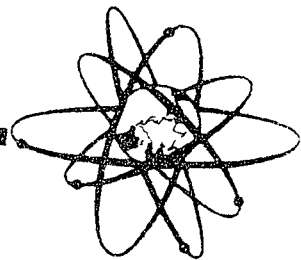


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BENCHMARK EXERCISE ON THE CHEMICAL MODELLING  
OF THE RELEASE OF RADIONUCLIDES  
DUE TO CORE-CONCRETE INTERACTIONS

(Part B)

December 1990



COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS

PRINCIPAL WORKING GROUP ON CONFINEMENT  
OF ACCIDENTAL RADIOACTIVE RELEASES

TASK GROUP ON FISSION PRODUCT  
PHENOMENA IN THE CONTAINMENT

(FPC)

**BENCHMARK EXERCISE ON THE CHEMICAL  
MODELLING OF THE RELEASE OF RADIONUCLIDES DUE TO  
CORE-CONCRETE INTERACTIONS:  
RESULTS OF PART B**

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October 1990

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### Executive Summary

This report is concerned with the second part of an exercise, Part B, to compare the calculational models for the release of radionuclides during core-concrete interaction in a severe accident in a nuclear reactor. The objective of this part of the exercise was to assess the uncertainties resulting from differences in the treatment of the solution phases, the composition of each phase and the choice of thermodynamic data in the modelling of core-concrete interactions. The problem consisted of the calculation of the equilibrium composition for a number of cases in which the input amounts of the components and the temperature and pressure of the system were specified. The method of treatment of the liquid phases, that is the components of the phases and the representation of the solutions as ideal or non-ideal, and the selection of thermodynamic data were chosen by the participants.

Six sets of solutions to the problems were received from participants using different codes and different assumptions in the modelling of the solution phases. The results from the first part of the exercise, Part A, had shown that there was good agreement between these codes in the method of calculating the chemical equilibrium. In the case of the submission using the VANESA code, the oxide and metal phases in the melt were not treated in equilibrium, a specification of the problem. However, the results were presented in order to discuss the influence on the composition of the gas phase over the melt of treating the oxide and metal solutions as separate layers.

The results from the exercise have shown that the adoption of various assumptions in the modelling of the solutions has resulted in considerable differences. In particular, the inclusion of complex stable molecules in an ideal solution phase or the use of binary interaction terms for non-ideal solutions that stabilise considerably certain components can reduce significantly the extent of release of species by vaporisation. Other smaller differences have arisen due to either variations in the thermodynamic values for particular species or the general expressions used to calculate the values over extended temperature ranges.

In order to reduce the uncertainties in the modelling of core-concrete melts, a thorough assessment of the thermodynamic data and the available phase diagrams for both oxide and metal systems should be performed and the modifications of the models made to account for the results from experimental programmes. For example, the results from the MCCI experiments of the ACE (Advanced Containment Experiments) Phase C programme is providing important information that will help to resolve some of the uncertainties.

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## 1. Introduction

The objective of the benchmark exercise is to assess the magnitude of the differences in the predicted releases of species by vaporisation in the chemical modelling of core-concrete interactions. These differences arise from the use of various models for the condensed phases in the codes and from the choice of the thermodynamic data for the species considered in the model. The purpose of Part A of the exercise was to establish whether the method of calculation of the chemical equilibria in itself introduces discrepancies in the results. A simplified standard problem was devised to test the numerical methods of the codes used by various organisations. The objective of Part B is to investigate the uncertainties resulting from differences in the chemical thermodynamic treatment of core-concrete melts.

## 2. Summary of the results from Part A

The results from this simplified problem have shown that, with the exception of the VANESA code, there is good agreement between the results using different codes and different versions of the same code used to determine the equilibrium composition of multicomponent systems [1]. In particular the extremely small releases of some of the species were accurately predicted. These codes determined the equilibria either by the direct minimization of the total Gibbs free energy of the system or by the Brinkley method. The latter method involves the solution of a number of equations expressed in terms of the equilibrium constant. The VANESA 1.01 code, which has been developed specifically to model the release of radionuclides and the generation of aerosols during core-concrete interactions, was not designed to treat the highly simplified problem in Part A. Modifications to the code and to the set problem were required in order to produce a fair comparison. The assessment of the results from the VANESA calculations showed that the equilibrium solver in the code is also capable of predicting extremely small releases of species. The differences in the results between the VANESA calculations and the others arises due to the specific assumptions used in VANESA to model dynamic core-concrete interactions.

## 3. Specification of the problem

Part B of the exercise is based on calculations of the chemical equilibria for three cases of more realistic composition than in Part A. The first calculation, Case A, considers an initial melt composition of high zirconium metal content relative to the other cases. In Cases B

and C, compositions of high silica and high calcia content respectively were considered. The ratio of gases to condensed phases in these cases is low and is intended to describe the situation during a few minutes of core-concrete interaction in a PWR cavity. It should be noted that the purpose of the exercise is to investigate the uncertainties resulting from differences in the chemical thermodynamic treatment of core-concrete melts and, therefore, not too much emphasis should be placed on the specification of the initial composition or the actual amounts of each element estimated by each participant to be in the gas phase.

Although the input amounts of certain species were specified in the problem, the method of treatment of the liquid and solid phases and the selection of thermodynamic data were chosen by the participants (.ie. the components of the phases, the representation of solutions as ideal or non-ideal, the consideration of the configuration of the melt).

### 3.1. Input parameters

In each of the Cases A, B and C, the system consists of a gas phase, a liquid oxide solution phase, a liquid metal solution phase and condensed solid phases all in chemical equilibrium. The initial components and the input amounts of the melt are shown in Table 1.

**Table 1** Initial compositions and input amounts

Component	Amount (moles)		
	Case A	Case B	Case C
UO <sub>2</sub>	10 <sup>5</sup>	10 <sup>5</sup>	10 <sup>5</sup>
Zr	10 <sup>5</sup>	10 <sup>4</sup>	10 <sup>4</sup>
SiO <sub>2</sub>	10 <sup>4</sup>	10 <sup>5</sup>	10 <sup>4</sup>
Fe	10 <sup>5</sup>	10 <sup>5</sup>	10 <sup>5</sup>
SrO	10 <sup>2</sup>	10 <sup>2</sup>	10 <sup>2</sup>
CaO	10 <sup>4</sup>	10 <sup>5</sup>	10 <sup>5</sup>
La <sub>2</sub> O <sub>3</sub>	10 <sup>2</sup>	10 <sup>2</sup>	10 <sup>2</sup>
CeO <sub>2</sub>	10 <sup>3</sup>	10 <sup>3</sup>	10 <sup>3</sup>
Mo	10 <sup>2</sup>	10 <sup>2</sup>	10 <sup>2</sup>
H <sub>2</sub> O	10 <sup>2</sup>	10 <sup>2</sup>	10 <sup>2</sup>
CO <sub>2</sub>	10 <sup>2</sup>	10 <sup>2</sup>	10 <sup>2</sup>

### 3.2 Equilibrium calculations

The calculation of the equilibrium composition for each case was to be carried out at temperatures of 2000K and 2500K and at a total pressure of 1 atmosphere. The results from these calculations were to be expressed as the number of moles of each element in the gas phase at equilibrium. In addition, the participants were requested to provide information regarding the type of solution models and thermodynamic data used in the exercise.

### 4. Participants

In this part of the benchmark exercise, six sets of solutions to the problem have been received from groups using different codes. A list of the participants and the organisations represented is shown in Table 2 together with the name of the code employed. A number of solutions was submitted by Powers for a particular case (Case B 2000K) in order to demonstrate the effect on the equilibrium composition of using different models for the solution phases.

Table 2 Participants in the Part B exercise

Participant	Organisation	Code*	Ref.
M A Mignanelli	AEA Technology, Harwell, UK	SGMX	MM(SGMX)
J Dufresne	CEA, Fontenay aux Roses, France	GEMINI	JD(MELE)
K Muramatsu	JAERI, Japan	MPEC2	KM(MPEC)
J J de Wolff	KEMA, Arnhem, Netherlands	SGMX-PV	JW(SGPV)
D A Powers	Sandia National Laboratory, USA	BRINKLEY	DP(BRIN)#
G Capponi	ENEA, Rome, Italy	VANESA 1.01	GC(VASA)## GC(VASB)

\* SGMX refers to the SOLGASMIX code developed by G Eriksson

SGMX-PV refers to the adaptation of the SOLGASMIX code by T Besmann, ORNL

BRINKLEY refers to code based on the Brinkley method

# Solutions for Case B 2000K are termed DP(BRIN),DP(BRI1),DP(BRI2) and DP(BRI3)

## GC(VASA) and GC(VASB) refer to calculations with and without coking resp.

## 5. Results

The results of the various calculations expressed as the number of moles of each element in the gas phase at equilibrium are shown in Figures 1 to 6; the results of the extra calculations performed by Powers are shown in Figure 3. The contributor for each set of results can be obtained by referring to the references in Table 2. An examination of the results showed that all the participants had used the correct input quantities for each calculation.

### 5.1. Comparison of the thermodynamic treatment

It can be seen from these figures that there are considerable differences between the results. It should be noted that, at present, it is not known which of the calculations, if any, are close to the *correct* solutions to the problems as different models for the melt have been employed based on various assumptions. In the following sections the models used by each participant are described first. The factors that have contributed to the variations between the results for each case, such as the choice of thermodynamic data, the composition of the gas phase and the treatment of the oxide and metal solutions as either ideal or non-ideal, are then discussed.

With the exception of the VANESA contribution, the thermodynamic data used by each participant and the source of the data were supplied with the results. An assessment of the data used is restricted to a comparison with the latest available data published in the open literature. In some cases the Gibbs energy of the substance is used,  $G^\circ$ , and in others the Gibbs energy of formation from the elements,  $\Delta_f G^\circ$ . A simple comparison between the values is therefore not informative.

The species that have been considered by each participant for the calculations can be seen in the appendix where all the results for Case B at 2000K are presented. In the assessment, the results from each participant have been compared with those from the author (ie MM(SGMX)). The comparison has been done only for convenience and is not intended to imply that the models used in MM(SGMX) or the code used, SOLGASMIX, are to be preferred. It was mentioned in section 4 that a number of solutions to the problem for Case B at 2000K were submitted by Powers. The results for this case are used, therefore, in the discussion of the influence of the thermodynamic treatment of the melts on the variation of the equilibrium composition.



### 5.1.1. Thermodynamic modelling

The central problem in the calculation of thermodynamic equilibria is to obtain a representation of the Gibbs free energy of the total system as a function of temperature, pressure and composition. The equilibrium state is simply given by the weighted sum of the Gibbs free energies of the individual phases at equilibrium. If the phase is a pure substance then its Gibbs free energy can usually be obtained from standard sources of thermochemical data. The Gibbs free energy for solution phases is more complicated to express. An important quantity for solution phases is the Gibbs free energy of mixing,  $\Delta G^{\text{mix}}$ , which is the change in Gibbs free energy accompanying the formation of the solution from its constituents. For an ideal solution,  $\Delta G^{\text{mix}}$  is given by the configurational entropy change on forming the solution. In a non-ideal solution, however,  $\Delta G^{\text{mix}}$  will be given by the ideal configurational entropy change plus an excess Gibbs free energy,  $G^{\text{XS}}$ . In order to derive the interaction parameters that describe the deviation from ideal behaviour it is common to express  $G^{\text{XS}}$  in terms of a polynomial in composition. For some solution phases a simple polynomial description of the excess Gibbs free energy is not sufficient to give a good representation. This is particularly true of systems in which there are strong interactions between atoms or molecules of the different components of the solution, which leads to pronounced minima in the Gibbs free energy at a particular composition. In such cases it may be appropriate to use, for example, an associated solution model in which an associate,  $A_p B_q$ , is allowed in the description of the solution between species A and B.

### 5.2. The MM(SGMX) calculations

The model consists of a gas phase, an oxide solution phase and a metal solution phase, both solutions being treated as ideal; the number of species in each phase are 56, 22 and 10 respectively. The constituents of the gas phase include the elements, the oxides and the mono and dihydroxides for each component. In the case of uranium, the oxyhydroxides were also considered in the data set. The thermodynamic data for the species have been obtained from standard reference tables [2-6] and from thermodynamic assessment studies [7-9]. The data for the mono and dihydroxides were obtained from the assessment of Jackson [8] and those for the oxyhydroxides from Krikorian [9], a correction being applied to allow for an error in the reported values. In the data set, expressions for the Gibbs energy of formation of the species, relative to the elements in their standard states at 298K, were in the form,

$$\Delta_f G^\circ = A + BT \quad (\text{J.mol}^{-1})$$

where T is the temperature in Kelvin and the coefficients A and B were obtained by fitting the available data over the temperature range 2000 to 2500K. Due to the lack of

data at high temperature for some of the species, the values for A and B were derived by extrapolation.

The model for the oxide solution considers the melt to be an ideal solution of assumed compounds involving the simple binary oxides (eg  $\text{UO}_2$ ,  $\text{ZrO}_2$ ,  $\text{CeO}_2$ ) and complex molecules formed by association (eg  $\text{SrSiO}_3$ ,  $\text{CaSiO}_3$ ,  $\text{SrZrO}_3$ ). This type of constitutional model was originally proposed by Schenck [10] and has been developed further by Hastie for the prediction of phase equilibria of multicomponent oxide mixtures [11]. The deviation of the simple component oxides from ideal thermodynamic activity is attributed to the formation of these stable complex molecules. By assuming an ideal mixture of all the constituents the thermodynamic activities and mole fractions at equilibrium are equivalent quantities in the model. In general the simple and complex constituents are established stable compounds that are represented in equilibrium phase diagrams. This modelling approach has been validated by Hastie by comparisons with experimentally determined activity data, derived mainly by high temperature mass spectrometry, for binary to sexternary mixtures of the components  $\text{Na}_2\text{O}$ ,  $\text{K}_2\text{O}$ ,  $\text{CaO}$ ,  $\text{MgO}$ ,  $\text{Al}_2\text{O}_3$  and  $\text{SiO}_2$ .

### 5.3 . *The JD(MELE) calculations*

#### 5.3.1 . *Model*

The models used in these calculations are complex and based on thermodynamic and phase diagram data compiled and assessed by the French organisation Thermodata. The system consists of a gas phase containing 73 species, an oxide liquid phase of 10 components, a metal liquid phase of 10 components, an ideal solid solution of 4 components and 33 condensed, stoichiometric phases. The components of the gas phase include elements, oxides, hydrides, organic species, carbides and some hydroxides, the mono and di-hydroxides of Ca, Sr and Fe. The oxide and metal liquids are both treated as non-ideal. In the case of the oxide liquid, only interaction terms describing a regular solution for the binary system  $\text{CaO-SiO}_2$  have been estimated. A number of binary interaction terms derived from an existing data base on metal alloys, THERMALLOY, were used to describe the metal liquid; these terms were evaluated by optimising the thermodynamic data and phase diagram information. As well as the interaction terms for the binary systems metal-metal and metal-carbon, values for the ternary system  $\text{Ca-Fe-Si}$  have also been determined. The values of  $\Delta_f G^\circ$  that were used in the calculations for the gas and condensed phases were obtained from standard reference tables [2][3].

### 5.3.2 . Results

The equilibrium compositions for all the cases consisted of gas and liquid and solid solution phases; no solid compounds were formed. The use of such a complicated model makes it difficult to determine the main reasons for the differences between these results and the values of MM(SGMX). There are, however, certain trends in the results for Case A and the results obtained for both Cases B and C. In the former case the oxygen potential of the system at equilibrium is low due to the high, initial zirconium content (i.e. an oxygen potential of  $-691\text{kJ.mol.}^{-1}$  for Case A at 2000K compared with values of  $-448\text{kJ.mol.}^{-1}$  and  $-463\text{kJ.mol.}^{-1}$  for Cases B and C respectively). For cases B and C the initial zirconium contents are the same but an order of magnitude lower than the amount specified in Case A.

The model used to describe the metal solution is the dominant factor in the more reducing system for Case A. The interaction terms are such that, relative to the ideal solution model, a higher proportion of the initial inventory of the components are partitioned into the metal liquid, in particular Sr, Ce and Si. Hence, the higher releases for Sr and Ce reflect the higher volatility of the metal compared to the oxide. The opposite is true in the case of Si, the partitioning of all of the inventory into the metal solution and the lower volatility of the metal compared to the oxide results in a lower gas release. In Cases B and C, the oxygen potential of the system is higher and the components are partitioned mainly to the oxide solutions. The liquid and solid solutions consist of the binary oxides only and apart from the inclusion of interaction terms for the CaO-SiO<sub>2</sub> system the solutions are treated as ideal. This would account for some of the observed differences; in particular the amount of Sr in the gas phase would be reduced if parameters describing the formation of SrZrO<sub>3</sub> were included in the model. The selection of MoO<sub>3</sub> as the only binary oxide of molybdenum in the liquid solution model, rather than the lower oxide MoO<sub>2</sub>, would account for the higher concentration of Mo in the gas. Other differences in the results compared to the values for MM(SGMX) are attributed to the inclusion of more species in the gas phase. The addition of LaO<sub>2</sub>(g) and, in particular, SiZrO<sub>4</sub>(g) into the data set of JD(MELE) and the choice of the values for the thermodynamic functions have resulted in a greater amount of La and Zr in the gas phase for Cases B and C, the systems at the higher oxygen potential at equilibrium. For example, the inclusion of SiZrO<sub>4</sub>(g) into the data set of MM(SGMX) results in an increase of six orders of magnitude in the Zr release.

