

**Description of non-ideal slag and metal systems by the  
intermediate-compound method**

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# **Description of non-ideal slag and metal systems by the intermediate-compound method**

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## **1 INTRODUCTION**

Pyrometallurgy is among the oldest branches of chemical technology. However, this discipline has lagged behind other fields in the chemical process industry in the application of thermodynamic techniques for the modelling of the non-ideal systems encountered. One obvious reason for this arises from the high temperatures that are routinely encountered in pyrometallurgical processes, and the concomitant difficulties involved in experimental measurements. Another more subtle reason lies in the complex nature of pyrometallurgical systems. Process simulation in the chemical industry has been most successful when thermodynamic techniques have been applied to model the interactions between two phases. Pyrometallurgical systems are seldom so simple. It is uncommon for less than three different phases to be involved, and it is not unusual to have even more phases present.

In the course of pyrometallurgical process simulations for the production of mass and energy balances, it is often necessary to determine the equilibrium composition of slag and metal systems. There are many ways to calculate chemical equilibrium, but the most generally applicable technique is that of free-energy minimization. Probably the most widely-used algorithm for the solution of the free-energy minimization problem is that developed by Eriksson<sup>1</sup>. This formulation requires that a list of possible species for each possible phase present at equilibrium is specified. This avoids the necessity for specifying individual chemical reactions and checking that they are in fact linearly independent.

In equilibrium calculations, it is assumed that the activity of each species in the specified system can be calculated from a chemical analysis of each phase. However, accurate activity data for components in slags and metals is limited. For example, data are often available for simple slag systems, but not for the more complex slags used in actual practice. The use of interaction parameters for dilute metallic solutions is a reasonable approach, but the theory is limited to the case of dilute solutions. Clearly, this approach is also not applicable to slags. There are numerous ways of modelling the activity relationships within complex slag and metal systems. For example, Flynn and Morris<sup>2</sup> obtained excellent agreement between their experimental data from the smelting of complex sulphides and their model, by using empirical functions of composition for the activity coefficients in the system. Of course, it is most desirable to have a generally applicable method that can be used on a wide range of systems, without the need for extensive experimental work.

In this paper, we will examine a model that attributes deviations from ideal-solution behaviour to the formation of complex component liquids and solid phases. The primary aim of this work is to enable equilibrium compositions of non-ideal slag and metal or matte systems to be predicted.

## **2 ACTIVITIES IN SOLUTIONS**

The activity of a component in a solution is defined as the ratio of its fugacity to its standard-state fugacity. The activity function can, at least in theory, be calculated from the equation of state of the solution. However, because of the low accuracy of liquid-phase equations of state in general, other techniques are required for the calculation of activities in slag and metal solutions.

Solution thermodynamics begins with the paradigm of an 'ideal solution'. The ideal-solution model, in which the activity of each component equals its mole fraction, is the simplest model of activities in a solution. In this model

$$a_i = x_i \tag{1}$$

where  $a_i$  is the activity and  $x_i$  is the mole fraction of species  $i$  in the solution. The ideal-solution model takes into account only the effect of dilution on activities, and ignores the chemical and physical effects of mixing. In fact, implicit in this model is the assumption that the enthalpy of mixing is zero, and the free energy of mixing is that arising solely from the configurational entropy of mixing. Solutions which follow this pattern obey Raoult's law (that the activity approaches the mole fraction tangentially as both approach unity) over the entire range of composition. Although very few metal solutions and even fewer oxide systems display the behaviour predicted by this model, this is chosen as the reference for solution behaviour. Solutions in which  $a_i > x_i$  are said to show positive deviations from ideal behaviour, while systems where  $a_i < x_i$  are said to show negative deviations.

The relation between activity and mole fraction is often expressed by means of an activity coefficient,  $\gamma_i$ .

$$a_i = \gamma_i x_i \tag{2}$$

Clearly, for positive deviations,  $\gamma_i > 1$ , and, for negative deviations,  $\gamma_i < 1$ . The activity coefficient is the gradient of the activity - composition curve, as shown in Figure 1.

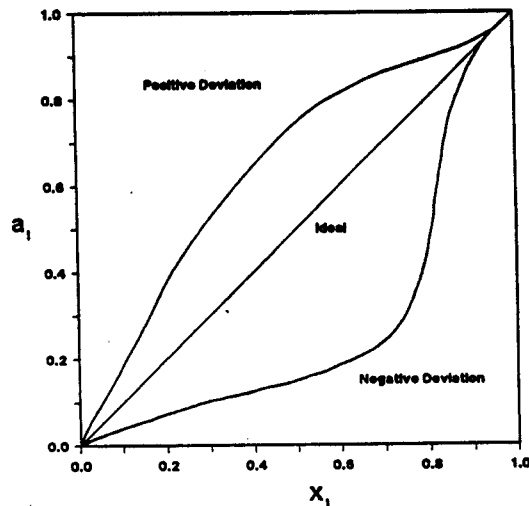


Figure 1: Activity - composition relationships in a binary solution

Henry's law defines another type of solution, in which the activity is directly proportional to the mole fraction, i.e. this implies an activity coefficient,  $f_i$ , which is constant.

$$a_i = f_i x_i \quad (3)$$

Henry's law is only obeyed at low concentrations, but can still be a useful basis for the consideration of dilute solutions.

