+        .1858≠-15 NO-      .4269≠-11 NO2-     .4237≠-12 NA+      .1840≠-13 O-       .2388≠-10 OH-      .1084≠-12 O2-
    .3500≠-17 SH-       .1714≠-15 SO-      .1313≠-09 SO2-
  GLASS ..........      .3500≠-02 AL2O3 L .4587≠-09 MULLITE .1211≠-01 CAO    L .0000≠+00 CSOH   L .1309≠-08 FEAL2O4L.1640≠ 00 FEO    L
    .4490≠-01 KALO2 L .7437≠ 00 K2SIO3 L.3296≠-03 NAOH   L .3139≠-01 SIO2   L
  SULF. AND CARB..      .6139≠-03 K2CO3 L .0000≠+00 K2CO3 C .9994≠ 00 K2SO4 L .0000≠+00 K2SO4 C

                                                   IDEALGAS    GLASS ..    SULF. AN     MIXTURE
MOLAR QUANTITY                   (GRAM-MOLES)      .5326≠+04   .5780≠+01   .6860≠+01   .5339≠+04
AVERAGE MOLECULAR WEIGHT                (AMU)      .3064≠+02   .1339≠+03   .1742≠+03   .3094≠+02
MASS                              (KILOGRAMS)      .1632≠+03   .7738≠ 00   .1195≠+01   .1652≠+03
VOLUME                         (CUBIC-METERS)      .6556≠+03   .2291≠-03   .4491≠-03   .6556≠+03
DENSITY             (KILOGRAMS/CUBIC METER)        .2489≠ 00   .3378≠+04   .2662≠+04   .2519≠ 00
ENTROPY                 (GRAMCALORIES/DEGK)        .3335≠+06   .5304≠+03   .8173≠+03   .3349≠+06
REACTION ENTHALPY               (KILOCALORIES)    -.9648≠+05  -.1481≠+04  -.1913≠+04  -.9987≠+05
HEAT OF FORMATION               (KILOCALORIES)    -.1536≠+06  -.1719≠+04  -.2276≠+04  -.1576≠+06
SENSIBLE HEAT                   (KILOCALORIES)     .5717≠+05   .2377≠+03   .3629≠+03   .5777≠+05
FROZEN CP                  (GMCAL/GMMOL-DEGK)      .9965≠+01   .3695≠+02   .4705≠+02   .1004≠+02
ADIABATIC EXPANSION COEFFICIENT                    .1249≠ +1    SONIC SPEED (METERS/SECOND)          .7130≠ +3

DEBYE LENGTH           (METERS).19315≠-04    ELECTRON DENSITY      (PER M↑3).95543≠+15   COLLISION FREQUENCY  (PER SEC).39965≠+12
COEFFICIENTS FOR OHM,S LAW..   SIGMA = SCALAR COND  (MHO/METER)   .6895≠-04     BETA1      (SQM-VOLT/NEWTON)          -.6533≠+04
BETA2  (ASSUMING ZERO ION SLIP)           (SQM-VOLT/TESLA-NEWTON)  .0000≠+00      THETA1      (VOLT/DEGK)               -.2053≠-04
MAGNETIC INDUCTION (ABS B)         (TESLA)  .0000≠+00    .2000≠+01    .4000≠+01    .6000≠+01    .8000≠+01    .1000≠+02    .1200≠+02
CHI                     (METER-OHM/TESLA)  .6681≠+04    .6617≠+04    .6570≠+04    .6552≠+04    .6544≠+04    .6540≠+04    .6538≠+04
HALL PARAMETER                              .0000≠+00    .9125≠ 00    .1812≠+01    .2710≠+01    .3610≠+01    .4509≠+01    .5409≠+01
PSI                  (METER-OHM/SQ TESLA)  .6457≠+02    .3674≠+02    .1603≠+02    .8262≠+01    .4923≠+01    .3240≠+01    .2285≠+01
THETA2                 (VOLT/TESLA-DEGK)   .8934≠-05    .5084≠-05    .2218≠-05    .1143≠-05    .6812≠-06    .4483≠-06    .3161≠-06
THETA3              (VOLT/SQ TESLA-DEGK)  -.3887≠-05   -.2212≠-05   -.9649≠-06   -.4974≠-06   -.2964≠-06   -.1950≠-06   -.1376≠-06
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U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                              5 11