#### 5.4 . The KM(MPEC) calculations

##### 5.4.1 . Model

The system is represented by a gas phase consisting of 52 species and ideal solutions for the oxide and metal liquids. The liquids are treated very simply; the oxide phase consists of FeO, CaO, SiO<sub>2</sub>, UO<sub>2</sub>, ZrO<sub>2</sub>, SrO, La<sub>2</sub>O<sub>3</sub> and CeO<sub>2</sub> and the metal phase consists of Fe, Mo and Zr only. In the case of the oxide liquid, interactions between the binary oxides are not taken into account and the oxides MoO<sub>2</sub> and Ce<sub>2</sub>O<sub>3</sub> are not included. The reduction of some of the oxides to the metal is prevented by the omission in the database of Ca, Si, U, Sr, La and Ce from the metal solution. The thermodynamic data used in the calculations were obtained from the VANESA code [12] which was received as part of the USNRC Source Term Code Package Mod. 1.1. An update of the data in the VANESA code has been made but the current values have not been used in the exercise. The results from this set of calculations for the benchmark exercise have recently been published [13].

##### 5.4.2 . Results

The values for the amount of each element in the gas phase at equilibrium, with the exception of hydrogen, are all significantly greater than those determined by MM(SGMX). These differences can be attributed almost entirely to the simple models used for the liquid phases.

#### 5.5. The JW(SGPV) calculations

##### 5.5.1. Model

The components of the gas and liquid phases in the system and the treatment of the solutions are similar to those in MM(SGMX). The oxide liquid is treated as an ideal solution consisting of both the binary oxides and complex oxide species. The number of species in the gas phase and oxide and metal solution phases are 41, 30 and 9 respectively. The main omissions in the composition of the phases are the gaseous hydroxides and elemental carbon. With the exception of the gaseous oxides [14-16], the thermodynamic data were obtained from standard reference tables [17]. The Gibbs free energy values were calculated using the approximation,

$$G^{\circ}_T = \Delta H^{\circ}_{298} - (S^{\circ}_{298})T = A + BT \quad (\text{J.mol}^{-1}).$$

As  $S^{\circ}_{298}$  values have been used the absolute Gibbs energy has been determined not  $\Delta G^{\circ}_T$ . The use of such an approximation results in an error in the  $G^{\circ}_T$  values from neglecting the  $H^{\circ}_T - H^{\circ}_{298}$  and  $S^{\circ}_T - S^{\circ}_{298}$  (.ie. the appropriate integration of the heat capacity  $C_p^{\circ}$ ) terms and the enthalpy and entropy contributions of any phase transitions. The magnitude of the

error in neglecting the  $C_p^\circ$  contributions is usually not significant although the error does increase with increase in temperature. However, a larger error is incurred in neglecting the thermodynamic values for phase transitions, in particular the contributions on melting. Such approximations should only be used when limited or no thermodynamic data are available.

#### 5.5.2. Results

The reasons for the differences in the results have been covered in the above section. Although the omission of carbon from the metal solution has contributed to some of the discrepancies, in particular the amount of C in the gas phase, the main reason for the difference is the use of an approximation to calculate the thermodynamic data.

### 5.6. The DP(BRIN) calculations

#### 5.6.1. Model

The model used in the calculations for Cases A, B and C consists of a gas phase, an oxide liquid phase and a metal liquid phase, all the mixtures being treated as ideal. The number of species in the gas phase is 64. These include elements, oxides, hydroxides and hydrides and are in the main species listed in the data base for the VANESA model. A molecular model of the oxide liquid phase was selected consisting of 20 components. These include binary oxides and the orthosilicates, metasilicates, zirconates and molybdates of the alkaline earths. The sesquioxides of Ce and La are represented by  $CeO_{1.5}$  and  $LaO_{1.5}$  and the orthosilicates of Ca and Sr by  $CaSi_{0.5}O_2$  and  $SrSi_{0.5}O_2$ . The metal phase consists of 8 species only; La and Ce are not considered as components.

In addition to the calculations performed using the above model, DP(BRIN), three more were carried out for Case B at 2000K to investigate the influence of various treatments of the solution phases on the results for the equilibrium composition [18]. The first, DP(BRI1), used a model with the same gas phase composition but with a much simpler description of the oxide and metal phases. The constituents of the oxide solution are now limited to the binary oxides and the metal solution only comprises Zr, Fe, Mo and C; both solution phases are still considered ideal. In order to determine the effect of non-ideality, a further calculation was performed using expressions derived from the ferrous-metallurgy literature [19] for the activity coefficients for Zr, U, Mo, Ca, Sr, Si and C (DP(BRI2)). The activity coefficient of Fe was assumed to be unity. The other details of the model, constituents of the phases and Gibbs free energy expressions, are the same as for the main calculations. The final factor investigated was the uncertainty in the thermodynamic properties of the gas phase species (DP(BRI3)). The main calculation was repeated using

values for the enthalpies of formation for all the gaseous species of Sr, Ce and La in the data set that increased the stability of these species; the values were set at the limit of the uncertainty ascribed in the literature.

### 5.6.2. Results

The results from the main calculations, DP(BRIN), for Cases A and C at both 2000K and 2500K are in reasonable agreement with the results from MM(SGMX). The values for U, Ca, Zr and La, however, do still differ by up to two orders of magnitude. The results for most of the elements for Case B, the system at the highest equilibrium oxygen potential, differ, particularly for the calculation at 2500K. A number of factors contribute to these differences in the results. The Gibbs free energy values for condensed  $\text{UO}_2$  in the data set for DP(BRIN) are more positive by  $72 \text{ kJ.mol}^{-1}$  which results in a higher oxygen potential for the system. The data selected in DP(BRIN) are estimated values for liquid urania whereas the values in MM(SGMX) are for the solid urania. This mainly affects the release of uranium but can also influence the releases of the other species (.eg. La). Another factor is the inclusion of  $\text{CaZrO}_3(\text{s})$  as a species in the oxide solution of DP(BRIN) which reduces the activity of the component binary oxides and hence reduces the extent of vaporisation of Ca and Zr. The selection of the stoichiometries for the meta and orthosilicates of Ca and Sr in the oxide phase also influences the gas phase composition (.ie.  $\text{MSiO}_3$  and  $\text{MSi}_{0.5}\text{O}_2$  respectively where  $\text{M}=\text{Ca}$  or  $\text{Sr}$ ).

The results obtained from the additional calculations for Case B at 2000K, DP(BRI1), DP(BRI2), DP(BRI3) [18], are best assessed with respect to the results for DP(BRIN). These data were also compared in the report submitted by the participant. The effect of the use of a simple model to describe the oxide and metal solutions on the composition of the gas phase, DP(BRI1), can be clearly seen in Figure 3. Whereas with the more complex model, the partial pressure of  $\text{SiO}(\text{g})$  was calculated to be only  $3.05 \times 10^{-2}$  atmospheres, with the simple model  $\text{SiO}(\text{g})$  is the dominant gas phase species, at a partial pressure  $9.81 \times 10^{-1}$  atmospheres. The amount of U, Ce, La and Sr is also increased by approximately three orders of magnitude. The results for all the elements are similar to those of KM(MPEC) in which a simple model for the oxide solution was used. The introduction of non-idealities into the model of the metal phase, DP(BRI2), enhanced the reduction of  $\text{SiO}_2$  to Si and inhibited the reduction of the oxide species of U, Zr, Sr and Ca. The equilibrium oxygen potential has also been increased by  $\sim 93 \text{ kJ.mol}^{-1}$ . In general, these factors have resulted in a decrease in the extent of release by vaporisation. The results from the calculations for DP(BRI3) show that the uncertainties in the thermodynamic properties of the gas phase species for Ce, La and Sr only have a small affect on the extent of vaporisation of these elements. The data for the Ce species had the largest uncertainty and resulted in an

increase in the vaporisation by a factor of three.

Although further calculations to examine the affect of the molecularity of the species in the oxide phase on the composition of the gas phase were not performed in Part B of the exercise, such an assessment was done for the simple problem in Part A. In addition to the calculation using the specified composition for the oxide phase,  $\text{UO}_2$ ,  $\text{U}_2\text{O}_{4.5}$ ,  $\text{ZrO}_2$ ,  $\text{Cr}_2\text{O}_3$ ,  $\text{La}_2\text{O}_3$  and  $\text{K}_2\text{O}$ , a second calculation was carried out with an oxide phase comprising of  $\text{UO}_2$ ,  $\text{UO}_{2.25}$ ,  $\text{ZrO}_2$ ,  $\text{CrO}_{1.5}$ ,  $\text{LaO}_{1.5}$  and  $\text{KO}_{0.5}$ . The results from these two calculations show that, although the gas phase compositions for most of the species and the oxygen potential of the systems are similar, the partial pressures of the lanthanum species differ by approximately an order of magnitude. The amount of La in the gas phase is 7.42 and 0.31 moles respectively; the difference is a direct result of the models used to describe the oxide solution .

### 5.7. *The GC(VASA) and GC(VASB) calculations*

#### 5.7.1. *Model*

The VANESA code was designed to deal with a dynamic core-concrete interaction and not with the somewhat artificial equilibrium problems set for Part B of this exercise. In order to perform the calculations a number of modifications have to be made to the code. A description of the type of modifications that are needed together with details of the assumptions in the VANESA code pertaining to the modelling of dynamic core-concrete interactions are discussed in the final report for Part A of the exercise [1]. It should be emphasised, however, that in the VANESA code there is no direct interaction between the two liquid phases; the metal and oxide phases are not in equilibrium and interact only via the gas. The gas is first equilibrated with the metal phase to set the oxygen potential for the total system; any metal liquid that is oxidised is transferred to the oxide liquid phase. The gas, containing vapour species from some of the metal components, is then allowed to interact with the oxide phase and the vaporisation of species from the melt is then calculated from the oxide phase only. As it was specified in the problem for Part B that the gas phase and liquid oxide and metal solutions are all to be treated in equilibrium, the results of these calculations using the VANESA code cannot be readily compared to the other results. However, the results of the VANESA calculations are presented in order to discuss the influence on the composition of the gas phase over the melt of treating the oxide and metal solutions as separate layers.

In each case, two sets of results from VANESA calculations were provided, one set in which coking, that is the precipitation of carbon, can occur, GC(VASA), and a set in

which carbon is not allowed to form, GC(VASB). In all these calculations, the system is described by a gas phase and an oxide and metal solution phase, the solutions being treated as ideal. The gas phase comprises 64 species which include elements, oxides, hydrides and mono and di-hydroxides. The components of the oxide and metal phases are  $\text{UO}_2$ ,  $\text{SiO}_2$ ,  $\text{CaO}$ ,  $\text{FeO}$ ,  $\text{ZrO}_2$ ,  $\text{SrO}$ ,  $\text{La}_2\text{O}_3$ ,  $\text{CeO}_2$  and U, Zr, Fe, Mo, La, C (for cases where coking is considered) respectively.

### 5.7.2 Results

The values for the amount of each element in the gas phase for the calculations without coking are approximately a factor of two greater than those with coking. When the formation of condensed species of carbon, either as metal carbides or as free carbon, is not allowed, the only equilibrium phases that can form are  $\text{CO}_2(\text{g})$  and  $\text{CO}(\text{g})$ , in these cases predominantly  $\text{CO}(\text{g})$ . As the partial pressures of the other gas phase species are essentially the same in the two cases, the increase in the number of moles of  $\text{CO}(\text{g})$  when coking is not allowed results in an increase in the amount of the other species in the gas phase at equilibrium.

One of the reasons for the differences in the results between the VANESA calculations and the other calculations is due to the treatment of the melt as a layered structure as opposed to a mixture of two immiscible liquids in equilibrium. Although the oxygen potentials in the two layers are equal in the VANESA calculations, this value is set in the absence of the oxide phase. An assessment of the effect of the structure of the melt during core-concrete interactions on the extent of vaporisation of species has been carried out [20]. In general, the releases for the layered melt with the metal layer on the bottom were found to be less than for the mixed melt, particularly for the components that have gas phase species of high vapour pressure over a metal liquid compared to an oxide liquid. In these calculations [20] the same database for the two cases were used and, for the layered structure, the oxygen potential for the metal and oxide phases was allowed to change.

The lower releases of Fe and Zr for the VANESA calculations for all of the cases compared to those determined by the other codes is due to the adoption of a layered configuration. In the case of Zr an additional factor, as described in the Part A report, is that the vaporisation of zirconium from the metal phase is neglected and so only the vaporisation from the oxide phase contributes to the Zr release. The other main reason for the differences in the results is the limited number of components describing the oxide and metal liquids chosen for these VANESA calculations. In general, the releases for Ce, Sr and Si are greater compared to the results of the calculations from MM(SGMX). In the case of Ce, this is due to the omission of the sesquioxide and metal in the VANESA database. The



inclusion of zirconates and silicates in the MM(SGMX) database has in effect reduced the activity of the component oxides in the liquid and hence the amount of Sr and Si in the gas phase.

## 6. Discussion

In order to determine the origin of the discrepancies between the results from each participant for all the cases, the differences in the releases of the elements, expressed in orders of magnitude, are shown in Table 3. For each case the maximum differences between all of the submissions (termed All) and between the submissions of MM(SGMX), JD(MELE) and DP(BRIN) (termed Sel.) are presented. The particular submissions in the latter comparison were selected as comprehensive solution models and, in general, sound thermodynamic data had been used in the calculations. It should be stressed again that the absolute values of the gaseous component fractions that have been calculated by the participants are mainly determined by the exercise specification which only considers a few minutes of interaction and so have no significance in the context of a real MCCI event.

Table 3 Differences, in orders of magnitude, in the releases of the elements between the various submissions#

Element	Case A 2000K		Case A 2500K		Case B 2000K		Case B 2500K		Case C 2000K		Case C 2500K	
	All*	Sel.*	All	Sel.	All	Sel.	All	Sel.	All	Sel.	All	Sel.
O	6.0	1.0	4.0	0.5	4.5	1.5	2.0	1.5	5	2.5	3	1
H	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	0	0	0
C	6.0	1.5	3.5	1.0	4.5	2.0	2.5	1	4.5	3	2.5	1.5
U	4.0	1.5	3.0	0.5	4.0	2.0	4.0	2.5	3.5	2	3.5	0.5
Zr	4.5	0.5	4.5	0.5	10.0	9.0	6.5	4.5	9	8.5	5.5	4
Fe	5.5	0.5	6.0	0.5	6.0	0.0	7.0	2	5.5	0	6.5	0
Si	10.0	4.5	7.0	3.0	5.0	1.0	2.5	2	5	1.5	3	0.5
Ca	4.5	2.0	3.0	1.0	5.5	2.0	2.5	2	6	3.5	4.5	2.5
Ce	4.5	2.0	4.0	2.0	4.0	0.0	2.5	1.5	4	1	3.5	1
La	4.0	1.0	4.5	1.5	5.0	3.5	4.5	2	4	2.5	5	3
Sr	5.5	5.5	4.5	4.0	7.0	2.0	2.5	0.5	5	2	3.5	1.5
Mo	2.0	1.0	2.0	1.0	2.5	1.0	3.5	1.5	2	1	2.5	1

# Difference =  $\max(\Delta \log_{10} r_i)$  where  $r_i$  is the amount in moles of element  $i$  released.

\* All - Differences between all the submissions;

Sel. - Differences between MM(SGMX), JD(MELE) and DP(BRIN).

As can be seen the calculated releases differ by many orders of magnitude when all of the submissions are considered, the differences being greater for the calculations at the lower

temperature. In general, these differences can be attributed to the use of both simple and complex solution models to describe the liquid phases in the set problems. However, considerable differences still exist even when the submissions that have employed extensive models are compared. In this case, the discrepancies can be ascribed to the different data sets, the components of each phase and the thermodynamic expressions, that have been used in each model. The extent these factors influence the overall release is dependent on the oxygen potential of the system at equilibrium. For example, the differences in the Zr release for Case A, the system at the lowest oxygen potential, are small compared to the values for Cases B and C. As discussed in section 5.3.2, this is due to the inclusion of  $\text{SiZrO}_4(\text{g})$  into the data set of JD(MELE). The variation in the La release, although not to the same extent, is also dependent on the oxygen potential of the system. The opposite trend exists for the releases of Sr and Si; the main discrepancies occur for the low oxygen potential system.

## 7. Conclusions

The objective of Part B of the exercise was to assess the uncertainties resulting from differences in the treatment of the solution phases, the composition of each phase and the choice of thermodynamic data in the modelling of core-concrete interactions. In order to simplify the exercise, one of the specifications of the problem was that the participants should treat the gas phase and liquid oxide and metal solutions as all in equilibrium. In the case of the submission using the VANESA code, the metal and oxide phases in the melt are not in equilibrium and interact only via the gas. Therefore, the results of these calculations using the VANESA code cannot be readily compared to the other results. However, the results are presented in order to discuss the influence on the composition of the gas phase over the melt of treating the oxide and metal solutions as separate layers. It must again be stressed that as different assumptions have been used in the calculations from each participants, it is not possible to know which, if any, are close to the *correct* solution to the set problems.

It can be seen from the figures presenting the results for the amount of each element in the gas phase that the adoption of various assumptions in the modelling of the solutions has resulted in considerable differences. In particular, the inclusion of complex stable molecules in an ideal solution phase or the use of binary interaction terms for non-ideal solutions that stabilise considerably certain components can reduce significantly the extent of release of species by vaporisation. Other differences have arisen due to either variations in the thermodynamic values for particular species or the general expressions used to calculate the values over extended temperature ranges.

The factors that have been raised during the assessment of the data that contribute to the uncertainty in the releases are, in order of decreasing importance:

1. The representation of the oxide solution as either a simple or complex phase - the use of associate models or interaction parameters to describe non-ideal behaviour.
2. The representation of the metal solution as either a simple or complex phase - the use of parameters to describe metal-metal and metal-carbon interactions.
3. The thermodynamic expressions estimated for the components of the liquid oxide phase in the ideal solution models where data are limited or unavailable.
4. The thermodynamic expressions estimated for species in the gas phase where data are limited or unavailable.
5. The estimation of high temperature thermodynamic data from measurements made at low temperature.
6. The uncertainties in the assessed thermodynamic expressions for the species in the gas phase.

Some of the uncertainties in the modelling of core-concrete melts will be reduced by the thorough assessment of the thermodynamic data and the available phase diagrams for both oxide and metal systems and the modification of the models to account for the results from experimental programmes. Although the task is complex, such studies are being performed at present by some of the participants of this exercise. The results from the MCCI experiments of the ACE (Advanced Containment Experiments) Phase C programme is providing important information that will help to resolve some of the uncertainties. The releases of Ba, Sr, La and Ce species from the melt during recent tests have been low, indicating that these elements are indeed stabilised in the melt.