Another simple model is that of the regular solution. This is defined as having an entropy of mixing equal to the ideal configurational entropy, and having an enthalpy of mixing that varies with composition according to a particular functional form. Some solutions closely approach regular behaviour, and this is often used as an assumption in the extrapolation of the activity coefficient from one temperature to another.

Although the solution models may be fictitious, they are useful for the derivation of expressions for the dependence of thermodynamic quantities on composition. The derived expressions are helpful in the extrapolation of data to other composition ranges, and in the estimation of the thermodynamic properties of related systems.

### 3 SLAG SYSTEMS

Slags are relatively concentrated solutions of oxides, and usually contain oxides such as  $\text{SiO}_2$ ,  $\text{CaO}$ ,  $\text{MgO}$ , and  $\text{Al}_2\text{O}_3$ , together with the metal oxides involved in the process. They are complex solutions in which each component influences the activity of the others, and hence their behaviour is not easily described. Some authors have derived solution models for slags based on the ideal or regular constitutional models, using various species as components. Others have adopted a structural approach, modelling the slag properties in terms of some hypothetical structure.

It is now generally accepted that slags are essentially ionic systems, although they have on occasion been viewed as having a molecular structure. The molecular theory rests

on the assumption that liquid slags are composed of individual oxides, sulphides, or fluorides such as  $\text{SiO}_2$ ,  $\text{CaO}$ ,  $\text{MgO}$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{CaS}$ , and  $\text{CaF}_2$ . Their molecules are envisaged as combining to form more complex (and unreactive) molecular structures, for example,  $2\text{CaO}\cdot\text{SiO}_2$ , which exist in dissociated equilibrium with the corresponding components. However, experimental measurements show a sharp increase in the electrical conductivity of slags upon melt-down. Together with other evidence, this demonstrates that slags consist of ions in the form of positively charged cations, such as  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Fe}^{2+}$ , and  $\text{Fe}^{3+}$ , and negatively charged anions, such as  $\text{O}^{2-}$ ,  $\text{SiO}_4^{4-}$ , and  $\text{AlO}_3^{3-}$ .

As explained by Turkdogan<sup>3</sup>, it is necessary to describe the thermodynamic properties of slags in terms of the constituent elements or oxides, despite the ionic nature of these polymeric melts. Since positive or negative ions cannot be added separately to an ionic solution, the individual contributions of the ionic species to the free energy of the system cannot be determined. Hence the activity or the activity coefficient of an individual ion cannot be determined. The thermodynamic quantities can be measured only for uncharged and electroneutral systems; therefore, only the activity of a neutral entity made up of at least two ionic species can be measured. The activity of an oxide in a polymeric melt is proportional to the product of the activities of the constituent ions, and is readily measured relative to the pure solid or liquid oxide.

The theory outlined in this paper is similar in some respects to the molecular theory for slags, but differs in that it does not require that a slag actually consist of molecular structures.

#### 4 METALLIC SYSTEMS

Many metallic systems are relatively dilute solutions. In this situation, it is often appropriate to use the activity coefficient at infinite dilution,  $\gamma^0$ . This value is the limiting value of the tangent to the curve of activity versus mole fraction as the mole fraction approaches zero.

Metallic systems are unlikely to be binary solutions in practice, so that the presence of other elements will affect the activity of solutes. In the case of dilute solutions, it is possible to handle this by the use of interaction coefficients. These coefficients essentially express the effect of one solute on the activity coefficient of another. Compilations of interaction coefficients are readily available, but it should be stressed that these data are only applicable to dilute solutions.

A solution model that can satisfactorily deal with non-dilute metallic solutions is therefore required.

## **5 IDEAL MIXING OF COMPLEX COMPONENTS**

The terminology used in the following section requires definition. The term 'components' refers to the usual reference-state oxides, such as  $\text{SiO}_2$ ,  $\text{CaO}$ ,  $\text{MgO}$ , and  $\text{Al}_2\text{O}_3$  in slag systems, and to the elements, such as  $\text{Fe}$  and  $\text{Si}$ , in metallic solutions. 'Complex components' refers to compounds (liquid or solid) of the simple components, such as  $2\text{MgO}\cdot\text{SiO}_2$  in a slag, or  $\text{Fe}_3\text{Si}$  in a metal.