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION   22%ASH
    .3988≠+02 AR      .3000≠ 00 ALO2    .1230≠+04 CO2     .7000≠-01 CA      .2800≠ 00 CL2     .0000≠+00 CS      .9500≠ 00 FE
    .6502≠+03 H2      .2900≠+02 K       .3396≠+04 N2      .1500≠ 00 NA      .3492≠+03 O2      .5000≠+01 S2      .4480≠+01 SIO2

PRESSURE =  1.00 ATM,  TEMPERATURE = 1400 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......    .3988≠+02  AR     .5901≠-13  ALO2    .1230≠+04  CO2     .5936≠-14  CA      .1528≠-10  CL2     .0000≠+00  CS
    .1533≠-09  FE     .1590≠-01  H2     .2609≠-02  K       .3396≠+04  N2      .9367≠-03  NA      .1796≠+01  O2      .2802≠-16  S2
    .3059≠-10  SIO2   .3377≠-07  E-     .3737≠-22 AL       .1709≠-17 ALO      .5144≠-06 AL(OH)2 .4398≠-30 AL2O     .6481≠-01 CO
    .9803≠-12 C O S   .6418≠-08 CAOH    .8053≠-05 CL       .0000≠+00 CSCL     .0000≠+00 CS O    .0000≠+00 CSOH     .1694≠-07 FEO
    .7880≠-03 FE(OH)2 .4453≠-04 H       .3505≠-02 HCL      .6494≠+03 H2O      .7297≠-11 H2S     .5194≠ 00 KCL      .1204≠-04 KO
    .1434≠+01 KOH     .1669≠-10 N       .1895≠-08 NH3      .1516≠ 00 NO       .4344≠-04 NO2     .3712≠-01 NACL     .5318≠-05 NAO
    .1075≠ 00 NAOH    .9186≠-04 O       .3506≠-01 OH       .4506≠-11 S        .2192≠-05 SO      .6444≠ 00 SO2      .7716≠-03 SO3
    .2174≠-27 SI      .7987≠-12 SIO     .5937≠-12 ALO2-    .1740≠-18 CN-      .0000≠+00 CO2-    .2294≠-05 CL-      .0000≠+00 CS+
    .2344≠-05 K+      .1763≠-13 NO-     .1587≠-08 NO2-     .1125≠-08 NA+      .1523≠-11 O-      .4671≠-08 OH-      .1664≠-10 O2-
    .4046≠-16 SH-     .2962≠-14 SO-     .1015≠-07 SO2-
  GLASS ..........    .4508≠-01 AL2O3 L .1304≠-06 MULLITE .7000≠-01 CAO    L .0000≠+00 CSOH  L .2298≠-08 FEAL2O4L.9492≠ 00 FEO    L
    .2098≠ 00 KALO2 L .4058≠+01 K2SIO3 L.4406≠-02 NAOH  L .4219≠ 00 SIO2   L
  SULF. AND CARB..    .4340≠-02 K2CO3 L .0000≠+00 K2CO3 C .9355≠+01 K2SO4 L .0000≠+00 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......    .7496≠-02  AR     .1109≠-16  ALO2    .2312≠ 00  CO2     .1116≠-17  CA      .2872≠-14  CL2     .0000≠+00  CS
    .2883≠-13  FE     .2988≠-05  H2     .4904≠-06  K       .6383≠ 00  N2      .1761≠-06  NA      .3377≠-03  O2      .5267≠-20  S2
    .5751≠-14  SIO2   .6348≠-11  E-     .7024≠-26 AL       .3212≠-21 ALO      .9669≠-10 AL(OH)2 .8268≠-34 AL2O     .1218≠-04 CO
    .1843≠-15 C O S   .1206≠-11 CAOH    .1514≠-08 CL       .0000≠+00 CSCL     .0000≠+00 CS O    .0000≠+00 CSOH     .3184≠-11 FEO
    .1481≠-06 FE(OH)2 .8370≠-08 H       .6588≠-06 HCL      .1221≠ 00 H2O      .1372≠-14 H2S     .9763≠-04 KCL      .2264≠-08 KO
    .2695≠-03 KOH     .3137≠-14 N       .3562≠-12 NH3      .2850≠-04 NO       .8166≠-08 NO2     .6978≠-05 NACL     .9997≠-09 NAO
    .2021≠-04 NAOH    .1727≠-07 O       .6591≠-05 OH       .8470≠-15 S        .4121≠-09 SO      .1211≠-03 SO2      .1450≠-06 SO3
    .4086≠-31 SI      .1501≠-15 SIO     .1116≠-15 ALO2-    .3271≠-22 CN-      .0000≠+00 CO2-    .4313≠-09 CL-      .0000≠+00 CS+
    .4405≠-09 K+      .3314≠-17 NO-     .2983≠-12 NO2-     .2114≠-12 NA+      .2863≠-15 O-      .8781≠-12 OH-      .3127≠-14 O2-
    .7605≠-20 SH-     .5568≠-18 SO-     .1909≠-11 SO2-
  GLASS ..........    .7828≠-02 AL2O3 L .2264≠-07 MULLITE .1216≠-01 CAO    L .0000≠+00 CSOH  L .3990≠-09 FEAL2O4L.1648≠ 00 FEO    L
    .3644≠-01 KALO2 L .7047≠ 00 K2SIO3 L.7651≠-03 NAOH  L .7327≠-01 SIO2   L
  SULF. AND CARB..    .4637≠-03 K2CO3 L .0000≠+00 K2CO3 C .9995≠ 00 K2SO4 L .0000≠+00 K2SO4 C