It must be noted that in order to use these improved models in a code to determine the effects of core-concrete interactions during reactor accidents, various other assumptions have to be made that also add to the uncertainty in the release of species from the melt. Whether the configuration of the melt is treated either as a mixture of immiscible liquids or as separate oxide and metal layers during the interaction and the influence of each liquid on setting the oxygen potential of the complete system are some of the factors which

have to be considered in the modelling of dynamic core-concrete interactions. The results from the VANESA calculations in this exercise provide an indication of the effect that these particular assumptions have on the releases.

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Amount of each element in the gas phase.

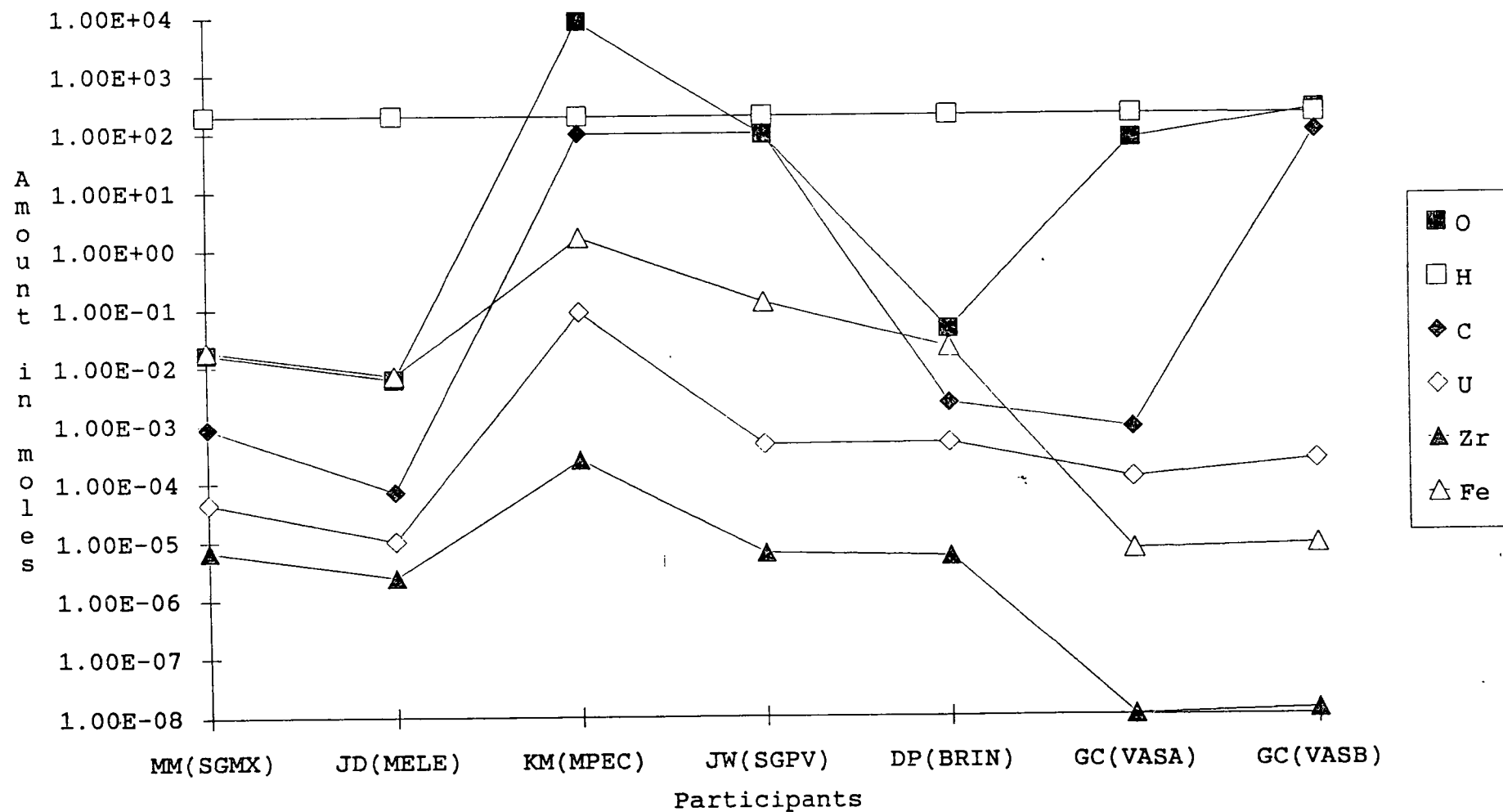


FIGURE 1 RESULTS OF THE CALCULATIONS FOR CASE A AT 2000K

Amount of each element in the gas phase.

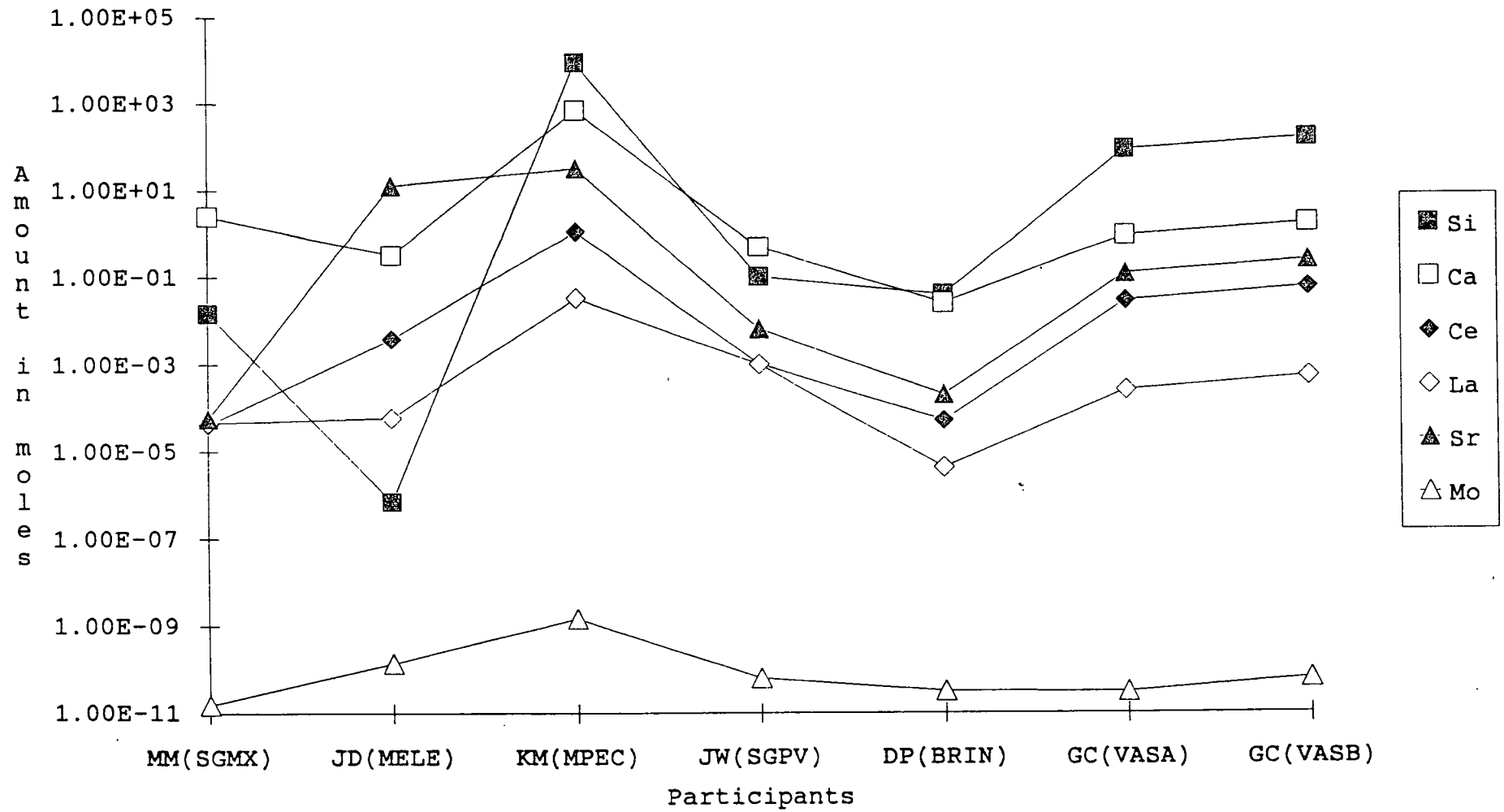


FIGURE 1 Continued

Amount of each element in the gas phase.

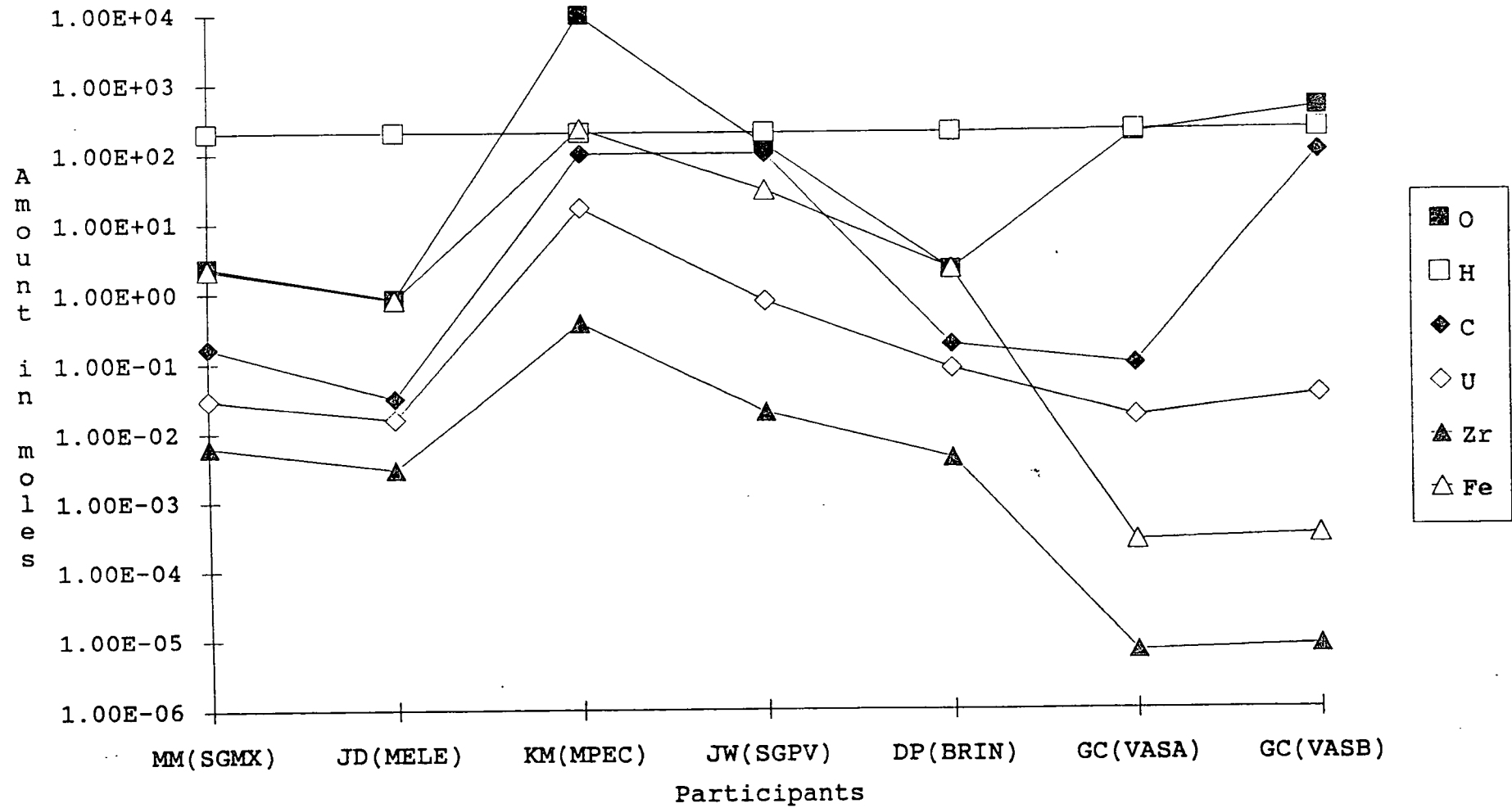


FIGURE 2 RESULTS OF THE CALCULATIONS FOR CASE A AT 2500K



Amount of each element in the gas phase.

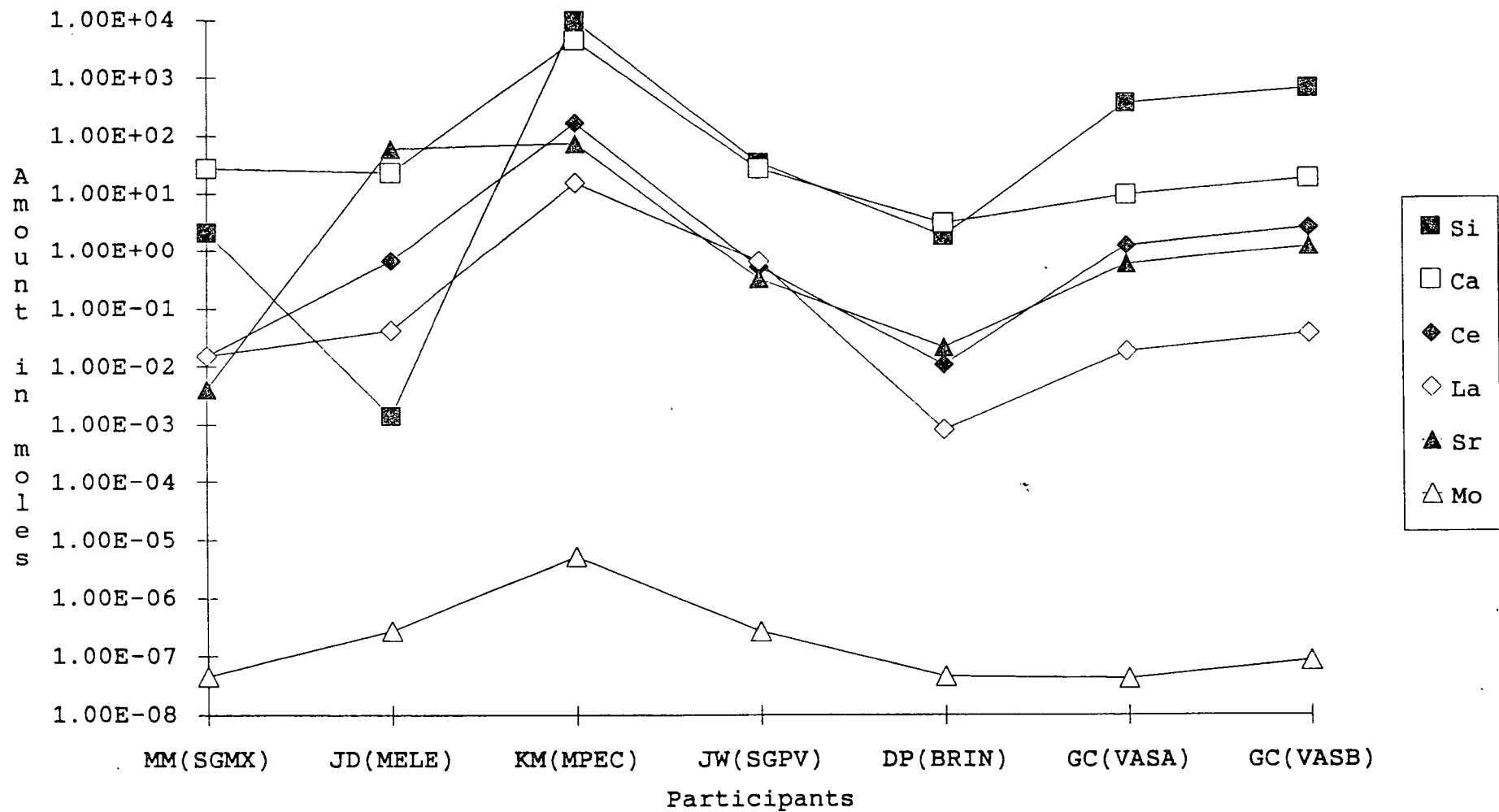


FIGURE 2 Continued

Amount of each element in the gas phase.