For systems as complex as metallurgical slags, the previously available solution models do not appear to be generally applicable, owing to the substantial, highly complex thermochemical interactions that occur on mixing. Many oxide systems are characterized by strong acid-base chemical interactions, leading to negative deviations in thermodynamic activities that are much larger than those predicted by the ideal-solution or regular-solution models. A notable property of silicate systems, for example, is the ability of the silica activity to vary from very high to very low values over a narrow compositional range. This characteristic is not found in metallic or organic solutions. An attempt has been made to account for these strong interactions by the consideration of the formation of complex liquids and solids as mixing components.

Turkdogan<sup>4</sup> maintains that Schenck<sup>5</sup> was the first author to introduce the concept of representing a slag composition in terms of assumed complex components. Hastie and

Bonnell<sup>6</sup>, however, trace the fundamental ideas back to the so-called 'chemical model' of Dolezalek<sup>7</sup>, which was applied to organic liquids. Further early work dealt with the application of this technique to alloys and several binary oxide systems. However, it is only recently that complex slags have been described by this model.

Hastie and Bonnell<sup>6,8,9</sup> have developed a model for the calculation of detailed equilibrium compositions of non-ideal systems such as oxide slags. The model is applicable to high-order systems and, among other applications, has been successfully used to describe oxide mixtures containing up to eight elements. This model has a thermodynamic basis, and does not rely on assumed molecular or ionic entities in the liquid phase, or on experimental information such as mixing thermochemistry or phase diagrams. This model has been validated<sup>6,8</sup> by comparisons with experimental activity data in systems ranging from binary to sexternary mixtures.

The model is based on the identification of complex components (such as alkali silicates) in solution. These complex components account for the non-ideal solution interactions. These complex components, together with the non-complexed constituent components, are explicitly included in a thermodynamic database from which standard Gibbs free energies of formation can be calculated. A multicomponent equilibrium calculation technique (such as the free-energy minimization technique developed by Eriksson<sup>1</sup>) is then used to determine the equilibrium distribution of each component in any phase, with the calculations being constrained to obey the Gibbs-Duhem activity and Gibbs phase-rule relationships. Hastie and Bonnell compared the experimental values with those predicted by the model, and found the equilibrium mole fractions of the uncomplexed components were equivalent to their activities. This approach thus enables a direct determination to be made of the activities of the putative components of the solution, without an analytical model of the activity function being required. Hastie and Bonnell found the model to be very reliable in predicting large departures from ideality, such as occur for alkalis in polymeric oxide slags.

The key assumption of the present model is that complex solution phases can be approximated as mixtures of known, or hypothetical, liquids based on melts of



established complex solids. The liquid components are not independent molecular or ionic species, but are essentially sub-phases that serve as models for the local associative order. Therefore, the complex thermodynamic interactions that occur between components are essentially contained in the Gibbs free energies for the complex components. A typical multicomponent oxide system can then be represented as an ideal mixture (or any other physical model) of many such component liquids and solids.

Once the equilibrium composition of the complex system has been derived, the thermodynamic activities are given simply by the final mole fractions of the component liquids. This approach is therefore a modified form of ideal-solution theory, but with the formation of complex components taken into account. This approach is referred to by Hastie and Bonnell as the Ideal Mixing of Complex Components (IMCC) model.

The use of molecular formulae in this model does not imply the actual presence of molecular species. The model deals only with liquids or solids as components of the mixture, and not with molecular or ionic species as is often the case with other solution models. Hence the complex components present in the model should not be taken as being indicative of the mixture speciation, but are strictly formal thermodynamic entities. It should also be noted that alternative definitions of ideality, such as Temkin's ionic model for slags, require structural assumptions that are not necessary in the present treatment. The component liquids considered in this paper are distinctly different from the hypothetical associated species used in other modelling approaches. For the most part, the component liquids are established neutral, stable, thermodynamic compounds, appearing in phase diagrams in equilibrium with congruently melting solids, and also in reference tables of thermodynamic functions. The free energies of formation,  $\Delta G_f^0$ , are either known or can be estimated for these complex component liquids (and solids).

The component and complex-component oxides formed are assumed to mix ideally, in accordance with Raoult's law. Hence thermodynamic activities and apparent mole fractions ( $x^*$ ) are equivalent quantities with this model. Here, the apparent mole fractions refer to the calculated equilibrium composition, with all possible liquid and

solid components present. This terminology should be distinguished from the use of  $x$  to denote the total mole fraction of components present when no complex-forming reactions are considered. Note that, in a slag,  $x_{\text{CaO}}^*$ , for example, may be much less than  $x_{\text{CaO}}$ , owing to the incorporation of CaO liquid into complex liquid species such as CaO.SiO<sub>2</sub>.