                                                    IDEALGAS    GLASS ..    SULF. AN    MIXTURE
MOLAR QUANTITY                   (GRAM-MOLES)      .5320≠+04   .5759≠+01   .9359≠+01   .5335≠+04
AVERAGE MOLECULAR WEIGHT                (AMU)      .3060≠+02   .1301≠+03   .1742≠+03   .3096≠+02
MASS                              (KILOGRAMS)      .1628≠+03   .7489≠ 00   .1631≠+01   .1652≠+03
VOLUME                         (CUBIC-METERS)      .6112≠+03   .2231≠-03   .6127≠-03   .6112≠+03
DENSITY             (KILOGRAMS/CUBIC METER)        .2664≠ 00   .3357≠+04   .2662≠+04   .2703≠ 00
ENTROPY                (GRAMCALORIES/DEGK)         .3293≠+06   .4988≠+03   .1085≠+04   .3308≠+06
REACTION ENTHALPY             (KILOCALORIES)      -.1016≠+06  -.1473≠+04  -.2655≠+04  -.1057≠+06
HEAT OF FORMATION             (KILOCALORIES)      -.1534≠+06  -.1682≠+04  -.3106≠+04  -.1582≠+06
SENSIBLE HEAT                 (KILOCALORIES)       .5181≠+05   .2093≠+03   .4511≠+03   .5247≠+05
FROZEN CP                 (GMCAL/GMMOL-DEGK)       .9850≠+01   .3575≠+02   .4705≠+02   .9943≠+01
ADIABATIC EXPANSION COEFFICIENT                    .1253≠ +1    SONIC SPEED (METERS/SECOND)          .6903≠ +3