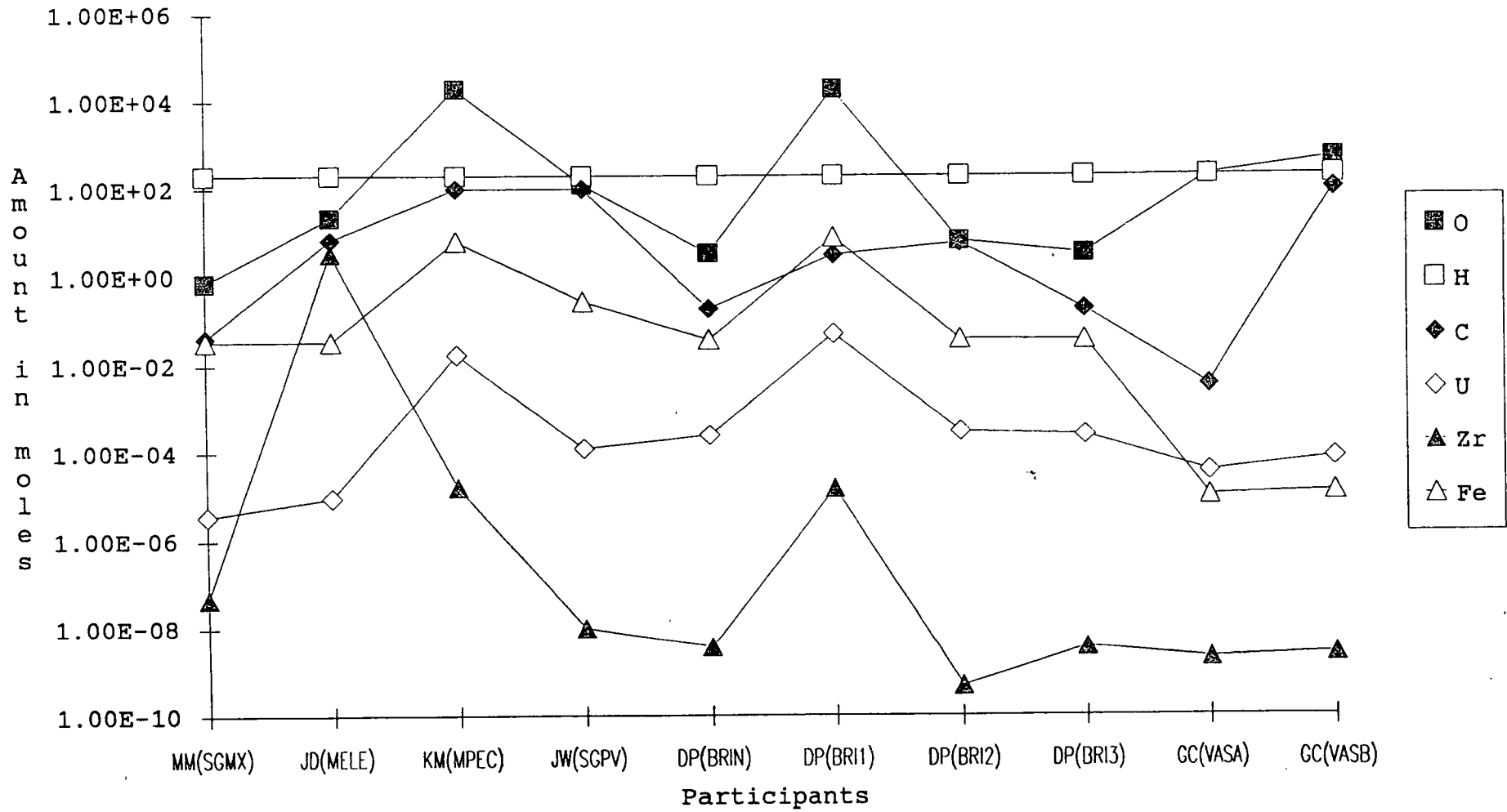


FIGURE 3 RESULTS OF THE CALCULATIONS FOR CASE B AT 2000K

Amount of each element in the gas phase.

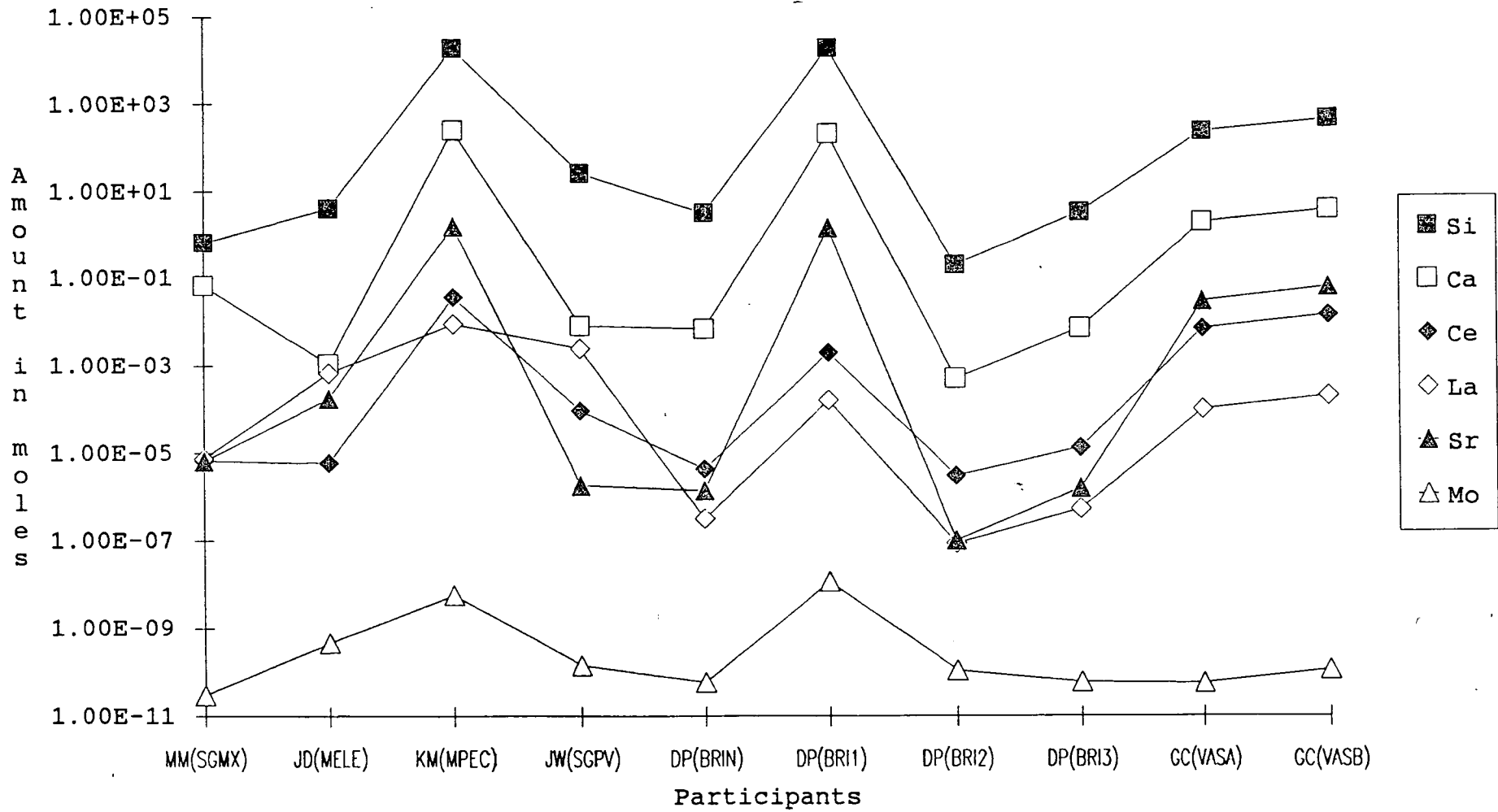


FIGURE 3 Continued

Amount of each element in the gas phase.

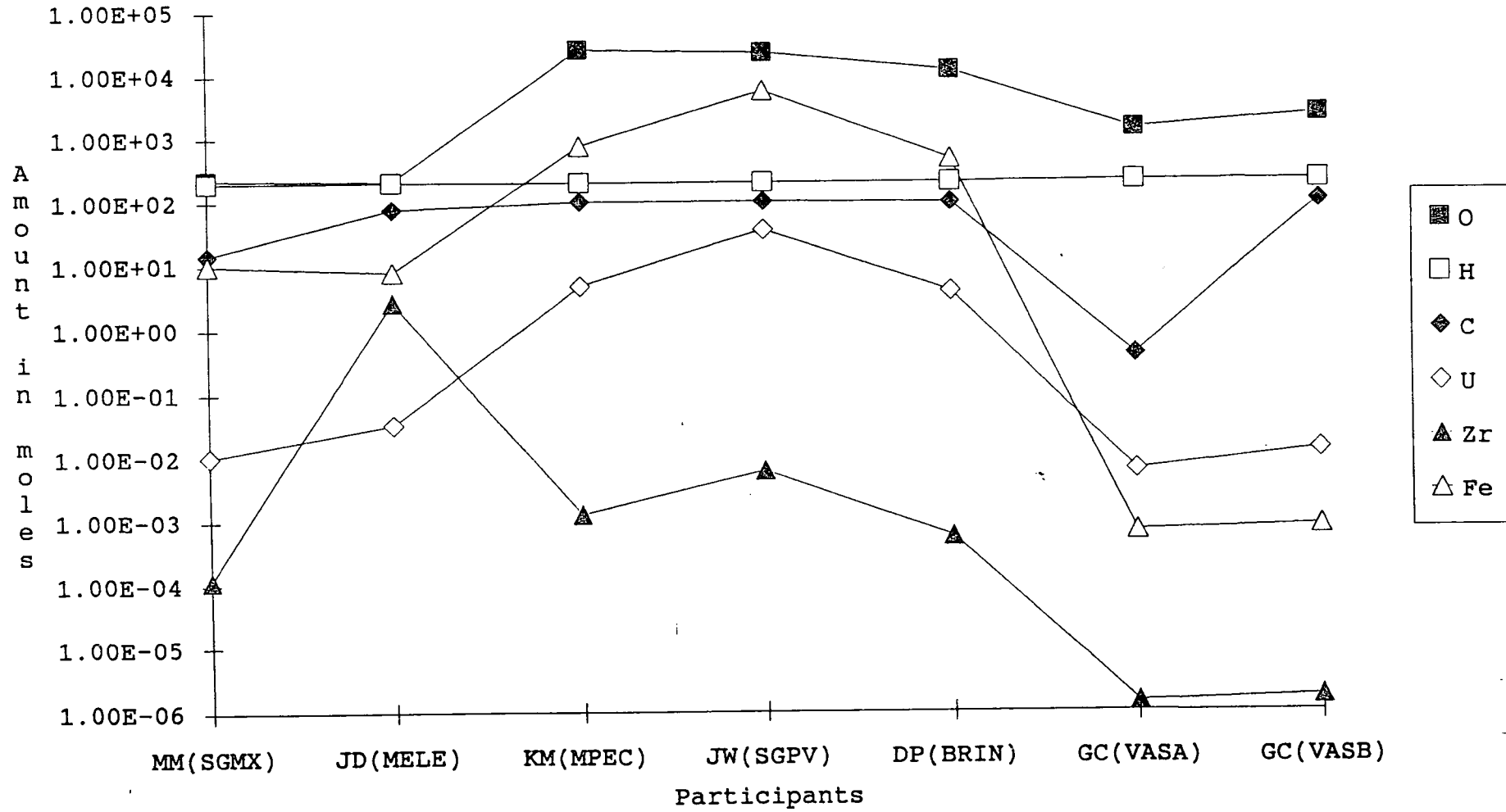


FIGURE 4 RESULTS OF THE CALCULATIONS FOR CASE B AT 2500K

Amount of each element in the gas phase.

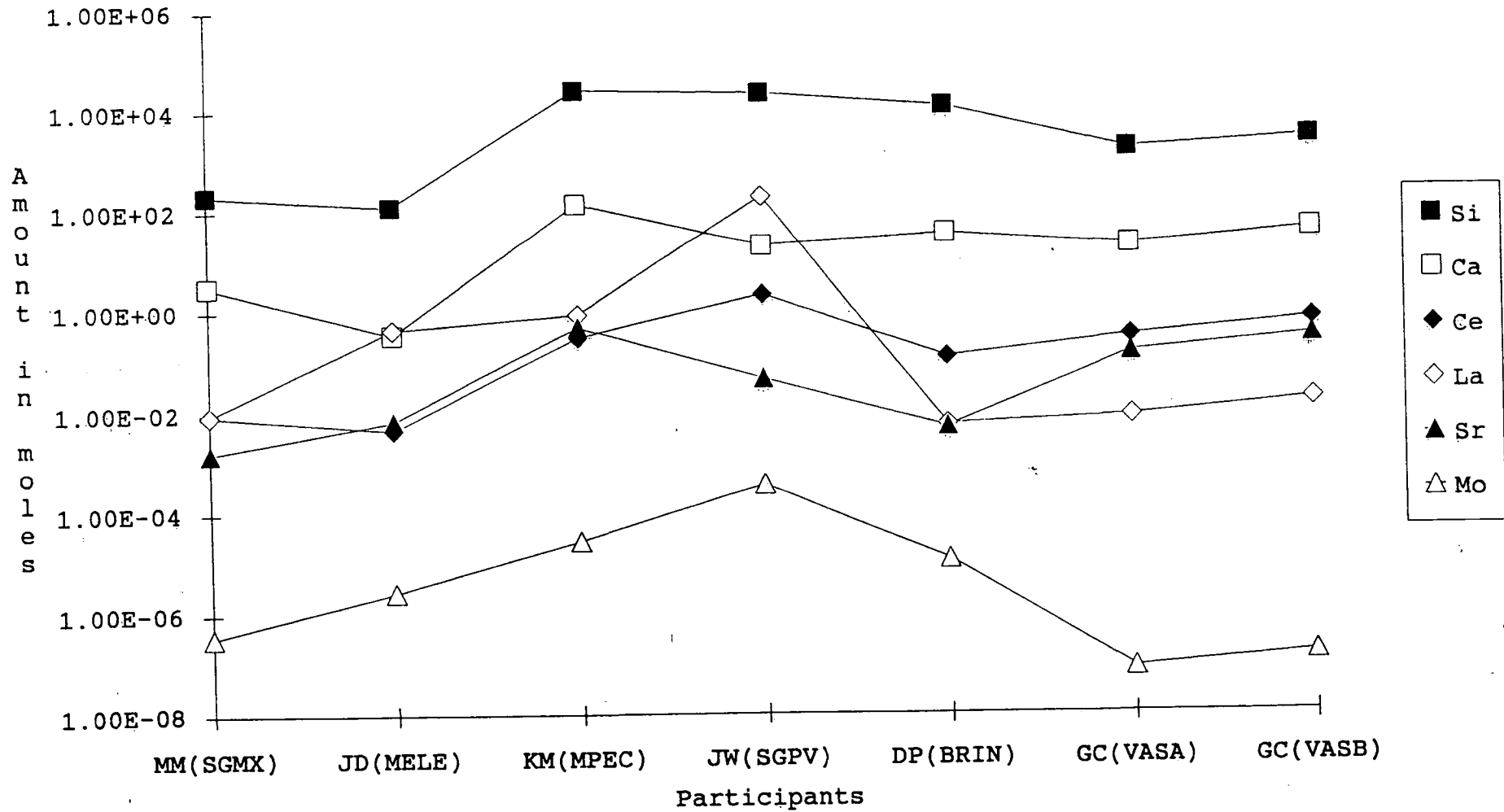


FIGURE 4 Continued

Amount of each element in the gas phase.

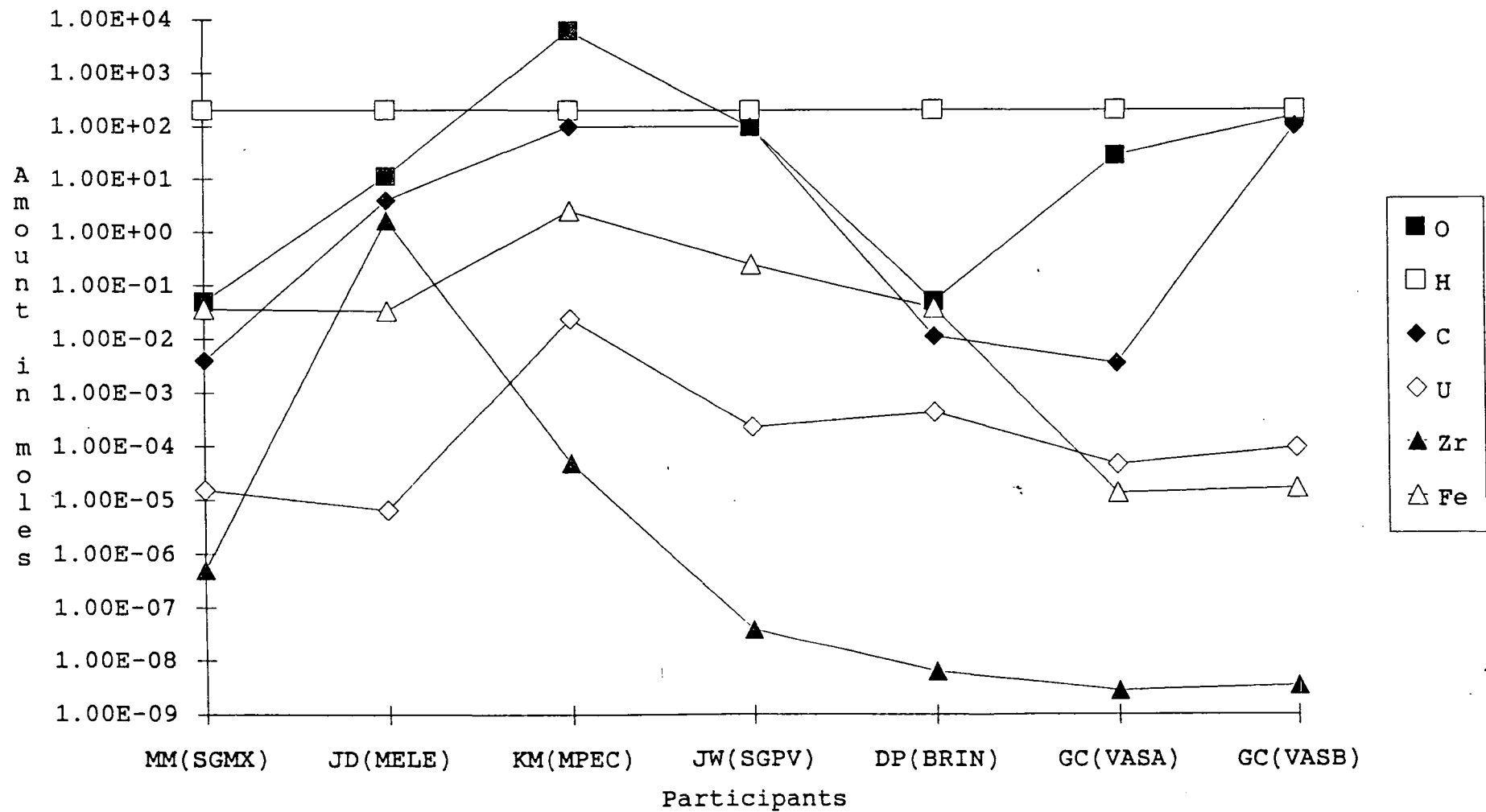


FIGURE 5 RESULTS OF THE CALCULATIONS FOR CASE C AT 2000K

Amount of each element in the gas phase.