In the IMCC model, it is implicit that the physical interactions (i.e. those not attributed to chemical bonding) among the complex components are considered negligible compared to the strong chemical interactions leading to their formation. It is noteworthy that this is the case for many metal-oxygen and metal-sulphur systems, as well as oxide ceramic mixtures and certain alloy systems, that are influenced primarily by the chemical interaction caused by the formation of associated species and secondarily by the physical interactions among all the species.

For the description of typical industrial slag systems, many solid and liquid complex components are required by the model. If sufficient data is available for the system of interest, this approach can effectively be used to represent binary, ternary, and quaternary interactions between the constituent oxide compounds.

One of the prime benefits of this predictive model is that it is equally capable of handling systems containing few or many components. The fact that this model can therefore be applied to systems where essentially no phase-stability information is available, represents a significant improvement in the prediction of activity relations for complex systems.

Other types of model require empirically based terms for the Gibbs energy of mixing. Such empirically based models serve primarily to allow theoretical extension of the experimental data to new compositions, but extensive extrapolations are risky, because new unaccounted-for complex species may form. According to Hastie and Bonnell, models with an empirical basis cannot be expected to apply, in the foreseeable future, to the great variety of industrially important complex systems.

In alloy mixtures, the extension from binary to higher-order systems is possible with little additional thermodynamic complexity. However, in slag systems, the number of significant component liquids may increase from two or three in a binary system to more than ten in a quaternary system. The presence of significant amounts of complex components containing three or four cations is a convincing argument against the extension of analytical models of binary oxide systems to higher-order systems without additional chemical interaction terms.

Because of the uncertainty in the available thermodynamic data, further refinement in the modelling of solution phases may not, in at least some cases, be warranted.

As an aside, it should be mentioned that the calculation of activities as functions of composition and temperature also provides sufficient information for the construction of phase diagrams. However, even modest uncertainties in thermodynamic data can lead to inconsistencies in phase diagram calculations. The phase boundaries calculated by Hastie and Bonnell<sup>9</sup>, using their model, are in good agreement with those in the experimental phase diagram found in the literature.

## **6 THERMODYNAMIC DATA**

The application of the IMCC model requires a thermodynamic database for the component and complex-component solids and liquids. Table 1 shows the Gibbs free energy function for the liquid species and solid phases used in the modelling of the CaO-MgO-SiO<sub>2</sub> system at a temperature of 1600°C. The reference state used for the enthalpy is that of the pure elements in their standard state at 25°C and 1 atmosphere, while the absolute entropy values are used. The values of the free energies were calculated using data from the F\*A\*C\*T thermodynamic database<sup>10</sup>.

Table 1: Gibbs free-energy function for solid phases and liquid species at 1600°C

Species	$\Delta G^\circ$ Solid (kJ/mol)	$\Delta G^\circ$ Liquid (kJ/mol)
CaO	-802	-774 *
MgO	-739	-709 *
SiO <sub>2</sub>	-1106	-1105 *
CaO.MgO	-1545 *	-1545 *
CaO.SiO <sub>2</sub>	-1994 **	-1997
2CaO.SiO <sub>2</sub>	-2850	-2850 ***
3CaO.SiO <sub>2</sub>	-3645 **	-3645 **
3CaO.2SiO <sub>2</sub>	-4845 **	-4845 **
MgO.SiO <sub>2</sub>	-1874 **	-1875
2MgO.SiO <sub>2</sub>	-2643	-2634 *
CaO.MgO.SiO <sub>2</sub>	-2765	-2765 **
CaO.MgO.2SiO <sub>2</sub>	-3885 **	-3902
2CaO.MgO.2SiO <sub>2</sub>	-4760 **	-4760 **
3CaO.MgO.2SiO <sub>2</sub>	-5626 **	-5626 **

\* = Extrapolated from the data for the liquid

\*\* = Extrapolated from the data for the solid

\*\*\* = Data for the solid phase

When the required data is not available for a particular liquid species or solid phase (either because no measurements exist or because of instability at the temperature of interest), it is necessary to extrapolate the free-energy data. This can be done in a number of ways. In cases where no literature data is available for a liquid, it is possible to use the data for the solid phase together with an estimate of the changes in enthalpy and entropy on melting. As a simpler alternative, the free-energy data can be extrapolated using the functional form of  $\Delta G_f^0$  for the phase region of interest. In cases where there is no data at all for a liquid, the free-energy function of the solid phase has been used instead. Although it is possible to correlate thermodynamic properties and their changes at phase boundaries with molecular structures, this was not done during the present investigation. The prime emphasis was on the development of a simple technique which is readily accessible, and which does not require an advanced knowledge of the estimation of thermodynamic properties. (It can be seen from Table 1 that in the case of MgO.SiO<sub>2</sub> (solid), for example, it would have been adequate to use the free-energy data for MgO.SiO<sub>2</sub> (liquid) directly, as the difference is very small.)