DEBYE LENGTH            (METERS).38121≠-04   ELECTRON DENSITY       (PER M↑3).33277≠+14   COLLISION FREQUENCY  (PER SEC).43950≠+12
COEFFICIENTS FOR OHM.S LAW..   SIGMA = SCALAR COND  (MHO/METER)   .2196≠-05     BETA1     (SQM-VOLT/NEWTON)             -.1876≠+06
BETA2  (ASSUMING ZERO ION SLIP)        (SQM-VOLT/TESLA-NEWTON)    .0000≠+00     THETA1      (VOLT/DEGK)                 -.2312≠-04
MAGNETIC INDUCTION (ABS B)        (TESLA)  .0000≠+00    .2000≠+01    .4000≠+01    .6000≠+01    .8000≠+01    .1000≠+02    .1200≠+02
CHI                   (METER-OHM/TESLA)    .1930≠+06    .1909≠+06    .1891≠+06    .1884≠+06    .1880≠+06    .1879≠+06    .1878≠+06
HALL PARAMETER                             .0000≠+00    .8384≠ 00    .1661≠+01    .2482≠+01    .3304≠+01    .4127≠+01    .4950≠+01
PSI                (METER-OHM/SQ TESLA)    .2173≠+04    .1319≠+04    .6055≠+03    .3184≠+03    .1914≠+03    .1265≠+03    .8943≠+02
THETA2                (VOLT/TESLA-DEGK)    .9300≠-05    .5646≠-05    .2592≠-05    .1363≠-05    .8191≠-06    .5414≠-06    .3828≠-06
THETA3             (VOLT/SQ TESLA-DEGK)   -.3740≠-05   -.2271≠-05   -.1042≠-05   -.5482≠-06   -.3295≠-06   -.2178≠-06   -.1540≠-06
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U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                         7 16

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION   22%ASH
    .3988≠+02 AR       .3000≠ 00 ALO2      .1230≠+04 CO2      .7000≠-01 CA       .2800≠ 00 CL2      .0000≠+00 CS       .9500≠ 00 FE
    .6502≠+03 H2       .2900≠+02 K         .3396≠+04 N2       .1500≠ 00 NA       .3492≠+03 O2       .5000≠+01 S2       .4480≠+01 SIO2