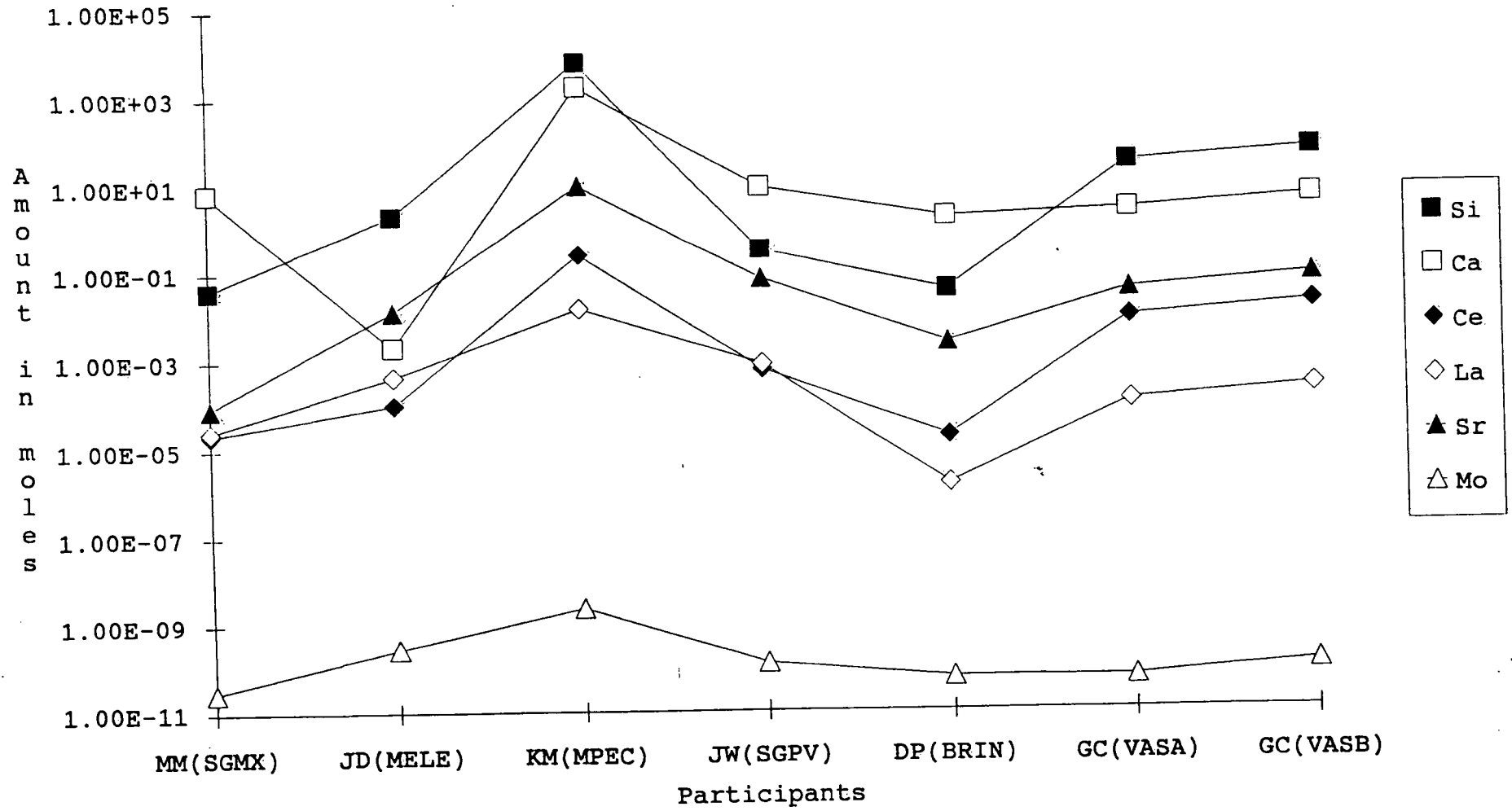


FIGURE 5 Continued

Amount of each element in the gas phase.

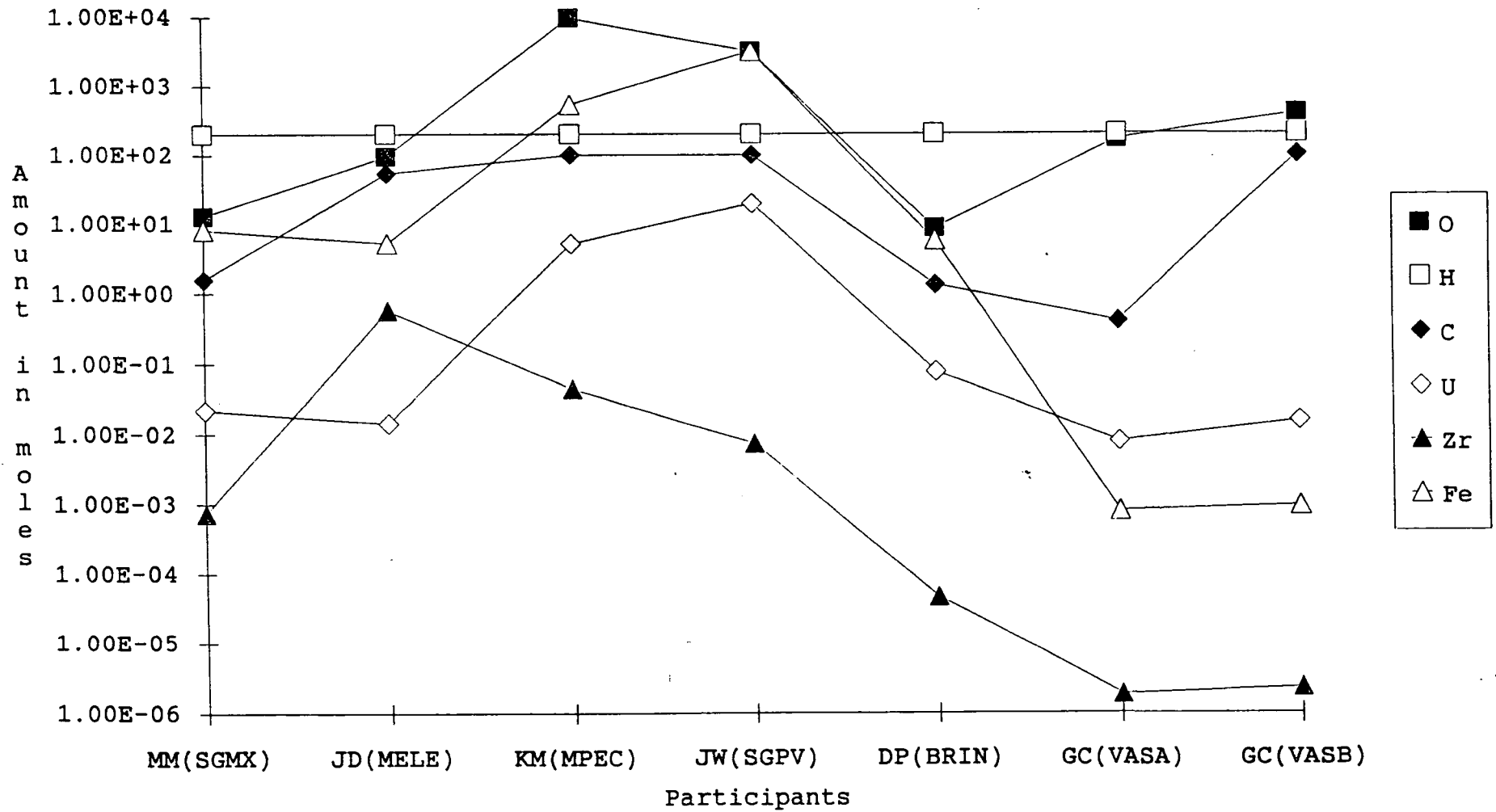


FIGURE 6 RESULTS OF THE CALCULATIONS FOR CASE C AT 2500K



Amount of each element in the gas phase.

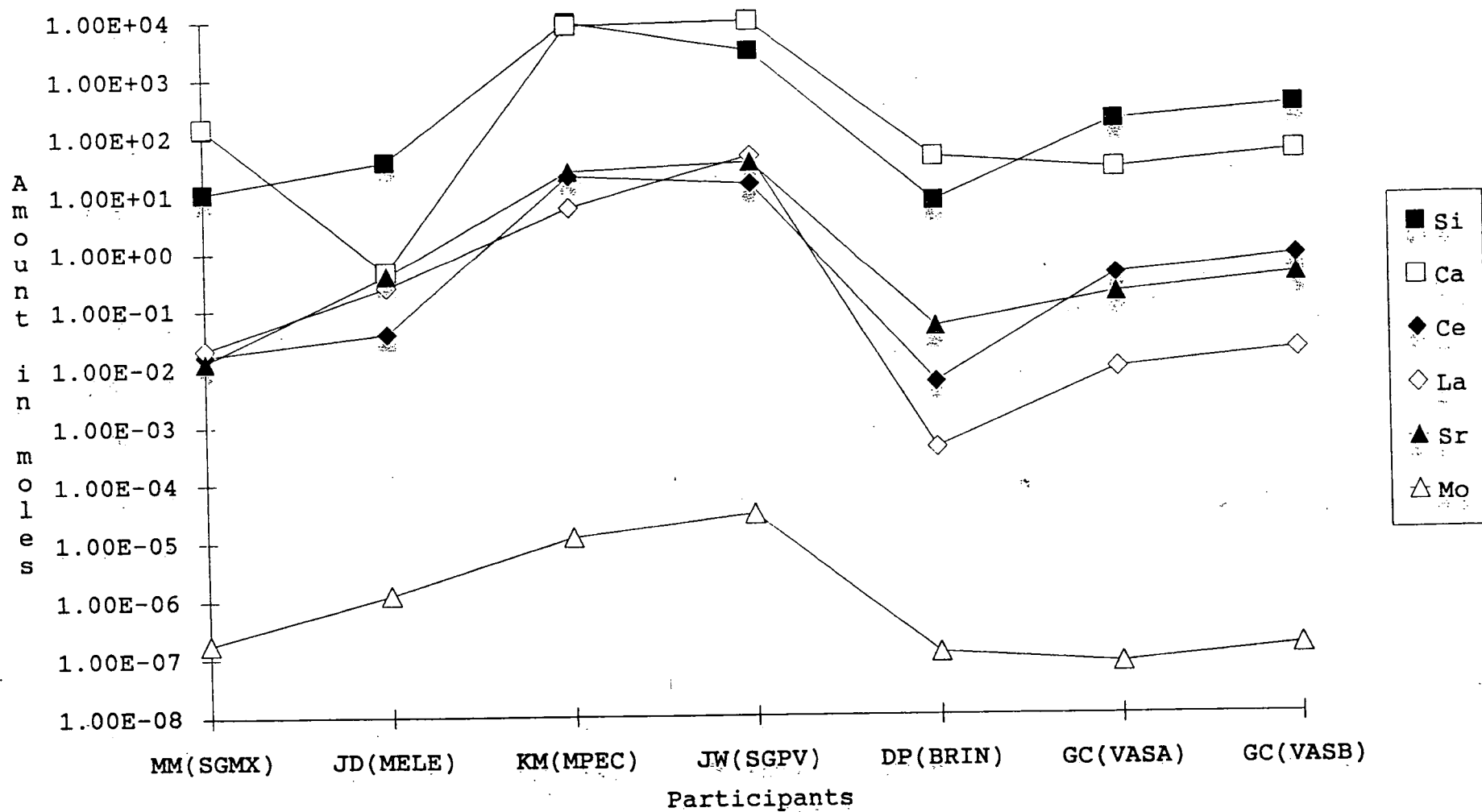


FIGURE 6 Continued



(b) JD(MELE)

.....BENCHMARK B:case B.....

T(K)=2000.0 P(atm)= 0.1000000D+01 V(l)= 0.1817135D+05

NOM PHASE	CONSTITUANT	NBRE DE MOLES	FRAC MOLLAIRE	DG/RT/MGL
METAL(L)		0.109662544D+06		-0.799564617D+00
	C	0.933757827D+02	0.851482913D-03	
	Ca	0.101298466D-02	0.923728945D-08	
	Ce	0.135459879D-02	0.123524290D-07	
	Fe	0.993350589D+05	0.905824860D+00	
	La	0.102978071D-03	0.939045061D-09	
	Mo	0.100000000D+03	0.911888380D-03	
	Si	0.101329711D+05	0.924013862D-01	
	Sr	0.904407894D-04	0.824719050D-09	
	U	0.997269377D-02	0.909398357D-07	
	Zr	0.112609503D+01	0.102687297D-04	
OXIDE(L)		0.150134518D+06		-0.322703505D+02
	CaO	0.465436475D+05	0.310012969D+00	
	CeO2	0.793552634D+03	0.528561084D-02	
	Ce2O3	0.103223003D+03	0.687536780D-03	
	FeO	0.664906990D+03	0.442874164D-02	
	La2O3	0.526461314D+01	0.350659877D-04	
	MoO3	0.344007239D-07	0.229132677D-12	
	SrO	0.999997340D+02	0.666067575D-03	
	SiO2	0.898630485D+05	0.598550199D+00	
	UO2	0.638130666D+04	0.425039275D-01	
	ZrO2	0.567957102D+04	0.378298815D-01	
OXIDE SS1		0.151485669D+06		-0.379596151D+02
	CaO(ss)	0.534563504D+05	0.352880578D+00	
	La2O3(ss)	0.947350048D+02	0.625372719D-03	
	UO2(ss)	0.936186834D+05	0.618003564D+00	
	ZrO2(ss)	0.431590034D+04	0.284904860D-01	
		NBRE DE MOLES	FRAC MOLLAIRE	P PART ou ACTI
H2(g)		0.994303082D+02	0.897965740D+00	0.897965740D+00
SiZrO4(g)		0.340265070D+01	0.307287990D-01	0.307287990D-01
CO(g)		0.561705551D+01	0.597593355D-01	0.597593355D-01
H2O(g)		0.484527226D+00	0.437581716D-02	0.437581716D-02
SiO(g)		0.580835811D+00	0.524559028D-02	0.524559028D-02
H1(g)		0.169806938D+00	0.153354461D-02	0.153354461D-02
Fe(g)		0.341322804D-01	0.308252272D-03	0.308252272D-03
CO2(g)		0.710279341D-02	0.641460864D-04	0.641460864D-04
LaO2(g)		0.656273414D-03	0.592687534D-05	0.592687534D-05
Ca(g)		0.898028686D-03	0.811019303D-05	0.811019303D-05
CaOH(g)		0.150257789D-03	0.135699415D-05	0.135699415D-05
CH4(g)		0.494356644D-04	0.446458768D-06	0.446458768D-06
H0(g)		0.849043831D-04	0.766780558D-06	0.766780558D-06
Sr(g)		0.146517080D-03	0.132321141D-05	0.132321141D-05
				LOG10(P)
				-0.467402328D-01
				-0.151245441D+01
				-0.122359424D+01
				-0.235894083D+01
				-0.228020563D+01
				-0.281430359D+01
				-0.351109371D+01
				-0.419282984D+01
				-0.522717421D+01
				-0.509096881D+01
				-0.586742202D+01
				-0.635021864D+01
				-0.611532891D+01
				-0.587837076D+01