The error due to the extrapolation is expected to be small. Certainly this error is less than the error in the measured values of  $\Delta G_f^0$ , which is estimated by Hastie and Bonnell<sup>6</sup> to be typically 4 to 12 kJ/mol.

## 7 COMPARISON WITH EXPERIMENTAL DATA

The IMCC approach has been used in the present work to model simple industrial slags. So that activities predicted by the use of the model could be compared with experimentally-determined values, three slag systems were investigated. The binary systems CaO-SiO<sub>2</sub> and MgO-SiO<sub>2</sub>, and the ternary system CaO-MgO-SiO<sub>2</sub>, were examined by means of the model, and the predicted data were compared with the experimentally-determined data of Rein and Chipman<sup>11</sup>.

For each of the systems, all possible species and phases for which thermodynamic data is available were considered as possible candidates for formation at equilibrium. For example, in the case of the CaO-SiO<sub>2</sub> binary system, the liquid phase was considered to comprise CaO(L), SiO<sub>2</sub>(L), CaO.SiO<sub>2</sub>(L), 2CaO.SiO<sub>2</sub>(L), 3CaO.SiO<sub>2</sub>(L), and 3CaO.2SiO<sub>2</sub>(L). The possible formation of some pure solid phases was considered from among CaO(S), SiO<sub>2</sub>(S), CaO.SiO<sub>2</sub>(S), 2CaO.SiO<sub>2</sub>(S), 3CaO.SiO<sub>2</sub>(S), and 3CaO.2SiO<sub>2</sub>(S), up to the limit imposed by the phase rule. The thermodynamic data in Table 1 were used in the free-energy minimization calculations.

The activities for the simple components in the slag were obtained from the results of the equilibrium calculations, in the manner outlined earlier. These calculated activities are relative to the pure components in the liquid state at 1600°C. However, the standard states used by Rein and Chipman are those of the solid oxides at 1600°C. This is an experimental convenience, because the compositional range for the liquid phase is often limited by saturation of the melt with the solid oxide at the temperature of the activity measurements. Before the experimental activity data could be used for the purposes of comparison, it had to be transformed by means of equation 4, where the subscripts S and L refer to the solid and liquid phases respectively.

$$\frac{a_L}{a_S} = \exp \left[ \frac{\Delta G_S - \Delta G_L}{RT} \right] \quad (4)$$

The above transformation is straightforward for the case of CaO and MgO. However, as 1600°C is near the melting point of SiO<sub>2</sub>, the difference in free energy between the solid and liquid needs to be determined with care, particularly as the ratio of the activities is an exponential function of the free-energy difference. In this case, the data of Hastie and Bonnell<sup>6</sup> was used to calculate a value (-2904 J/mol) for the change in free energy from SiO<sub>2</sub> solid to SiO<sub>2</sub> liquid at 1600°C.

Figures 2 and 3 show the activity - mole-fraction relationships for the two binary systems under consideration. So that a comparison can be made with the experimental data, the graphs pertain to that portion of the phase diagram where only a liquid is present, although the model is able to deal with the presence of solids as well. The composition boundaries are indicated on the diagrams. From these figures, a comparison can be made between the calculated activities, the experimentally determined activities, and the ideal activities. Where the activity curves lie close to the x-axis, an enlarged portion of this part of the graph is also presented.