PRESSURE =  1.00 ATM,  TEMPERATURE = 1200 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......     .3988≠+02  AR      .1265≠-16  ALO2    .1230≠+04  CO2     .2084≠-18  CA      .5515≠-10  CL2     .0000≠+00  CS
    .1539≠-13  FE      .4886≠-03  H2      .1517≠-04  K       .3396≠+04  N2      .2096≠-04  NA      .1499≠+01  O2      .5610≠-27  S2
    .6243≠-14  SIO2    .1275≠-10  E-      .6748≠-29 AL       .9362≠-23 ALO      .3072≠-08 AL(OH)2 .1172≠-38 AL2O     .1262≠-02 CO
    .3051≠-18 C O S    .1141≠-10 CAOH     .2545≠-05 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .1767≠-10 FEO
    .8216≠-04 FE(OH)2 .3164≠-06 H         .4542≠-02 HCL      .6501≠+03 H2O      .3669≠-17 H2S      .4538≠ 00 KCL      .8240≠-07 KO
    .1317≠ 00 KOH      .1784≠-13 N        .2276≠-10 NH3      .3788≠-01 NO       .2277≠-04 NO2      .1017≠ 00 NACL     .1532≠-06 NAO
    .3019≠-01 NAOH     .2222≠-05 O        .3231≠-02 OH       .9044≠-18 S        .2106≠-10 SO       .4269≠-03 SO2      .1859≠-05 SO3
    .1065≠-35 SI       .1003≠-16 SIO      .1985≠-16 ALO2-    .1607≠-24 CN-      .0000≠+00 CO2-     .6100≠-07 CL-      .0000≠+00 CS+
    .6099≠-07 K+       .2517≠-17 NO-      .1213≠-10 NO2-     .3739≠-10 NA+      .1550≠-15 O-       .3034≠-11 OH-      .1395≠-13 O2-
    .1389≠-24 SH-      .6547≠-22 SO-      .1698≠-13 SO2-
  GLASS ..........     .6196≠-01 AL2O3 L .1672≠-06 MULLITE .7000≠-01 CAO   L .0000≠+00 CSOH  L .2131≠-10 FEAL2O4L.9499≠ 00 FEO   L
    .1761≠ 00 KALO2 L .4093≠+01 K2SIO3 L.1812≠-01 NAOH  L .3870≠ 00 SIO2  L
  SULF. AND CARB..     .2670≠-01 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .1000≠+02 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......     .7499≠-02  AR      .2379≠-20  ALO2    .2313≠ 00  CO2     .3918≠-22  CA      .1037≠-13  CL2     .0000≠+00  CS
    .2895≠-17  FE      .9188≠-07  H2      .2852≠-08  K       .6386≠ 00  N2      .3941≠-08  NA      .2818≠-03  O2      .1055≠-30  S2
    .1174≠-17  SIO2    .2397≠-14  E-      .1269≠-32 AL       .1760≠-26 ALO      .5776≠-12 AL(OH)2 .2203≠-42 AL2O     .2372≠-06 CO
    .5736≠-22 C O S    .2145≠-14 CAOH     .4785≠-09 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .3323≠-14 FEO
    .1545≠-07 FE(OH)2 .5950≠-10 H         .8541≠-06 HCL      .1222≠ 00 H2O      .6900≠-21 H2S      .8533≠-04 KCL      .1549≠-10 KO
    .2476≠-04 KOH      .3355≠-17 N        .4280≠-14 NH3      .7122≠-05 NO       .4281≠-08 NO2      .1912≠-04 NACL     .2881≠-10 NAO
    .5677≠-05 NAOH     .4178≠-09 O        .6076≠-06 OH       .1701≠-21 S        .3959≠-14 SO       .8028≠-07 SO2      .3496≠-09 SO3
    .2003≠-39 SI       .1887≠-20 SIO      .3733≠-20 ALO2-    .3023≠-28 CN-      .0000≠+00 CO2-     .1147≠-10 CL-      .0000≠+00 CS+
    .1147≠-10 K+       .4733≠-21 NO-      .2282≠-14 NO2-     .7030≠-14 NA+      .2915≠-19 O-       .5705≠-15 OH-      .2622≠-17 O2-
    .2612≠-28 SH-      .1231≠-25 SO-      .3192≠-17 SO2-
  GLASS ..........     .1076≠-01 AL2O3 L .2904≠-07 MULLITE .1216≠-01 CAO   L .0000≠+00 CSOH  L .3702≠-11 FEAL2O4L.1650≠ 00 FEO   L
    .3059≠-01 KALO2 L .7111≠ 00 K2SIO3 L.3148≠-02 NAOH  L .6724≠-01 SIO2  L
  SULF. AND CARB..     .2663≠-02 K2CO3 L .0000≠+00 K2CO3 C .0000≠+00 K2SO4 L .9973≠ 00 K2SO4 C

                                                       IDEALGAS     GLASS ..     SULF. AN     MIXTURE
MOLAR QUANTITY                         (GRAM-MOLES)    .5318≠+04    .5756≠+01    .1003≠+02    .5334≠+04
AVERAGE MOLECULAR WEIGHT                      (AMU)    .3059≠+02    .1305≠+03    .1742≠+03    .3097≠+02
MASS                                    (KILOGRAMS)    .1627≠+03    .7512≠ 00    .1746≠+01    .1652≠+03
VOLUME                               (CUBIC-METERS)    .5237≠+03    .2229≠-03    .6565≠-03    .5237≠+03
DENSITY                 (KILOGRAMS/CUBIC METER)        .3106≠ 00    .3370≠+04    .2660≠+04    .3154≠ 00
ENTROPY                       (GRAMCALORIES/DEGK)      .3211≠+06    .4689≠+03    .1018≠+04    .3226≠+06
REACTION ENTHALPY                  (KILOCALORIES)     -.1119≠+06   -.1517≠+04   -.3032≠+04   -.1164≠+06
HEAT OF FORMATION                  (KILOCALORIES)     -.1533≠+06   -.1686≠+04   -.3442≠+04   -.1584≠+06
SENSIBLE HEAT                      (KILOCALORIES)      .4144≠+05    .1688≠+03    .4104≠+03    .4202≠+05
FROZEN CP                     (GMCAL/GMMOL-DEGK)       .9580≠+01    .3586≠+02    .5134≠+02    .9686≠+01
ADIABATIC EXPANSION COEFFICIENT                        .1262≠ +1    SONIC SPEED (METERS/SECOND)              .6415≠ +3