CaOH2(g)	0.1750310190-04	0.1580723840-06	0.1580723840-06	-0.6801144000+01
SrOH(g)	0.2702810190-04	0.2440936770-06	0.2440936770-06	-0.6612443470+01
SiO2(g)	0.1009741430-04	0.9119082780-07	0.9119082780-07	-0.7040048840+01
UO2(g)	0.7287539400-05	0.6581454710-07	0.6581454710-07	-0.7181678100+01
CH2O(g)	0.3858539400-05	0.3484688170-07	0.3484688170-07	-0.7457836080+01
CeO(l)	0.5930226900-05	0.5355651290-07	0.5355651290-07	-0.7271187710+01
CH4O(g)	0.3525164400-05	0.3183613640-07	0.3183613640-07	-0.7497079640+01
SrO2H2(g)	0.1876148780-05	0.1694370010-07	0.1694370010-07	-0.7770991740+01
FeH2O2(g)	0.1786851900-05	0.1613725050-07	0.1613725050-07	-0.7792170460+01
CH3(g)	0.2108320650-05	0.1904046910-07	0.1904046910-07	-0.7720322360+01
UO3(g)	0.1990743360-05	0.1797861600-07	0.1797861600-07	-0.7745243740+01
FeO(g)	0.3537070790-05	0.3194366430-07	0.3194366430-07	-0.7495615270+01
SiH(g)	0.2322633150-05	0.2097594820-07	0.2097594820-07	-0.7678278400+01
Si(g)	0.3528619220-05	0.3186733730-07	0.3186733730-07	-0.7496654220+01
LaO(g)	0.9075889630-06	0.8196532920-08	0.8196532920-08	-0.8086369810+01
SrO(g)	0.9119088430-07	0.8235546220-09	0.8235546220-09	-0.9084307590+01
U1(g)	0.1032595930-06	0.9325484240-09	0.9325484240-09	-0.9030328610+01
CaO(g)	0.3643149920-07	0.3290167630-09	0.3290167630-09	-0.9482781970+01
H2MoO4(g)	0.1167620290-12	0.1054490370-14	0.1054490370-14	-0.1497693740+02
CH2(g)	0.5730734230-08	0.5175487330-10	0.5175487330-10	-0.1028604880+02
Si3(g)	0.4437871860-14	0.4007889500-16	0.4007889500-16	-0.1639708430+02
HO2(g)	0.6656985830-12	0.6011995050-14	0.6011995050-14	-0.1422098140+02
ZrO2(g)	0.5121931350-09	0.4625670940-11	0.4625670940-11	-0.1133482530+02
MoO2(g)	0.2988489160-10	0.2698936500-12	0.2698936500-12	-0.1256880730+02
CH12Si(g)	0.6696337640-32	0.6047534080-34	0.6047534080-34	-0.3421842170+02
C2H4(g)	0.9729274050-09	0.8786611370-11	0.8786611370-11	-0.1105617860+02
La(g)	0.1471444320-11	0.1328877090-13	0.1328877090-13	-0.1387651520+02
C5FeO5(g)	0.2313927020-28	0.2089732220-30	0.2089732220-30	-0.3067990940+02
Ce(g)	0.2258286320-10	0.2039482510-12	0.2039482510-12	-0.1269048000+02
C2H4O(g)	0.5028712800-16	0.4541484270-18	0.4541484270-18	-0.1834280220+02
C2O2(g)	0.1896499000-12	0.1712748520-14	0.1712748520-14	-0.1476630640+02
C5T(g)	0.3269425450-26	0.2952653060-28	0.2952653060-28	-0.2852978760+02
U(g)	0.1994616900-12	0.1801359840-14	0.1801359840-14	-0.1474439950+02
MoO3(g)	0.4981133140-12	0.4498514570-14	0.4498514570-14	-0.1434693090+02
La2O2(g)	0.1175780830-12	0.1061860240-14	0.1061860240-14	-0.1497393260+02
C4(g)	0.1260455260-23	0.1138330610-25	0.1138330610-25	-0.2594373160+02
H2O2(g)	0.1280344190-11	0.1156292520-13	0.1156292520-13	-0.1393693230+02
LA2O(g)	0.6150186550-17	0.5554299210-19	0.5554299210-19	-0.1925537070+02
Mo3(g)	0.0000000000+00	0.0000000000+00	0.1000000000-35	-0.3600000000+02
O3(g)	0.1587127780-22	0.1433352060-24	0.1433352060-24	-0.2484364710+02
C2O(g)	0.2352608270-10	0.2124665680-12	0.2124665680-12	-0.1267270940+02
C3(g)	0.1354389680-16	0.1223163790-18	0.1223163790-18	-0.1891251540+02
Si2C(g)	0.1926208800-11	0.1739579750-13	0.1739579750-13	-0.1375955570+02
SiC2(g)	0.3068491740-12	0.2771187690-14	0.2771187690-14	-0.1455733410+02
C2H(g)	0.3705912300-09	0.3346849000-11	0.3346849000-11	-0.1147536390+02
C2H2(g)	0.4321585000-12	0.3902869600-14	0.3902869600-14	-0.1440861600+02
Si2(g)	0.2770573890-10	0.2502134890-12	0.2502134890-12	-0.1260168930+02
UO(g)	0.2091015940-13	0.1888418840-15	0.1888418840-15	-0.1572390170+02
ZrO(g)	0.3269016810-09	0.2952284020-11	0.2952284020-11	-0.1152984190+02
MoO(g)	0.3786610130-09	0.3419728080-11	0.3419728080-11	-0.1146600840+02
C2(g)	0.3671584290-15	0.3315847010-17	0.3315847010-17	-0.1747940550+02
CH(g)	0.3039064310-10	0.2744611460-12	0.2744611460-12	-0.1256151910+02
Ca2(g)	0.5181184470-11	0.4679183060-13	0.4679183060-13	-0.1332983000+02
SiC(g)	0.9497474760-13	0.8577270950-15	0.8577270950-15	-0.1506665090+02
ZrH(g)	0.3701255520-14	0.3342643420-16	0.3342643420-16	-0.1647390970+02
Mo(g)	0.3860327180-10	0.3486302730-12	0.3486302730-12	-0.1245763490+02
Zr(g)	0.7860162020-15	0.7098596330-17	0.7098596330-17	-0.1714882750+02
C(g)	0.5308044480-11	0.4793751700-13	0.4793751700-13	-0.1331932450+02
O2(g)	0.2182138840-09	0.1970712910-11	0.1970712910-11	-0.1170537660+02
LaO2Zr(g)	0.0000000000+00	0.0000000000+00	0.5305760410+00	

U2(M.5(s)	0.000000000D+00	0.279741992D-03
MoO2(s)	0.000000000D+00	0.449620896D-08
MoSi2(s)	0.000000000D+00	0.441846710D-06
(eU2(s)	0.000000000D+00	0.112249959D-01
Zr(s)	0.000000000D+00	0.647308479D-08
Cl(s)	0.000000000D+00	0.143663952D-02
Mol(s)	0.000000000D+00	0.117669268D-02
SrO(s)	0.000000000D+00	0.625769069D-02
SiC(s)	0.000000000D+00	0.173478060D-04
UC(s)	0.000000000D+00	0.142867361D-07
Mo3C2(s)	0.000000000D+00	0.103720297D-11
U2C3(s)	0.000000000D+00	0.404542457D-18
Ce2O3(s)	0.000000000D+00	0.146003051D-02
Mo2C(s)	0.000000000D+00	0.887675979D-07
Mo2.9c2.1(s)	0.000000000D+00	0.795203143D-12
Mo3Si(s)	0.000000000D+00	0.697835476D-09
Mo5Si3(s)	0.000000000D+00	0.347830565D-16
Ca2O4Si(s)	0.000000000D+00	0.000000000D+00
CaO3Si(s)	0.000000000D+00	0.000000000D+00
Ca3O7Si2(s)	0.000000000D+00	0.000000000D+00
Ce2C3(s)	0.000000000D+00	0.522743027D-18
CeC2(s)	0.000000000D+00	0.690625430D-11
CaC2(s)	0.000000000D+00	0.450237932D-08
UC1.9(s)	0.000000000D+00	0.281753708D-07
UC1.93(s)	0.000000000D+00	0.388141132D-10
ZrC(s)	0.000000000D+00	0.471980521D-06
Ca3O5Si(s)	0.000000000D+00	0.000000000D+00

CONSTITUANT	PHASES SOLUTIONS	COMP DEFINIS	GAZ	TOTAL	ACTIVITE
C	0.933757827D+02	0.000000000D+00	0.662421724D+01	0.100000000D+03	0.143663952D-02
Ca	0.999999989D+05	0.000000000D+00	0.106582602D-02	0.100000000D+06	0.810800856D-05
Ce	0.99999994D+03	0.000000000D+00	0.593024948D-05	0.100000000D+04	0.188774199D-07
Fe	0.999999659D+05	0.000000000D+00	0.341376043D-01	0.100000000D+06	0.874437048D+00
H	0.000000000D+00	0.000000000D+00	0.200000000D+03	0.200000000D+03	0.947610542D+00
La	0.199999343D+03	0.000000000D+00	0.657181005D-03	0.200000000D+03	0.143230283D-08
Mo	0.100000000D+03	0.000000000D+00	0.447764052D-09	0.100000000D+03	0.117669268D-02
O	0.502678691D+06	0.000000000D+00	0.213085027D+02	0.502700000D+06	0.140382083D-05
Si	0.999960166D+05	0.000000000D+00	0.398340245D+01	0.100000000D+06	0.740027626D-03
Sr	0.999998245D+02	0.000000000D+00	0.175512521D-03	0.100000000D+03	0.132133558D-05
U	0.100000000D+06	0.000000000D+00	0.927828298D-05	0.100000000D+06	0.170901106D-07
Zr	0.999659745D+04	0.000000000D+00	0.340255070D+01	0.100000000D+05	0.606239368D-08
G/RT	-0.106829135D+08	-0.281044597D-05	-0.434380646D+03	-0.10683347875812D+08	

(c) KM(MPEC)

\*\*\* MPEC \*\* CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION  
 CSAMI/GHEST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART 0  
 CASE 3 TEMPERATURE (K)= 3000.00 (CONSTANT PRESSURE) PRESSURE(ATM)= 1.000 GAS VOLUME (M+3)= 3.267E+03 SR  
 INPUT GRAM-ATOMS OF ELEMENTS C FE MO CA SI U ZR  
 5.027E+05 2.000E+02 1.000E+02 1.000E+02 1.000E+05 1.000E+05 1.000E+04 1.000E+02  
 LA CE  
 2.000E+02 1.000E+03

NO.	SPECIES	MIXTURE	G/R1	MOLES	ACTIVITY	PARTIAL PRESSURE(ATM)
1	H	1	6.422	2.2784E+00	1.1473E-04	1.1473E-04
2	OH	1	20.595	8.6470E-15	4.3746E-19	4.3746E-19
3	O	1	5.704	3.6040E-07	1.8149E-11	1.8149E-11
4	O2	1	0.0	5.9111E-13	2.9767E-17	2.9767E-17
5	CO2	1	-23.832	4.3669E-04	2.1990E-08	2.1990E-08
6	CO	1	-17.147	9.9999E+01	5.0357E-03	5.0357E-03
7	FE	1	8.025	6.4853E+00	3.2659E-04	3.2659E-04
8	FE0	1	3.736	2.5794E-06	1.2989E-10	1.2989E-10
9	FE(OH)2	1	7.872	4.8794E-07	2.4571E-11	2.4571E-11
10	FE(OH)2	1	21.942	2.8864E-11	1.4527E-15	1.4527E-15
11	MO	1	11.360	5.8590E-09	2.9504E-13	2.9504E-13
12	MOO	1	-5.076	1.0444E-12	5.2605E-17	5.2605E-17
13	MOO2	1	-14.579	6.9088E-14	4.7609E-18	4.7609E-18
14	MOO3	1	-26.237	3.9774E-15	3.4791E-22	3.4791E-22
15	MOO2(OH)2	1	-16.361	0.0	2.0039E-19	2.0039E-19
16	(MOO3)2	1	-17.097	0.0	0.0	0.0
17	(MOO3)3	1	0.0	0.0	1.2005E-02	1.2005E-02
18	CA	1	-3.456	4.3945E-05	2.2130E-09	2.2130E-09
19	CAO	1	-1.0137E-02	1.0137E-02	5.1147E-07	5.1147E-07
20	CA(OH)2	1	-23.036	3.8037E-07	1.9165E-11	1.9165E-11
21	SI	1	10.132	2.9349E+01	1.4779E-03	1.4779E-03
22	SI0	1	-15.386	1.9365E+04	9.7510E-01	9.7510E-01
23	SI02	1	-17.912	1.3206E-03	6.6501E-08	6.6501E-08
24	SI(OH)2	1	-0.991	7.6518E-04	3.8532E-08	3.8532E-08
25	SI(OH)2	1	-14.613	2.4270E-07	1.2222E-11	1.2222E-11
26	U	1	16.408	1.8599E-05	9.3662E-10	9.3662E-10
27	UO	1	-7.249	1.9049E-03	9.6026E-08	9.6026E-08
28	UO2	1	-28.359	1.5311E-02	7.7104E-07	7.7104E-07
29	UO3	1	-40.692	1.8978E-05	9.5549E-10	9.5549E-10
30	UO2(OH)2	1	-48.824	1.7534E-12	8.8296E-17	8.8296E-17
31	ZR	1	-5.430	1.3241E-08	6.6677E-13	6.6677E-13
32	ZR0	1	-19.430	8.6322E-05	8.2195E-10	8.2195E-10
33	ZR02	1	-1.194	9.8047E-08	4.9374E-12	4.9374E-12
34	ZR(OH)2	1	-16.302	2.3665E-11	8.3925E-13	8.3925E-13
35	ZR(OH)2	1	0.0	1.5783E+00	7.9482E-05	7.9482E-05
36	SRO	1	-6.045	3.6331E-08	1.8296E-10	1.8296E-10
37	SROH	1	-11.795	8.0321E-05	4.0549E-09	4.0549E-09
38	SRO(OH)2	1	-22.683	1.6602E-09	8.3604E-14	8.3604E-14
39	LA	1	10.926	1.2963E-06	6.5291E-11	6.5291E-11
40	LA0	1	-16.936	8.9091E-03	4.4864E-07	4.4864E-07
41	LA(OH)2	1	-6.153	1.3038E-08	6.5659E-13	6.5659E-13
42	LA(OH)2	1	-24.848	4.8001E-09	2.4575E-13	2.4575E-13
43	CE	1	11.621	1.0423E-04	5.2406E-09	5.2406E-09
44	CE0	1	-13.248	3.5916E-02	1.8086E-04	1.8086E-04
45	CE(OH)2	1	-4.952	8.3230E-07	3.1841E-11	3.1841E-11
46	CE(OH)2	1	-20.060	8.8646E-10	4.4640E-14	4.4640E-14
47	MO	1	0.0	3.4575E-16	1.7411E-20	1.7411E-20
48	MOO	1	0.0	2.0223E-19	1.0184E-23	1.0184E-23
49	MOO2	1	0.0	1.8712E-03	9.4229E-08	9.4229E-08
50	(MOO3)2	1	-8.152	9.8653E+01	6.9780E-03	6.9780E-03
51	H2O	1	0.0	1.9048E+01	6.0984E-05	6.0984E-05
52	FEN(L)	1	-8.922	9.7635E+04	3.4319E-01	3.4319E-01
53	CAO(L)	2	-22.312	8.0805E+04	2.7652E-01	2.7652E-01
54	SI(O2(L))	2	-33.152	9.9999E+04	3.4506E-01	3.4506E-01
55	UO2(L)	2	-41.364	9.9337E+03	3.4079E-02	3.4079E-02
56	ZR(O2(L))	2	-41.997	9.8642E+01	3.3764E-04	3.3764E-04
57	SRO(L)	2	-20.473	9.9994E+01	3.4504E-04	3.4504E-04
58	LA(O2(L))	2	-74.155	9.9995E+02	3.4505E-03	3.4505E-03
59	ZR(O2(L))	2	-39.822	9.9982E+04	9.9934E-01	9.9934E-01
60	CE(O2(L))	2	0.0	1.0000E+02	6.6045E-04	6.6045E-04
61	FE(L)	3	0.0	6.6142E+01	0.0	0.0
62	MO(L)	3	0.0	0.0	0.0	0.0
63	ZR(L)	3	0.0	0.0	0.0	0.0

\*\*\* (CONST. PRESSURE) TOTAL Gibbs FREE ENERGY = -1.6905E+11 JUMIE  
 \*\*\* ELEMENT C WAS REPLACED BY SPECIES CU  
 \*\* CONVERGED, ITERATION= 5 (LIMIT= 1) TIME (MS)= 111.000 TIME FOR INITIAL GUESS (MS)= 22.000

(d) JW(SGPV)

OT = 2000.00 K  
P = 1.000E+00 ATM

	X*/MOLE	Y/MOLE	P/ATM	ACTIVITY			MOLE FRACTION		
O (g)	0.00000E+00	0.52293E-08	0.23166E-10	0.23166E-10	Zr (m)	0.10000E+05	0.20099E+00	0.18313E-05	0.18313E-05
O2 (g)	0.25135E+06	0.97415E-12	0.43152E-14	0.43152E-14	Fe (m)	0.10000E+06	0.99974E+05	0.91093E+00	0.91093E+00
H (g)	0.00000E+00	0.11550E+00	0.51162E-03	0.51162E-03	Mo (m)	0.10000E+03	0.10000E+03	0.91116E-03	0.91116E-03
H2 (g)	0.00000E+00	0.99788E+02	0.44203E+00	0.44203E+00	U (m)	0.00000E+00	0.11910E+01	0.10852E-04	0.10852E-04
UH (g)	0.00000E+00	0.63631E-05	0.28186E-07	0.28186E-07	Si (m)	0.00000E+00	0.96743E+04	0.88148E-01	0.88148E-01
H2O (g)	0.10000E+03	0.64792E-01	0.28700E-03	0.28700E-03	Sr (m)	0.00000E+00	0.23645E-03	0.21544E-08	0.21544E-08
C (g)	0.00000E+00	0.73830E-09	0.32704E-11	0.32704E-11	Ca (m)	0.00000E+00	0.20909E+00	0.19051E-05	0.19051E-05
CO (g)	0.00000E+00	0.99750E+02	0.44275E+00	0.44275E+00	La (m)	0.00000E+00	0.26279E-01	0.23944E-06	0.23944E-06
CO2 (g)	0.10000E+03	0.48933E-02	0.21676E-04	0.21676E-04	Ce (m)	0.00000E+00	0.78303E-01	0.71347E-06	0.71347E-06
CH4 (g)	0.00000E+00	0.44631E-01	0.19770E-03	0.19770E-03					
Zr (g)	0.00000E+00	0.14218E-11	0.62982E-14	0.62982E-14	ZrO2 (o)	0.00000E+00	0.67652E+04	0.33191E-01	0.33191E-01
Fe (g)	0.00000E+00	0.27756E+00	0.12295E-02	0.12295E-02	FeO (o)	0.00000E+00	0.25733E+02	0.12625E-03	0.12625E-03
Mo (g)	0.00000E+00	0.13567E-09	0.60099E-12	0.60099E-12	Fe2O3(o)	0.00000E+00	0.70634E-09	0.34654E-14	0.34654E-14
U (g)	0.00000E+00	0.16328E-08	0.72327E-11	0.72327E-11	Fe3O4(o)	0.00000E+00	0.27838E-12	0.13658E-17	0.13658E-17
Si (g)	0.00000E+00	0.15491E-02	0.68620E-05	0.68620E-05	MoO2 (o)	0.00000E+00	0.30934E-06	0.15176E-11	0.15176E-11
Sr (g)	0.00000E+00	0.18208E-04	0.80656E-07	0.80656E-07	MoO3 (o)	0.00000E+00	0.46967E-13	0.23043E-18	0.23043E-18
Ca (g)	0.00000E+00	0.80574E-02	0.35691E-04	0.35691E-04	FeMoO4(o)	0.00000E+00	0.94564E-16	0.46394E-21	0.46394E-21
La (g)	0.00000E+00	0.10728E-08	0.47523E-11	0.47523E-11	UO2 (o)	0.10000E+06	0.99998E+05	0.49060E+00	0.49060E+00
Ce (g)	0.00000E+00	0.26021E-08	0.11527E-10	0.11527E-10	UO3 (o)	0.00000E+00	0.12139E-02	0.59554E-08	0.59554E-08
ZrO (g)	0.00000E+00	0.57818E-08	0.25611E-10	0.25611E-10	U3O8 (o)	0.00000E+00	0.22458E-09	0.11018E-14	0.11018E-14
ZrO2 (g)	0.00000E+00	0.42662E-08	0.18879E-10	0.18879E-10	SiO2 (o)	0.10000E+06	0.14701E+05	0.72124E-01	0.72124E-01
FeO (g)	0.00000E+00	0.27046E-06	0.11980E-08	0.11980E-08	ZrSiO4(o)	0.00000E+00	0.68577E+03	0.33645E-02	0.33645E-02
MoO (g)	0.00000E+00	0.53481E-11	0.23690E-13	0.23690E-13	Fe2SiO4(o)	0.00000E+00	0.25985E-03	0.12749E-08	0.12749E-08
MoO2 (g)	0.00000E+00	0.27794E-12	0.12312E-14	0.12312E-14	SrO (o)	0.10000E+03	0.47157E+00	0.23136E-05	0.23136E-05
MoO3 (g)	0.00000E+00	0.14153E-15	0.62694E-18	0.62694E-18	SrCO3(o)	0.00000E+00	0.15930E-07	0.78153E-13	0.78153E-13
Mo2O6(g)	0.00000E+00	0.19472E-31	0.86256E-34	0.86256E-34	SrSiO3(o)	0.00000E+00	0.94617E+02	0.46420E-03	0.46420E-03
Mo3O9(g)	0.00000E+00	0.13235E-47	0.58627E-50	0.58627E-50	Sr2SiO4(o)	0.00000E+00	0.31444E-01	0.15427E-06	0.15427E-06
UO (g)	0.00000E+00	0.26540E-05	0.11756E-07	0.11756E-07	SrZrO3(o)	0.00000E+00	0.48487E+01	0.23788E-04	0.23788E-04
UO2 (g)	0.00000E+00	0.11918E-03	0.52793E-06	0.52793E-06	CaO (o)	0.10000E+06	0.35368E+04	0.17352E-01	0.17352E-01
UO3 (g)	0.00000E+00	0.15426E-05	0.68330E-08	0.68330E-08	CaCO3(o)	0.00000E+00	0.14240E-04	0.69861E-10	0.69861E-10
SiO (g)	0.00000E+00	0.25493E+02	0.11293E+00	0.11293E+00	CaSiO3(o)	0.00000E+00	0.55719E+05	0.27337E+00	0.27337E+00
SiO2 (g)	0.00000E+00	0.38031E-04	0.16846E-06	0.16846E-06	Ca2SiO4(o)	0.00000E+00	0.19100E+05	0.93705E-01	0.93705E-01
SrO (g)	0.00000E+00	0.29467E-09	0.13053E-11	0.13053E-11	CaZrO3(o)	0.00000E+00	0.25440E+04	0.12481E-01	0.12481E-01
FAKE (g)	0.00000E+00	0.14108-284	0.62492-287	0.62492-287	CaMoO4(o)	0.00000E+00	0.24472E-10	0.12006E-15	0.12006E-15
Sr2O (g)	0.00000E+00	0.21958E-12	0.97265E-15	0.97265E-15	CaUO4(o)	0.00000E+00	0.31014E+00	0.15216E-05	0.15216E-05
CaO (g)	0.00000E+00	0.17749E-07	0.78710E-10	0.78710E-10	CaFe2O4(o)	0.00000E+00	0.43001E-08	0.21097E-13	0.21097E-13
LaO (g)	0.00000E+00	0.79817E-04	0.35356E-06	0.35356E-06	Ca2Fe2O5	0.00000E+00	0.43980E-10	0.21577E-15	0.21577E-15
LaO2 (g)	0.00000E+00	0.23352E-02	0.10344E-04	0.10344E-04	La2O3(o)	0.10000E+03	0.99986E+02	0.49054E-03	0.49054E-03
La2O (g)	0.00000E+00	0.51352E-12	0.22747E-14	0.22747E-14	CeO2 (o)	0.10000E+04	0.10221E+03	0.50147E-03	0.50147E-03
La2O2(g)	0.00000E+00	0.36413E-09	0.16130E-11	0.16130E-11	Ce2O3(o)	0.00000E+00	0.44885E+03	0.22021E-02	0.22021E-02
CeO (g)	0.00000E+00	0.91803E-04	0.40665E-06	0.40665E-06					