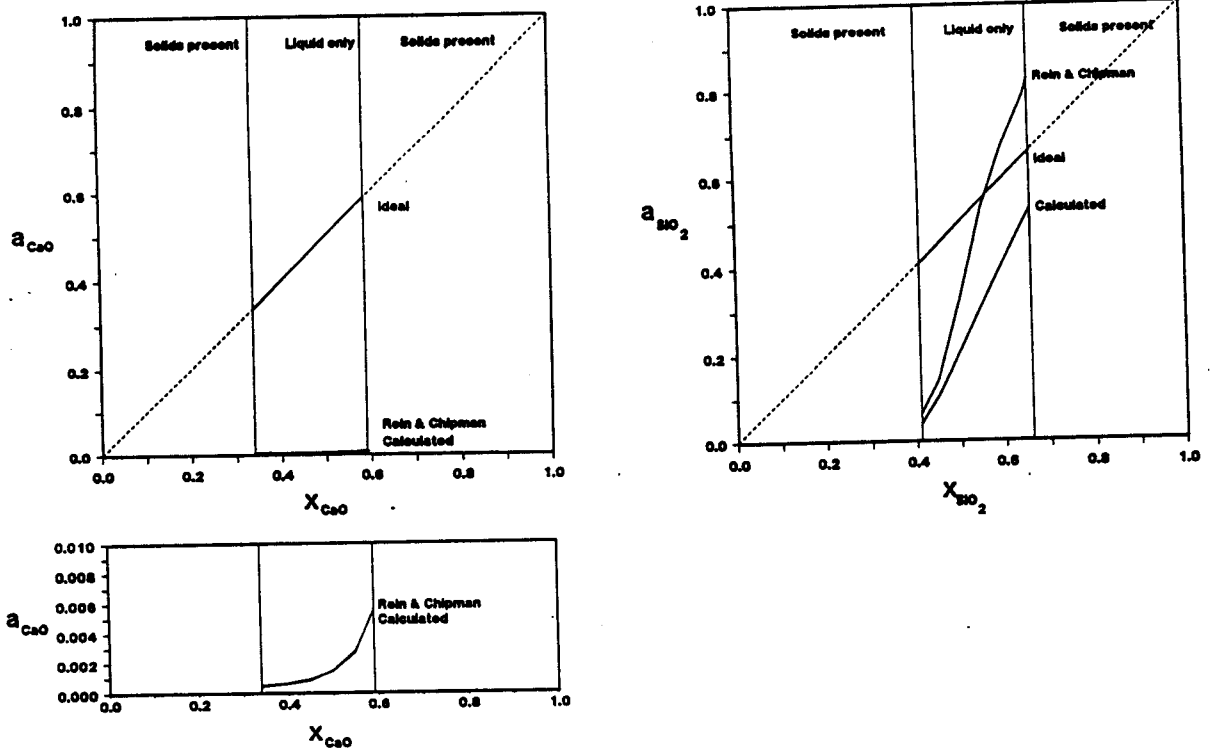


Figure 2: Activity - mole fraction curves for the system CaO-SiO<sub>2</sub> at 1600°C

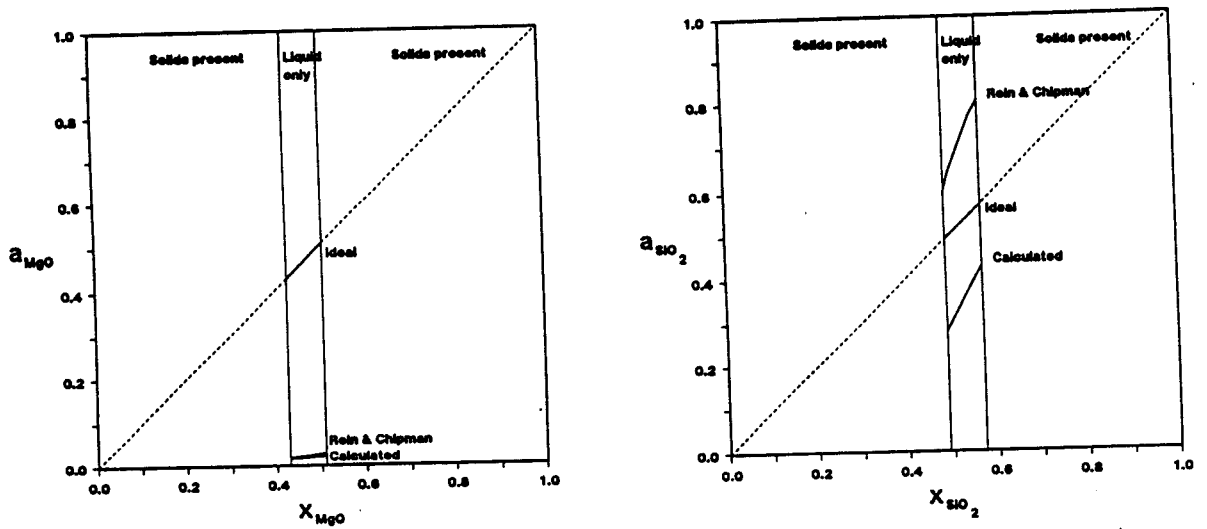


Figure 3: Activity - mole fraction curves for the system MgO-SiO<sub>2</sub> at 1600°C

There is excellent agreement between the calculated and experimentally determined activities of CaO and MgO in the binary systems. It is also important to note the large discrepancies that would result if the assumption of an ideal solution was made. The agreement between the various curves for the activity of SiO<sub>2</sub> is not quite as good as for CaO and MgO. In the CaO-SiO<sub>2</sub> binary, the agreement is better at lower SiO<sub>2</sub> contents. In the case of the MgO-SiO<sub>2</sub> system, the calculated SiO<sub>2</sub> activity is rather close to that predicted for an ideal solution. However, the discrepancies for SiO<sub>2</sub> activity should be seen in the context of the likely errors in experimental determinations of activity. According to Turkdogan<sup>12</sup>, uncertainties in activity data of up to ±30% are not considered unusual for a given set of experiments. In fact, Turkdogan has also noted that, when experimental activities are recalculated relative to the pure liquid oxide components, there should be marked negative deviations from Raoult's law in almost all the binary oxide melts consisting of the oxides of a network modifier and a network former, e.g. MO-SiO<sub>2</sub>.