DEBYE LENGTH              (METERS).20179≠-03   ELECTRON DENSITY      (PER M↑3).14660≠+11   COLLISION FREQUENCY  (PER SEC).53867≠+12
COEFFICIENTS FOR OHM,S LAW..   SIGMA = SCALAR COND  (MHO/METER)    .7948≠-09    BETA1     (SQM-VOLT/NEWTON)          -.4258≠+09
BETA2  (ASSUMING ZERO ION SLIP)           (SQM-VOLT/TESLA-NEWTON)  .0000≠+00     THETA1     (VOLT/DEGK)              -.2594≠-04
MAGNETIC INDUCTION (ABS B)         (TESLA)  .0000≠+00   .2000≠+01   .4000≠+01   .6000≠+01   .8000≠+01   .1000≠+02   .1200≠+02
CHI                     (METER-OHM/TESLA)  .4412≠+09   .4364≠+09   .4313≠+09   .4288≠+09   .4276≠+09   .4270≠+09   .4267≠+09
HALL PARAMETER                             .0000≠+00   .6937≠ 00   .1371≠+01   .2045≠+01   .2719≠+01   .3394≠+01   .4069≠+01
PSI                 (METER-OHM/SQ TESLA)   .5189≠+07   .3573≠+07   .1847≠+07   .1023≠+07   .6300≠+06   .4216≠+06   .3002≠+06
THETA2                 (VOLT/TESLA-DEGK)   .8722≠-05   .6006≠-05   .3105≠-05   .1720≠-05   .1059≠-05   .7087≠-06   .5047≠-06
THETA3              (VOLT/SQ TESLA-DEGK)  -.2933≠-05  -.2020≠-05  -.1044≠-05  -.5784≠-06  -.3561≠-06  -.2383≠-06  -.1697≠-06
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U S BU MINES   PGH ENERGY RES CTR   MULTIPHASE EQUILIBRIUM PROGRAM (ALGOL) 01MAY72 VERSION6                              5 17

STOICHIOMETRY (GMOL) FOR CASE IDENTIFIED AS SPENCER/ORNING 3-PHASE DEMONSTRATION   22%ASH
    .3988≠+02 AR      .3000≠ 00 AL02    .1230≠+04 CO2     .7000≠-01 CA      .2800≠ 00 CL2     .0000≠+00 CS      .9500≠ 00 FE
    .6502≠+03 H2      .2900≠+02 K       .3396≠+04 N2      .1500≠ 00 NA      .3492≠+03 02      .5000≠+01 S2      .4480≠+01 SI02