(e) DP(BRIN)

Results Obtained in the Case B Problem  
with T = 2000 K

SPECIES	MOLES	MOLE FRACTION	PRESSURE (ATMS)	FREE-ENERGY (CAL/MOLE)	SPECIES	MOLES	MOLE FRACTION	PRESSURE (ATMS)	FREE-ENERGY (CAL/MOLE)
METALS									
U metal	2.503e-01	2.280e-04		-44487	Fe(g)	3.855e-02	3.726e-04		497
Zr metal	1.835e-01	1.672e-06		-33602	FeO(g)	1.660e-07	1.604e-09		-73079
Fe metal	9.989e-04	9.102e-01		-30507	FeOH	2.384e-07	2.384e-09		-113267
Mo metal	1.000e-02	9.112e-04		-24151	Fe(OH) <sub>2</sub>	4.399e-09	4.251e-11		-258830
Sr metal	2.659e-04	2.423e-09		-43187	Mo(g)	5.835e-11	5.639e-13		60117
Ca metal	1.967e-00	1.793e-05		-36758	MoO	1.385e-13	1.335e-15		-38535
Si metal	9.632e-03	8.776e-02		-23348	MoO <sub>2</sub> (g)	1.563e-13	1.511e-15		-161709
C graphite	9.981e-01	9.094e-04		-10998	MoO <sub>3</sub> (g)	1.421e-16	1.374e-18		-256559
OXIDES									
UO <sub>2</sub> (s)	9.997e-04	4.372e-01		-319892	MoO <sub>2</sub> (OH) <sub>2</sub>	1.103e-18	1.066e-20		-437426
SiO <sub>2</sub> (s)	2.355e-04	1.030e-01		-269347	Co(g)	6.663e-03	6.440e-05		-41840
CaO(s)	5.568e-03	2.435e-02		-188111	CoO(g)	1.369e-08	1.323e-10		-112476
LaO <sub>1.5</sub> (s)	2.000e-02	8.747e-04		-272569	Co(OH)	5.693e-05	5.693e-07		-184478
CoO <sub>2</sub> (s)	1.969e-01	8.611e-05		-321816	Co(OH) <sub>2</sub>	3.529e-07	3.410e-09		-325570
MoO <sub>2</sub> (s)	2.589e-06	1.132e-11		-197168	CoH	2.604e-05	2.516e-07		-58552
FeO(s)	1.087e-02	4.754e-04		-123154	Co <sub>2</sub>	5.049e-10	4.880e-12		-56874
ZrO <sub>2</sub> (s)	3.716e-03	1.625e-02		-315457	Sr(g)	1.359e-06	1.313e-08		-49903
CaO <sub>1.5</sub> (s)	9.803e-02	4.287e-03		-276006	SrO(g)	4.144e-11	4.005e-13		-131262
CaSiO <sub>3</sub>	4.532e-04	1.982e-01		-474825	SrOH	1.250e-08	1.250e-10		-192837
CaSiO <sub>3</sub> .5O <sub>2</sub>	4.283e-04	1.873e-01		-335410	Sr(OH) <sub>2</sub>	1.857e-11	1.795e-13		-328251
SrSiO <sub>3</sub>	7.178e-01	3.139e-04		-491035	SrH	5.203e-09	5.029e-11		-66535
SrO(s)	1.636e-01	7.156e-07		-188475	La(g)	1.466e-11	1.417e-13		1049
SrSiO <sub>3</sub> .5O <sub>2</sub>	2.644e-01	1.157e-04		-347876	LaO(g)	3.152e-07	3.046e-09		-161279
CaMoO <sub>4</sub>	2.661e-08	1.164e-13		-504532	LaOH	2.058e-11	1.989e-13		-161730
SrMoO <sub>4</sub>	1.055e-13	4.816e-19		-496937	La(OH) <sub>2</sub>	1.354e-09	1.308e-11		-399797
CaZrO <sub>3</sub>	6.282e-03	2.748e-02		-520420	La <sub>2</sub> O	1.278e-17	1.235e-19		-182712
SrZrO <sub>3</sub>	1.630e-00	7.131e-06		-529442	(LaO) <sub>2</sub>	3.063e-14	2.960e-16		-336321
MoO <sub>3</sub> (s)	2.633e-22	1.151e-27		-173496	Co(g)	1.605e-10	1.551e-12		-5583
GASES									
H <sub>2</sub>	9.989e-01	9.654e-01		-77358	CoO	3.792e-06	3.665e-08		-168286
H	1.645e-01	1.589e-03		-13137	CoO <sub>2</sub> (g)	5.382e-07	5.201e-09		-283208
OH	4.021e-06	3.886e-08		-93615	CoOH	1.872e-10	1.809e-12		-167624
O	4.728e-09	4.569e-11		-20057	Co(OH) <sub>2</sub>	4.619e-11	4.464e-13		-323492
H <sub>2</sub> O	2.385e-02	2.385e-04		-166894	(CoO) <sub>2</sub>	1.249e-11	1.200e-13		-354451
U(g)	4.125e-09	3.987e-11		17350	CO	1.900e-01	1.836e-03		-136472
UC	9.481e-06	9.163e-08		-136092	CO <sub>2</sub>	1.001e-05	9.675e-08		-220003
UO <sub>2</sub> (g)	2.414e-04	2.333e-06		-271640	Si(g)	3.001e-04	3.674e-06		18718
UO <sub>3</sub>	3.700e-06	3.576e-08		-377716	SiO	3.153e-00	3.048e-02		-141826
UOH	4.966e-10	4.799e-12		-135665	SiO <sub>2</sub> (g)	2.691e-06	2.601e-08		-200970
U(OH) <sub>2</sub>	1.361e-11	1.316e-13		-202001	SiOH	1.464e-06	1.415e-08		-122619
UO <sub>2</sub> (OH) <sub>2</sub>	4.095e-10	3.957e-12		-541692	Si(OH) <sub>2</sub>	8.064e-08	7.793e-10		-272526
Zr(g)	2.019e-13	1.952e-15		48145	SiH	2.671e-04	2.581e-06		-20627
ZrO	3.344e-09	3.232e-11		-113146	SiH <sub>4</sub>	8.339e-06	8.059e-08		-123097
ZrO <sub>2</sub> (g)	2.602e-10	2.515e-12		-225679	Si <sub>2</sub>	3.647e-07	3.525e-09		11318
ZrOH	7.903e-13	7.637e-15		-118708	O <sub>2</sub>	4.893e-13	4.729e-15		-114270
Zr(OH) <sub>2</sub>	5.457e-12	5.274e-14		-207818	Co <sub>2</sub> O	3.234e-20	3.126e-22		-153100
					LaO <sub>2</sub>	3.494e-24	3.377e-26		-120000
					Sr <sub>2</sub> O	1.009e-19	9.754e-22		-174469
					(SiO) <sub>2</sub>	7.103e-09	6.865e-11		-210392



(f) DP(BRI1)

Results Obtained for Case B at 2000 K with  
a Simpler Solution Model

SPECIES	MOLES	MOLE FRACTION	PRESSURE (ATMS)	FREE-ENERGY (CAL/MOLE)	SPECIES	MOLES	MOLE FRACTION	PRESSURE (ATMS)	FREE-ENERGY (CAL/MOLE)
METALS									
Zr metal	5.889e-01	4.897e-04		-33602	Fe(g)	7.828e-08	4.883e-04		-497
Fe metal	8.998e-04	8.875e-01		-38587	FeO(g)	2.822e-06	1.472e-10		-73879
Mo metal	1.888e-02	8.877e-04		-24151	FeOH	2.852e-07	1.548e-11		-113267
C graphite	8.687e-01	8.665e-04		-18998	Fe(OH) <sub>2</sub>	3.322e-11	1.733e-15		-258830
OXIDES									
UO <sub>2</sub> (c)	1.888e-05	3.422e-01		-319892	Mo(g)	1.184e-08	6.175e-13		60117
SiO <sub>2</sub> (c)	8.114e-04	2.777e-01		-269347	MoO	2.346e-12	1.224e-16		-38535
CaO(c)	8.979e-04	3.415e-01		-188111	MoO <sub>2</sub> (g)	2.224e-13	1.168e-17		-161789
LaO <sub>1.5</sub> (c)	2.888e-02	6.845e-04		-272569	MoO <sub>3</sub> (g)	1.693e-17	8.832e-22		-256559
CaO <sub>2</sub> (c)	5.778e-08	1.977e-05		-321816	MoO <sub>2</sub> (OH) <sub>2</sub>	5.833e-23	3.843e-27		-437426
MoO <sub>2</sub> (c)	2.548e-08	6.694e-14		-197168	Co(g)	2.868e-02	1.878e-02		-41848
FeO(c)	1.275e-01	4.363e-05		-123154	Co <sub>2</sub> (g)	3.557e-05	1.855e-09		-112476
ZrO <sub>2</sub> (c)	8.958e-03	3.485e-02		-315457	Co(OH)	1.115e-02	5.815e-07		-184478
CaO <sub>1.5</sub> (c)	8.842e-02	3.483e-03		-276886	Co(OH) <sub>2</sub>	4.872e-07	2.124e-11		-325578
SrO(c)	8.858e-01	3.374e-04		-188475	CoH	5.884e-02	3.868e-06		-58552
MoO <sub>3</sub> (c)	2.922e-21	1.888e-26		-173496	Co <sub>2</sub>	2.625e-03	1.368e-07		-56874
GASES									
H <sub>2</sub>	8.816e-01		5.128e-03	-77358	Sr(g)	1.417e-08	7.393e-05		-49983
H	2.218e-08		1.157e-04	-13137	SrO(g)	3.628e-06	1.888e-10		-131262
OH	4.543e-06		2.378e-18	-93615	SrOH	8.228e-05	4.283e-09		-192837
O	7.335e-08		3.826e-12	-28857	Sr(OH) <sub>2</sub>	7.285e-18	3.758e-14		-328251
H <sub>2</sub> O	1.963e-03		1.824e-07	-166894	SrH	3.853e-04	2.862e-08		-66535
U(g)	8.533e-05		4.451e-09	17350	La(g)	8.774e-08	4.576e-12		1848
UO	1.642e-02		8.565e-07	-136892	LaO(g)	1.578e-04	8.238e-09		-161279
UO <sub>2</sub> (g)	3.581e-02		1.826e-06	-271640	LaOH	7.511e-10	3.818e-14		-161738
UO <sub>3</sub>	4.494e-05		2.344e-09	-377716	La(OH) <sub>2</sub>	3.812e-18	1.571e-14		-339797
UOH	6.263e-08		3.267e-12	-135665	La <sub>2</sub> O	2.868e-13	1.878e-17		-182712
U(OH) <sub>2</sub>	1.847e-11		5.462e-16	-282881	(LaO) <sub>2</sub>	4.158e-11	2.165e-15		-336321
UO <sub>2</sub> (OH) <sub>2</sub>	2.288e-12		1.152e-16	-541692	Co(g)	8.741e-07	5.881e-11		-5583
Zr(g)	1.118e-08		5.832e-13	48145	CoO	1.927e-03	1.885e-07		-168286
ZrO	1.558e-05		8.887e-18	-113146	Co <sub>2</sub> (g)	2.298e-05	1.195e-09		-283288
ZrO <sub>2</sub> (g)	1.818e-07		5.268e-12	-225679	CoOH	6.828e-09	3.813e-13		-167624
ZrOH	2.666e-10		1.392e-14	-118788	Co(OH) <sub>2</sub>	1.842e-11	5.437e-16		-323492
Zr(OH) <sub>2</sub>	1.124e-11		5.861e-16	-287818	(CoO) <sub>2</sub>	1.741e-08	8.883e-13		-354451
					CO	3.132e-08	1.634e-04		-136472
					CO <sub>2</sub>	1.382e-05	7.289e-18		-228883
					Si(g)	2.788e-01	1.413e-03		16718
					SiO	1.881e-04	9.813e-01		-141626
					SiO <sub>2</sub> (g)	1.344e-03	7.813e-08		-288978
					SiOH	6.362e-04	3.319e-08		-122619
					Si(OH) <sub>2</sub>	2.136e-07	1.114e-11		-272526
					SiH	1.386e-08	7.228e-05		-28627
					SiH <sub>4</sub>	1.671e-05	8.717e-18		-123897
					Si <sub>2</sub>	8.893e-08	5.212e-04		11318
					O <sub>2</sub>	6.357e-13	3.316e-17		-114278
					Co <sub>2</sub> O	5.383e-16	2.888e-28		-153188
					La <sub>2</sub> O <sub>2</sub>	1.466e-22	7.846e-27		-128888
					Sr <sub>2</sub> O	4.864e-11	2.589e-15		-174469
					(SiO) <sub>2</sub>	1.365e-03	7.118e-08		-218392

(g) DP(BRI2)