It should be pointed out that the determination of phase boundaries in phase diagrams is extremely sensitive to errors in the free-energy data. For example, if the value for the free energy of liquid SiO<sub>2</sub> were altered by only 5 kJ/mol, the predicted boundary between solid SiO<sub>2</sub> plus liquid and the liquid only in the CaO-SiO<sub>2</sub> system at 1600°C, would shift by 20 mole % CaO.

It is clear from the experimental data that the activity of CaO in the CaO-SiO<sub>2</sub> system and the activity of MgO in the MgO-SiO<sub>2</sub> system show negative departures from ideality. Treatment of the liquid phase as an ideal solution of the simple oxide components and complex components, with homogeneous equilibrium among these species, would automatically introduce approximately the right degree of departure from the simple oxide ideality.

In order to demonstrate the use of the IMCC model for a ternary slag system, a slice through the CaO-MgO-SiO<sub>2</sub> system was investigated. Figure 4 shows the activity - mole-fraction relationships in the CaO-MgO-SiO<sub>2</sub> system at a constant level of 30 mole % CaO.



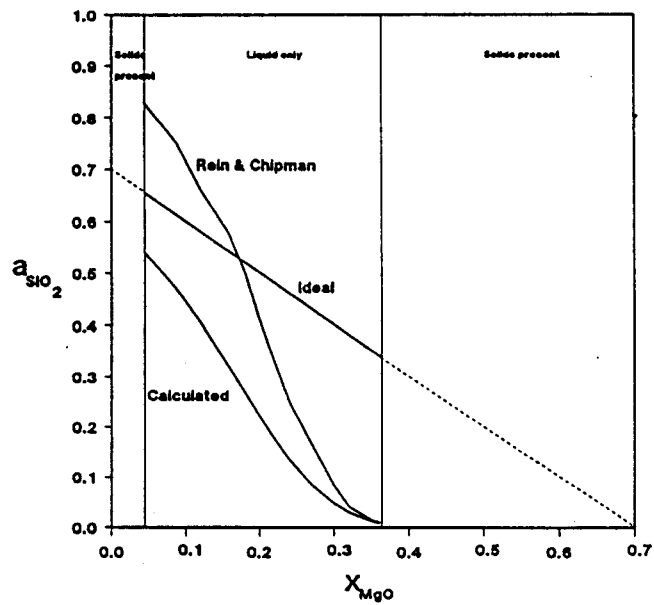
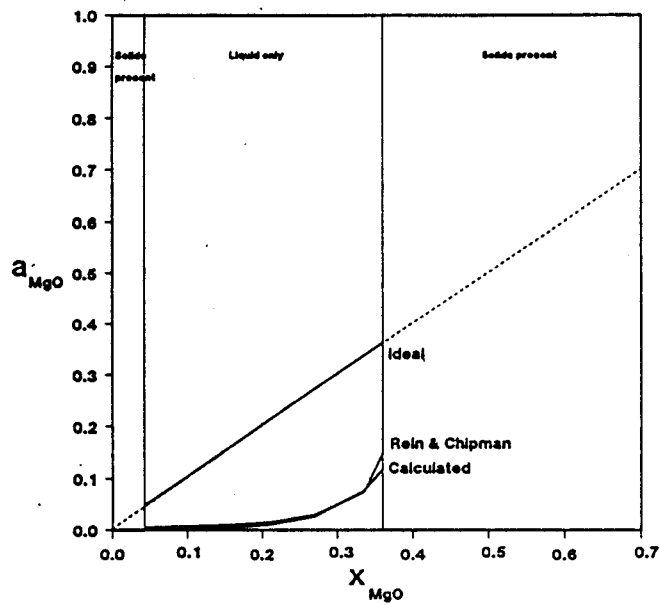
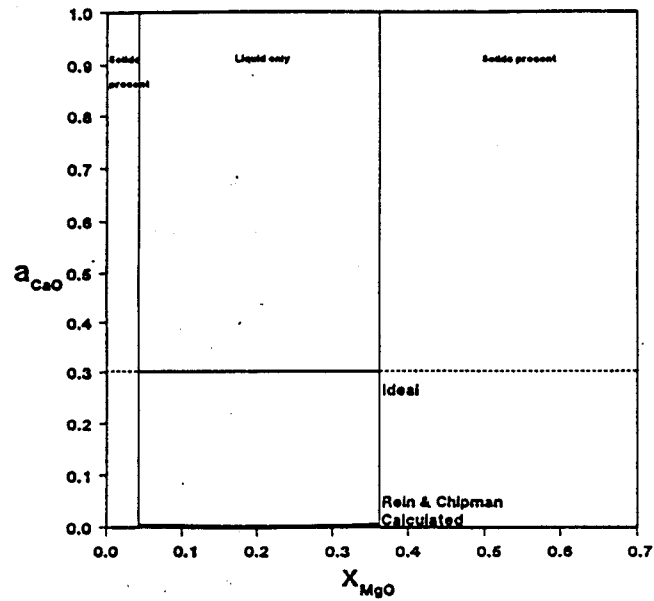


Figure 4: Activity - mole fraction curves for the system CaO-MgO-SiO<sub>2</sub> (at 30% CaO) at 1600°C

Once again, there is excellent agreement between the calculated and experimentally determined activities for CaO and MgO, together with moderately good agreement between the activity curves for SiO<sub>2</sub>.