PRESSURE =  1.00 ATM,  TEMPERATURE = 1000 DEGK

EQUILIBRIUM MOLAR QUANTITIES
  IDEALGAS .......     .3988≠+02  AR      .1016≠-21  AL02    .1230≠+04  CO2     .9968≠-25  CA      .1068≠-08  CL2     .0000≠+00  CS
    .3071≠-19  FE      .3342≠-05  H2      .7165≠-08  K       .3396≠+04  N2      .1701≠-07  NA      .1514≠+01  02      .4249≠-42  S2
    .6836≠-19  SI02    .1311≠-15  E-      .2038≠-38 AL       .3815≠-30 ALO      .2104≠-11 AL(OH)2 .8993≠-51 AL20     .4381≠-05 CO
    .1774≠-27 C O S    .1446≠-14 CAOH     .9210≠-06 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .1056≠-14 FEO
    .3350≠-05 FE(OH)2 .3011≠-09 H         .1100≠-01 HCL      .6502≠+03 H20      .4229≠-26 H2S      .4262≠ 00 KCL      .5578≠-10 KO
    .3219≠-02 KOH      .1260≠-17 N        .3915≠-13 NH3      .6218≠-02 NO       .1210≠-04 NO2      .1228≠ 00 NACL     .2023≠-09 NAO
    .9167≠-03 NAOH     .1400≠-07 O        .1236≠-03 OH       .3258≠-27 S        .1928≠-17 SO       .1685≠-07 SO2      .5160≠-09 SO3
    .3022≠-47 SI       .1908≠-23 SIO      .6898≠-23 AL02-    .2540≠-33 CN-      .0000≠+00 CO2-     .4010≠-09 CL-      .0000≠+00 CS+
    .4010≠-09 K+       .6977≠-23 NO-      .1018≠-13 NO2-     .9009≠-13 NA+      .2698≠-21 0-       .6579≠-16 OH-      .5239≠-18 02-
    .9250≠-37 SH-      .7133≠-33 SO-      .9089≠-22 SO2-
  GLASS ..........     .1126≠ 00 AL2O3 L .1065≠-05 MULLITE .7000≠-01 CAO    L .0000≠+00 CSOH  L .3158≠-13 FEAL204L.9500≠ 00 FEO    L
    .7472≠-01 KALO2 L .3902≠+01 K2SIO3 L.2626≠-01 NAOH   L .5781≠ 00 SIO2   L
  SULF. AND CARB..     .0000≠+00 K2CO3 L .3460≠ 00 K2CO3 C .0000≠+00 K2SO4 L .1000≠+02 K2SO4 C

MOLAR FRACTIONS WITHIN PHASES
  IDEALGAS .......     .7499≠-02  AR      .1910≠-25  AL02    .2312≠ 00  CO2     .1875≠-28  CA      .2009≠-12  CL2     .0000≠+00  CS
    .5775≠-23  FE      .6284≠-09  H2      .1347≠-11  K       .6386≠ 00  N2      .3199≠-11  NA      .2848≠-03  02      .7990≠-46  S2
    .1286≠-22  SI02    .2466≠-19  E-      .3833≠-42 AL       .7174≠-34 ALO      .3956≠-15 AL(OH)2 .1691≠-54 AL20     .8238≠-09 CO
    .3335≠-31 C O S    .2718≠-18 CAOH     .1732≠-09 CL       .0000≠+00 CSCL     .0000≠+00 CS O     .0000≠+00 CSOH     .1985≠-18 FEO
    .6299≠-09 FE(OH)2 .5663≠-13 H         .2069≠-05 HCL      .1223≠ 00 H20      .7953≠-30 H2S      .8014≠-04 KCL      .1049≠-13 KO
    .6053≠-06 KOH      .2369≠-21 N        .7361≠-17 NH3      .1169≠-05 NO       .2276≠-08 NO2      .2310≠-04 NACL     .3804≠-13 NAO
    .1724≠-06 NAOH     .2633≠-11 O        .2324≠-07 OH       .6127≠-31 S        .3626≠-21 SO       .3169≠-11 SO2      .9703≠-13 SO3
    .5684≠-51 SI       .3588≠-27 SIO      .1297≠-26 AL02-    .4777≠-37 CN-      .0000≠+00 CO2-     .7542≠-13 CL-      .0000≠+00 CS+
    .7540≠-13 K+       .1312≠-26 NO-      .1915≠-17 NO2-     .1694≠-16 NA+      .5073≠-25 0-       .1237≠-19 OH-      .9853≠-22 02-
    .1739≠-40 SH-      .1341≠-36 SO-      .1709≠-25 SO2-
  GLASS ..........     .1971≠-01 AL2O3 L .1864≠-06 MULLITE .1225≠-01 CAO    L .0000≠+00 CSOH  L .5528≠-14 FEAL204L.1663≠ 00 FEO    L
    .1308≠-01 KALO2 L .6829≠ 00 K2SIO3 L.4595≠-02 NAOH   L .1012≠ 00 SIO2   L
  SULF. AND CARB..     .0000≠+00 K2CO3 L .3344≠-01 K2CO3 C .0000≠+00 K2SO4 L .9666≠ 00 K2SO4 C