Results Obtained for Case B at 2000 K with  
a Non-ideal Metal Phase

SPECIES	MOLES	MOLE FRACTION	PRESSURE (ATMS)	FREE-ENERGY (CAL/MOLE)	SPECIES	MOLES	MOLE FRACTION	PRESSURE (ATMS)	FREE-ENERGY (CAL/MOLE)
METALS									
U metal	2.586e-08	2.380e-05		-44487	Fe (g)	3.928e-02		3.591e-04	497
Zr metal	2.492e-02	2.287e-07		-33602	FeO (g)	2.756e-06		2.595e-06	-73079
Fe metal	9.823e-04	9.018e-01		-30507	FeOH	3.900e-06		3.673e-08	-113267
Mo metal	1.000e-02	9.180e-04		-24151	Fe(OH) <sub>2</sub>	1.158e-06		1.091e-08	-258030
Sr metal	2.895e-08	1.923e-13		-43187	Mo (g)	5.813e-11		5.662e-13	60117
Ca metal	1.543e-04	1.417e-09		-36758	MoO	2.324e-12		2.188e-14	-38535
Si metal	1.050e-04	9.642e-02		-23348	MoO <sub>2</sub> (g)	4.296e-11		4.045e-13	-161709
C graphite	9.413e-01	8.641e-04		-10998	MoO <sub>3</sub> (g)	6.380e-13		6.008e-15	-256559
OXIDES									
UO <sub>2</sub> (s)	1.000e-05	4.353e-01		-319892	MoO <sub>2</sub> (OH) <sub>2</sub>	7.847e-14		7.390e-16	-437426
SiO <sub>2</sub> (s)	2.296e-04	9.996e-02		-269347	Co (g)	4.256e-04		4.008e-06	-41840
CaO (s)	5.685e-03	2.475e-02		-188111	CoO (g)	1.428e-08		1.345e-10	-112476
LaO <sub>1.5</sub> (s)	2.000e-02	8.707e-04		-272569	Co (OH)	6.054e-05		5.701e-07	-184478
CoO <sub>2</sub> (s)	7.507e-01	3.268e-04		-321816	Co(OH) <sub>2</sub>	5.836e-06		5.496e-08	-325570
MoO <sub>2</sub> (s)	5.966e-04	3.033e-09		-197168	CoH	1.639e-06		1.543e-08	-58552
FeO (s)	1.767e-03	7.692e-03		-123154	Co <sub>2</sub>	2.007e-12		1.890e-14	-56674
ZrO <sub>2</sub> (s)	3.678e-03	1.601e-02		-315457	Sr (g)	8.718e-08		8.210e-10	-49903
CoO <sub>1.5</sub> (s)	9.249e-02	4.027e-03		-276006	SrO (g)	4.344e-11		4.090e-13	-131262
CoSiO <sub>3</sub>	4.491e-04	1.955e-01		-474825	SrOH	1.336e-08		1.258e-10	-192637
CoSi <sub>2</sub> O <sub>7</sub>	4.309e-04	1.876e-01		-335410	Sr(OH) <sub>2</sub>	3.086e-10		2.906e-12	-328251
SrSiO <sub>3</sub>	7.146e-01	3.111e-04		-491835	SrH	3.290e-10		3.098e-12	-66535
SrO (s)	1.679e-01	7.300e-07		-188475	La (g)	2.270e-13		2.137e-15	1049
SrSi <sub>3</sub> O <sub>10</sub>	2.673e-01	1.164e-04		-347876	LaO (g)	7.968e-08		7.503e-10	-161279
CoMoO <sub>4</sub>	1.188e-04	5.172e-10		-504532	LaOH	5.127e-12		4.828e-14	-161730
SrMoO <sub>4</sub>	4.736e-10	2.062e-15		-496937	La(OH) <sub>2</sub>	5.425e-09		5.109e-11	-339797
CoZrO <sub>3</sub>	6.320e-03	2.752e-02		-520420	La <sub>2</sub> O	4.873e-20		4.589e-22	-162712
SrZrO <sub>3</sub>	1.648e-00	7.175e-06		-529442	(LaO) <sub>2</sub>	1.907e-15		1.786e-17	-336321
MoO <sub>3</sub> (s)	1.157e-18	5.036e-24		-173496	Co (g)	2.344e-12		2.208e-14	-5583
GASES									
H <sub>2</sub>	9.953e-01		9.373e-01	-77358	CoO	9.044e-07		8.517e-09	-168286
H	1.663e-01		1.566e-03	-13137	CoO <sub>2</sub> (g)	2.096e-06		1.974e-08	-283208
OH	6.641e-05		6.253e-07	-93615	CoOH	4.399e-11		4.143e-13	-167624
O	7.924e-08		7.463e-10	-28057	Co(OH) <sub>2</sub>	1.747e-10		1.645e-12	-323492
H <sub>2</sub> O	3.062e-01		3.655e-03	-166894	(CoO) <sub>2</sub>	6.925e-13		6.522e-15	-354451
U (g)	1.580e-11		1.488e-13	17350	CO	5.868e-00		5.526e-02	-136472
UO	5.931e-07		5.586e-09	-136092	CO <sub>2</sub>	5.051e-03		4.757e-05	-220003
UO <sub>2</sub> (g)	2.467e-04		2.323e-06	-271640	Si (g)	1.420e-06		1.337e-08	16718
UO <sub>3</sub>	6.175e-05		5.815e-07	-377716	SiO	1.923e-01		1.811e-03	-141826
UOH	3.061e-11		2.883e-13	-135665	SiO <sub>2</sub> (g)	2.681e-06		2.524e-08	-208970
U(OH) <sub>2</sub>	1.350e-11		1.272e-13	-282801	SiOH	8.800e-08		8.207e-10	-122619
UO <sub>2</sub> (OH) <sub>2</sub>	1.003e-07		1.020e-09	-541692	Si(OH) <sub>2</sub>	7.798e-08		7.343e-10	-272526
Zr (g)	7.655e-16		7.209e-18	48145	SiH	9.027e-07		8.254e-09	-28627
ZrO	2.070e-10		1.950e-12	-113146	SiH <sub>4</sub>	2.035e-08		2.764e-10	-123097
ZrO <sub>2</sub> (g)	2.631e-10		2.477e-12	-225679	Si <sub>2</sub>	4.956e-12		4.667e-14	11318
ZrOH	4.821e-14		4.540e-16	-118708	O <sub>2</sub>	1.339e-10		1.261e-12	-114270
Zr(OH) <sub>2</sub>	5.357e-12		5.045e-14	-287818	Co <sub>2</sub> O	1.098e-22		1.034e-24	-153180
					LaO <sub>2</sub>	1.442e-23		1.358e-25	-128000
					Sr <sub>2</sub> O	6.814e-21		6.229e-23	-174469
					(SiO) <sub>2</sub>	2.575e-11		2.424e-13	-218392

(h) DP(BRI3)

Results Obtained for Case B at 2000 K with Lower Bound Free - Energy Data for some Vapor Species.

SPECIES	MOLES	MOLE FRACTION	PRESSURE (ATMS)	FREE-ENERGY (CAL/MOLE)	SPECIES	MOLES	MOLE FRACTION	PRESSURE (ATMS)	FREE-ENERGY (CAL/MOLE)
METALS									
U metal	2.503e-01	2.280e-04		-44487	Fe(g)	3.855e-02	3.726e-04		497
Zr metal	1.835e-01	1.672e-06		-39602	FeO(g)	1.660e-07	1.604e-09		-73079
Fe metal	9.989e-04	9.102e-01		-30507	FeOH	2.384e-07	2.384e-09		-113267
Mo metal	1.000e-02	9.112e-04		-24151	Fe(OH) <sub>2</sub>	4.399e-09	4.251e-11		-258830
Sr metal	2.659e-04	2.423e-09		-43187	Mo(g)	5.835e-11	5.639e-13		60117
Ca metal	1.967e-03	1.793e-05		-36758	MoO	1.381e-13	1.335e-15		-38535
Si metal	9.632e-03	8.776e-02		-23348	MoO <sub>2</sub> (g)	1.563e-13	1.511e-15		-161709
C graphite	9.981e-01	9.894e-04		-18998	MoO <sub>3</sub> (g)	1.421e-16	1.374e-18		-256559
OXIDES									
UO <sub>2</sub> (s)	9.997e-04	4.372e-01		-319892	MoO <sub>2</sub> (OH) <sub>2</sub>	1.103e-18	1.066e-20		-437426
SiO <sub>2</sub> (s)	2.355e-04	1.830e-01		-269347	Co(g)	6.663e-03	6.440e-05		-41848
CaO(s)	5.568e-03	2.435e-02		-188111	CoO(g)	1.369e-08	1.323e-10		-112476
LaO <sub>1.5</sub> (s)	2.000e-02	8.747e-04		-272569	Co(OH)	5.898e-05	5.693e-07		-184478
CoO <sub>2</sub> (s)	1.969e-01	8.611e-05		-321816	Co(OH) <sub>2</sub>	3.529e-07	3.410e-09		-325570
MoO <sub>2</sub> (s)	2.589e-06	1.132e-11		-197168	CoH	2.604e-05	2.516e-07		-58552
FeO(s)	1.887e-02	4.754e-04		-123154	Co <sub>2</sub>	5.049e-10	4.888e-12		-56874
ZrO <sub>2</sub> (s)	3.716e-03	1.625e-02		-315457	Sr(g)	1.502e-06	1.452e-08		-50303
CaO <sub>1.5</sub> (s)	9.803e-02	4.287e-03		-276806	SrO(g)	1.134e-10	1.096e-12		-135262
CaSiO <sub>3</sub>	4.532e-04	1.882e-01		-474825	SrOH	4.552e-08	4.399e-10		-107837
CaSiO <sub>3</sub> .5O <sub>2</sub>	4.283e-04	1.873e-01		-335410	Sr(OH) <sub>2</sub>	2.229e-10	2.222e-12		-398251
SrSiO <sub>3</sub>	7.176e-01	3.139e-04		-491035	SrH	1.831e-08	1.769e-10		-71535
SrO(s)	1.636e-01	7.156e-07		-188475	La(g)	1.883e-11	1.820e-13		55
SrSiO <sub>3</sub> .5O <sub>2</sub>	2.644e-01	1.157e-04		-347876	LaO(g)	5.197e-07	5.022e-09		-163266
CaMoO <sub>4</sub>	2.661e-08	1.164e-13		-504532	LaOH	2.058e-11	1.989e-13		-161738
SrMoO <sub>4</sub>	1.055e-13	4.616e-19		-496937	La(OH) <sub>2</sub>	1.354e-09	1.308e-11		-339797
CaZrO <sub>3</sub>	6.282e-03	2.748e-02		-520420	La <sub>2</sub> O	4.232e-16	4.090e-18		-196621
SrZrO <sub>3</sub>	1.638e-00	7.131e-06		-529442	(LaO) <sub>2</sub>	2.756e-12	2.664e-14		-354204
MoO <sub>3</sub> (s)	2.633e-22	1.151e-27		-173496	Ca(g)	1.865e-10	1.802e-12		-6179
GASES									
H <sub>2</sub>	9.989e-01		9.654e-01	-77358	CaO	1.031e-05	9.862e-08		-172260
H	1.645e-01		1.589e-03	-13137	CaO <sub>2</sub> (g)	2.412e-06	2.331e-08		-289169
OH	4.021e-06		3.806e-08	-93615	CaOH	1.872e-10	1.809e-12		-167624
O	4.728e-09		4.569e-11	-28057	Ca(OH) <sub>2</sub>	4.619e-11	4.464e-13		-323492
H <sub>2</sub> O	2.385e-02		2.385e-04	-166894	(CaO) <sub>2</sub>	6.819e-10	6.591e-12		-370347
U(g)	4.125e-09		3.987e-11	17350	CO	1.800e-01	1.836e-03		-136472
UO	9.481e-06		9.163e-08	-136092	CO <sub>2</sub>	9.675e-08	9.675e-08		-220003
UO <sub>2</sub> (g)	2.414e-04		2.333e-06	-271640	Si(g)	3.801e-04	3.674e-06		16718
UO <sub>3</sub>	3.700e-06		3.576e-08	-377716	SiO	3.153e-00	3.048e-02		-141826
UOH	4.966e-10		4.789e-12	-135665	SiO <sub>2</sub> (g)	2.891e-06	2.601e-08		-208970
U(OH) <sub>2</sub>	1.361e-11		1.316e-13	-202801	SiOH	1.464e-06	1.415e-08		-122619
UO <sub>2</sub> (OH) <sub>2</sub>	4.095e-10		3.957e-12	-541692	Si(OH) <sub>2</sub>	8.064e-08	7.783e-10		-272526
Zr(g)	2.018e-13		1.952e-15	48145	SiH	2.671e-04	2.581e-06		-20627
ZrO	3.344e-09		3.232e-11	-113146	SiH <sub>4</sub>	8.339e-06	8.059e-08		-123097
ZrO <sub>2</sub> (g)	2.602e-10		2.515e-12	-225679	Si <sub>2</sub>	3.647e-07	3.525e-09		11318
ZrOH	7.983e-13		7.637e-15	-118788	O <sub>2</sub>	4.893e-13	4.728e-15		-114270
Zr(OH) <sub>2</sub>	5.457e-12		5.274e-14	-287818	Co <sub>2</sub> O	2.918e-18	2.813e-20		-171071

(i) GC(VASA)

GRESt-Benchmark Part B Case B(2000 K) : 'not as reducing' coking considered

----VANESA results

-- Equilibrium composition

H2O(g)	H2(g)	H(g)	OH(g)	O(g)	O2(g)	CO2(g)	CO(g)	C(l)
0.8062D-03	0.1000D+03	0.1618D+00	0.1335D-06	0.1543D-09	0.5390D-15	0.6369D-08	0.3576D-02	0.1000D+03
Fe(l)	FeO(l)	Fe(g)	FeO(g)	FeOH(g)	Fe(OH)2(g)			
0.1000D+06	0.2393D-02	0.1061D-04	0.1877D-11	0.2742D-11	0.1739D-14			
Mo(l)	Mo(g)	MoO(g)	MoO2(g)	MoO3(g)	H2MoO4(g)	(MoO3)2	(MoO3)3	MoOH(g)
0.1000D+03	0.5622D-10	0.4493D-14	0.1718D-15	0.5275D-20	0.1429D-23	0.0	0.0	0.3194D-14
CaO(l)	Ca(g)	CaO(g)	CaOH(g)	Ca(OH)2(g)	CaH(g)	Ca2(g)		
0.1000D+06	0.1789D+01	0.1321D-06	0.5786D-03	0.1191D-06	0.7565D-02	0.4804D-04		
SiO2(l)	Si(g)	SiO(g)	SiO2(g)	SiOH(g)	Si(OH)2(g)	SiH(g)	SiH4(g)	Si2(g)
0.9974D+05	0.7580D+00	0.2109D+03	0.6116D-05	0.1003D-03	0.1899D-06	0.5415D+00	0.1778D-01	0.1689D+01
UO2(l)	U(l)	U(g)	UO(g)	UO2(g)	UO3(g)	UO2(OH)2(g)	UOH(g)	U(OH)2(g)
0.1000D+06	0.0	0.2550D-06	0.1980D-04	0.1702D-04	0.8805D-08	0.3399D-13	0.1054D-08	0.9912D-12
ZrO2(l)	Zr(l)	Zr(g)	ZrO(g)	ZrO2(g)	ZrOH(g)	Zr(OH)2(g)	ZrH(g)	
0.1501D+03	0.9850D+04	0.3660D-11	0.2054D-08	0.5393D-11	0.4925D-12	0.1169D-12	0.1647D-10	
SrO(l)	Sr(g)	SrO(g)	SrOH(g)	Sr(OH)2(g)	SrH(g)			
0.9997D+02	0.2763D-01	0.2843D-07	0.9027D-05	0.1105D-08	0.1076D-03			
La2O3(l)	La(g)	LaO(g)	LaOH(g)	La(OH)2(g)	La2O(g)	La2O2(g)		
0.1000D+03	0.5806D-07	0.4218D-04	0.2799D-08	0.6323D-08	0.2648D-04	0.5818D-09		
CeO2(l)	Ce(g)	CeO(g)	CeOH(g)	Ce(OH)2(g)	CeO2(g)	Ce2O2(g)		
0.1000D+04	0.8028D-05	0.6408D-02	0.3214D-06	0.2722D-08	0.3070D-04	0.4117D-04		

(j) GC(VASB)

GREY-Benchmark Part B Case B(2000 K) : 'not as reducing' no coking

----VANESA results

-- Equilibrium composition

H2O(g)	H2(g)	H(g)	OH(g)	O(g)	O2(g)	CO2(g)	CO(g)	C(l)
0.8046D-03	0.9997D+02	0.2282D+00	0.1880D-06	0.3079D-09	0.1074D-14	0.1776D-03	0.1000D+03	0.0
Fe(l)	FeO(l)	Fe(g)	FeO(g)	FeOH(g)	Fe(OH)2(g)			
0.1000D+06	0.1587D-02	0.1313D-04	0.2342D-11	0.2463D-11	0.1127D-14			
Mo(l)	Mo(g)	MoO(g)	MoO2(g)	MoO3(g)	H2MoO4(g)	(MoO3)2	(MoO3)3	MoOH(g)
0.1000D+03	0.1122D-09	0.8940D-14	0.3409D-15	0.1044D-19	0.1411D-23	0.0	0.0	0.4485D-14
CaO(l)	Ca(g)	CaO(g)	CaOH(g)	Ca(OH)2(g)	CaH(g)	Ca2(g)		
0.1000D+06	0.3457D+01	0.2549D-06	0.8021D-03	0.1189D-06	0.1051D-01	0.9104D-04		
SiO2(l)	Si(g)	SiO(g)	SiO2(g)	SiOH(g)	Si(OH)2(g)	SiH(g)	SiH4(g)	Si2(g)
0.9954D+05	0.1466D+01	0.4009D+03	0.1178D-04	0.1391D-03	0.1897D-06	0.7524D+00	0.9392D-02	0.3204D+01
UO2(l)	U(l)	U(g)	UO(g)	UO2(g)	UO3(g)	UO2(OH)2(g)	UOH(g)	U(OH)2(g)
0.1000D+06	0.0	0.5285D-06	0.4097D-04	0.3518D-04	0.1817D-07	0.3390D-13	0.1514D-08	0.9913D-12
ZrO2(l)	Zr(l)	Zr(g)	ZrO(g)	ZrO2(g)	ZrOH(g)	Zr(OH)2(g)	ZrH(g)	
0.1001D+03	0.9900D+04	0.4602D-11	0.2577D-08	0.6754D-11	0.4450D-12	0.7626D-13	0.1491D-10	
SrO(l)	Sr(g)	SrO(g)	SrOH(g)	Sr(OH)2(g)	SrH(g)			
0.9994D+02	0.5717D-01	0.5874D-07	0.1295D-04	0.1104D-08	0.1545D-03			
La2O3(l)	La(l)	La(g)	LaO(g)	LaOH(g)	La(OH)2(g)	La2O(g)	La2O2(g)	
0.1000D+03	0.0	0.1183D-06	0.8580D-04	0.3985D-08	0.6318D-08	0.5391D-04	0.1204D-08	
CeO2(l)	Ce(g)	CeO(g)	CeOH(g)	Ce(OH)2(g)	CeO2(g)	Ce2O2(g)		
0.1000D+04	0.1664D-04	0.1326D-01	0.4618D-06	0.2722D-08	0.6344D-04	0.8792D-04		