## **8 APPLICATION TO A COMPLEX SYSTEM**

As discussed earlier, so that a complex equilibrium system can be specified, it is necessary to list all the possible species in each phase. As an example, a specification is given in Table 2 for the gas, slag, and metal phases that are present at equilibrium in the production of ferrochromium. It should be borne in mind that solid phases might also be present, depending on the process temperature, up to the limit prescribed by the phase rule. It is obviously quite reasonable to neglect the inclusion of those species known to be unstable. However, it should be noted that there is no harm done in specifying a species to be present in a particular phase, even if it is unstable in that phase. The free-energy minimization, subject to the constraints of mass conservation, takes care of the amount of each substance that is formed.

Table 2: Specification of possible complex components for ferrochromium production

Phase	Components
Gas	CO CO <sub>2</sub> H <sub>2</sub> H <sub>2</sub> O N <sub>2</sub> SiO Mg
Slag	Cr <sub>2</sub> O <sub>3</sub> CrO <sub>2</sub> CrO <sub>3</sub> Cr <sub>5</sub> O <sub>12</sub> Cr <sub>8</sub> O <sub>21</sub> FeO Fe <sub>2</sub> O <sub>3</sub> Fe <sub>3</sub> O <sub>4</sub> SiO <sub>2</sub> CaO CaO <sub>2</sub> MgO Al <sub>2</sub> O <sub>3</sub> FeO.Cr <sub>2</sub> O <sub>3</sub> MgO.Cr <sub>2</sub> O <sub>3</sub> FeO.Al <sub>2</sub> O <sub>3</sub> MgO.Fe <sub>2</sub> O <sub>3</sub> CaO.Fe <sub>2</sub> O <sub>3</sub> 2CaO.Fe <sub>2</sub> O <sub>3</sub> FeO.SiO <sub>2</sub> 2FeO.SiO <sub>2</sub> CaO.SiO <sub>2</sub> 2CaO.SiO <sub>2</sub> 3CaO.SiO <sub>2</sub> 3CaO.2SiO <sub>2</sub> CaO.Al <sub>2</sub> O <sub>3</sub> CaO.2Al <sub>2</sub> O <sub>3</sub> 3CaO.Al <sub>2</sub> O <sub>3</sub> 12CaO.7Al <sub>2</sub> O <sub>3</sub> CaO.MgO MgO.SiO <sub>2</sub> 2MgO.SiO <sub>2</sub> Al <sub>2</sub> O <sub>3</sub> .SiO <sub>2</sub> Al <sub>2</sub> O <sub>3</sub> .2SiO <sub>2</sub> 3Al <sub>2</sub> O <sub>3</sub> .2SiO <sub>2</sub> CaO.MgO.SiO <sub>2</sub> CaO.MgO.2SiO <sub>2</sub> 2CaO.MgO.2SiO <sub>2</sub> 3CaO.MgO.2SiO <sub>2</sub> CaO.Al <sub>2</sub> O <sub>3</sub> .SiO <sub>2</sub> CaO.Al <sub>2</sub> O <sub>3</sub> .2SiO <sub>2</sub> 2CaO.Al <sub>2</sub> O <sub>3</sub> .SiO <sub>2</sub> 3CaO.Al <sub>2</sub> O <sub>3</sub> .3SiO <sub>2</sub> 2MgO.2Al <sub>2</sub> O <sub>3</sub> .5SiO <sub>2</sub>
Metal	Cr Fe Si C Cr <sub>3</sub> C <sub>2</sub> Cr <sub>4</sub> C Cr <sub>7</sub> C <sub>3</sub> Cr <sub>23</sub> C <sub>6</sub> Fe <sub>3</sub> C SiC FeSi FeSi <sub>2</sub> Fe <sub>3</sub> Si Fe <sub>3</sub> Si <sub>7</sub> CrSi <sub>2</sub> Cr <sub>3</sub> Si Cr <sub>5</sub> Si <sub>3</sub>

## 9 CONCLUSION

The Ideal Mixing of Complex Components (IMCC) solution model has been shown to be applicable to the prediction of activities in complex solutions where chemical interactions are dominant over physical interactions. Such systems are often encountered in pyrometallurgical systems. This solution model works well and is easy to use in equilibrium calculations within a computer program for pyrometallurgical process simulation such as PYROSIM<sup>13</sup>.

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