                                                       IDEALGAS    GLASS ..    SULF. AN    MIXTURE
MOLAR QUANTITY                       (GRAM-MOLES)     .5318≠+04   .5714≠+01   .1035≠+02   .5334≠+04
AVERAGE MOLECULAR WEIGHT                    (AMU)     .3059≠+02   .1276≠+03   .1731≠+03   .3097≠+02
MASS                                  (KILOGRAMS)     .1627≠+03   .7288≠ 00   .1790≠+01   .1652≠+03
VOLUME                            (CUBIC-METERS)      .4364≠+03   .2163≠-03   .6786≠-03   .4364≠+03
DENSITY                 (KILOGRAMS/CUBIC METER)       .3727≠ 00   .3369≠+04   .2639≠+04   .3785≠ 00
ENTROPY                    (GRAMCALORIES/DEGK)        .3120≠+06   .4179≠+03   .9580≠+03   .3133≠+06
REACTION ENTHALPY                 (KILOCALORIES)     -.1218≠+06  -.1529≠+04  -.3208≠+04  -.1266≠+06
HEAT OF FORMATION                 (KILOCALORIES)     -.1533≠+06  -.1653≠+04  -.3531≠+04  -.1584≠+06
SENSIBLE HEAT                     (KILOCALORIES)      .3142≠+05   .1239≠+03   .3222≠+03   .3187≠+05
FROZEN CP                    (GMCAL/GMMOL-DEGK)       .9237≠+01   .3454≠+02   .4577≠+02   .9335≠+01
ADIABATIC EXPANSION COEFFICIENT                       .1274≠ +1    SONIC SPEED (METERS/SECOND)          .5885≠ +3

DEBYE LENGTH              (METERS).20741≠-02   ELECTRON DENSITY       (PER M+3).18099≠+06   COLLISION FREQUENCY  (PER SEC).66160≠+12
COEFFICIENTS FOR OHM,S LAW..   SIGMA = SCALAR COND  (MHO/METER)    .8027≠-14      BETA1      (SQM-VOLT/NEWTON)            -.3449≠+14
BETA2  (ASSUMING ZERO ION SLIP)          (SQM-VOLT/TESLA-NEWTON)   .0000≠+00      THETA1      (VOLT/DEGK)                 -.2786≠-04
MAGNETIC INDUCTION (ABS B)         (TESLA)  .0000≠+00    .2000≠+01    .4000≠+01    .6000≠+01    .8000≠+01    .1000≠+02    .1200≠+02
CHI                         (METER-OHM/TESLA)  .3593≠+14    .3558≠+14    .3513≠+14    .3486≠+14    .3473≠+14    .3465≠+14    .3460≠+14
HALL PARAMETER                                 .0000≠+00    .5713≠ 00    .1128≠+01    .1679≠+01    .2230≠+01    .2781≠+01    .3333≠+01
PSI                   (METER-OHM/SQ TESLA)  .4035≠+12    .3072≠+12    .1791≠+12    .1056≠+12    .6709≠+11    .4567≠+11    .3285≠+11
THETA2                  (VOLT/TESLA-DEGK)  .7797≠-05    .5937≠-05    .3460≠-05    .2041≠-05    .1296≠-05    .8826≠-06    .6349≠-06
THETA3               (VOLT/SQ TESLA-DEGK) -.2182≠-05   -.1652≠-05   -.9684≠-06   -.5712≠-06   -.3629≠-06   -.2470≠-06   -.1777≠-06
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