Exploring Compositional Space in Metallurgical Slag Systems

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Abstract: Critical to our understanding of the relative stabilities of metallurgical reaction systems is knowledge of equilibrium phase chemistry, and how the phases and their chemical compositions might change as functions of key process variables. Despite the extensive research that has been undertaken to determine the thermodynamic properties of slag-forming systems there is still much more that needs to be done to

- Improve the accuracy of existing data,
- Describe the behaviour of complex multi-component, multi-phase systems, and
- Characterise new combinations of elements arising from the manufacture of new materials

The main themes that will be examined include:

- A review of some of the modern experimental and modeling tools that are available to characterize the elements and phases present in high temperature slag systems,
- How complex multi-component systems can be described in understandable and useful forms, and how these approaches can be used to systematically explore the sequences of phase changes during processing,
- Identifying critical experimental data, and the development of research strategies to accurately and optimally determine phase equilibria,
- What lies ahead? Future challenges and directions.

Keywords: phase diagrams, slags, liquidus

1. Introduction

In the preface of the classic text on “Phase Diagrams for Metallurgy” Rhines [1] provides a short summary of the history of development of phase equilibria studies and those who contributed to establishing the guidelines and ways of representing equilibria in multi-component, multi-phase systems. It is a little over 100 years since the scientific community began to present the measurements of chemical equilibria in heterogeneous systems in diagrammatic form, as functions of key thermodynamic variables of composition, temperature and pressure. Over that timeframe the approach has proved to be invaluable in understanding geological/earth processes, phase changes in metal alloys and ceramic materials, and the chemistry of process metallurgy.

The purpose of the present paper is not to attempt comprehensive analysis and review of the field but rather to highlight some of the more recent developments in experimental techniques and theoretically based tools, to illustrate different ways in which phase equilibria can be presented to users and to indicate areas of future research.

2. Experimental techniques and modeling tools

A wide range of experimental techniques have been used to determine the phases present at equilibrium, their crystal structures, compositions, stoichiometry, oxidation states of individual elements and thermodynamic properties [2]

As researchers we are, to certain extent, limited by the physical and theoretical tools that are available to us at any given time. Looking beyond the many phase diagrams that we now accept as "well established" back to the original papers it becomes clear that most early phase equilibria studies from the early to the mid-20th century relied on a small number of experimental techniques; principally bulk chemical analysis, optical microscopy, XRD, TGA and DTA. These techniques have served and continue to serve us well; they have provided the bulk of the scientific knowledge we have today and are still relevant. As the design and instrumentation associated with these analytical techniques have improved so to have the accuracies of the data that can be obtained and used to characterise first and second order phase transformations, i.e. those having discrete phase boundaries, and those exhibiting internal structural changes within particular phases respectively.

In addition, however, a wide range of relatively new and sophisticated measurement techniques are now available that are increasingly used by researchers of phase equilibria; these include – Knudsen cell mass spectrometry KCMS; electrochemical techniques; spectroscopic techniques XPS, SIMS, XANES, Mossbauer, FTIR, Raman; Micro-analytical techniques EDS, EPMA; Electron microscopy SEM, TEM [3, 4]. Examples of the thermodynamic and phase equilibria measurements in high temperature systems undertaken in recent studies are summarized and referenced in Table 1.

Table 1. Summary of recent research on property measurements undertaken in high temperature slag systems.

Property	**References see details in Appendix A**
Activity	A1-A5
Oxidation state	A6-A11
Partitioning of minor elements between phases	A12-A22
Phase equilibria	A23-A50
Thermodynamic modelling	A51-A63

3. The "hidden" elements

It is well established that some elements e.g. the transition metals, can exist in more than one oxidation state, and that each of the ions can behave essentially as different and additional components in the system. The relative proportions of species of different oxidation states depend, as with any other chemical species on the bulk composition, temperature and oxygen pressure in the system. From a thermodynamic point of view establishing these data is important if accurate descriptions of the relative stabilities of different phases are to be obtained.

The conventional approach to the determination of the relative proportions of the different oxidation states of an element has been to undertake bulk wet chemical analysis on single phase materials. These approaches become difficult when trying to characterise multi-element systems, and cannot be used to quantitatively determine the species present when more than one phase is present in the system.

More recently developed spectroscopic techniques offer some promise for future research in this area, but these are not without their own difficulties. In particular, the spectra are complex in shape, in many cases the differences in spectra between the ions of the same element are small and often overlap each other. Improvements in resolution of the instruments, the ability to distinguish between signals obtained at a given wavelength, have helped but this does not solve all of the difficulties. Since these are comparative measurements developing suitable standards for the measurements is important. There are also some current limitations on the special resolution of the techniques, that is, the minimum size of the sample that can be analysed.

Recent studies on the use of XPS have shown that accurate measurement of Fe^{2+}/Fe^{3+} ratio in oxides can be obtained within scanning area as small as 100μm square [5, 6]. This was demonstrated after a) selecting a suitable peak for measurement; avoiding the strong but more complex multi-peak shape of the 2p and instead using the weaker but much simpler to describe 3p peak shape, (Figure 1) b) careful analysis and optimization of the model parameters used to describe the peak shape for each standard, and c) the selection of unambiguously defined standards for each ion. In this case stoichiometric fayalite, $2FeO.SiO_2$, was used (see Figure 2) for the Fe^{2+} standard rather than wustites, the former contains only Fe^{2+} ions whereas the latter, which had previously been employed without success, are known from metallurgical research to contain variable concentrations of both Fe^{2+} and Fe^{3+} depending on preparation history. Thus the contributions from each the two species can be unambiguously measured. The accuracy of the procedure can be tested by reference to another “unknown” in the form of stoichiometric magnetite, $FeO.Fe_2O_3$, as an (see Figure 3).

In the future it is expected that the spacial and spectral resolutions of these XPS instruments will be further improved, which will enable the accurate analysis of oxidation states of elements in individual phases in multiphase systems. It may also be possible to use this approach to simultaneously quantify the species in complex slag systems containing a number of transition metals.

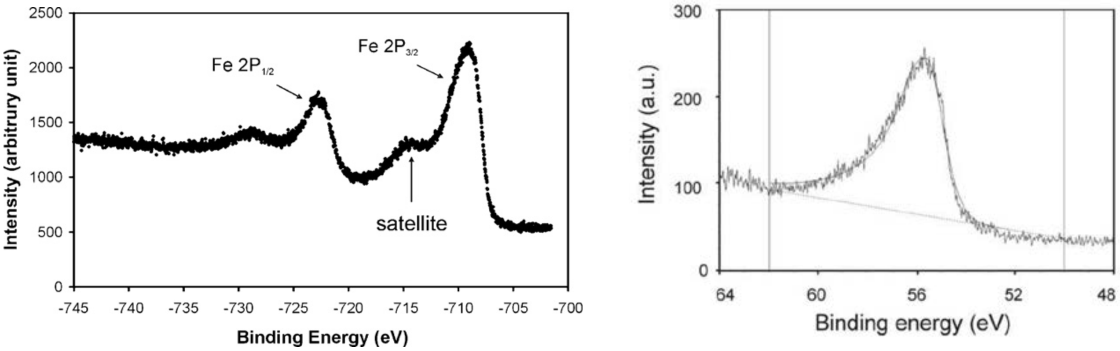


Figure 1. XPS spectra from a fractured Fe_2O_3 standard sample a) 2p, and b) 3p [6]

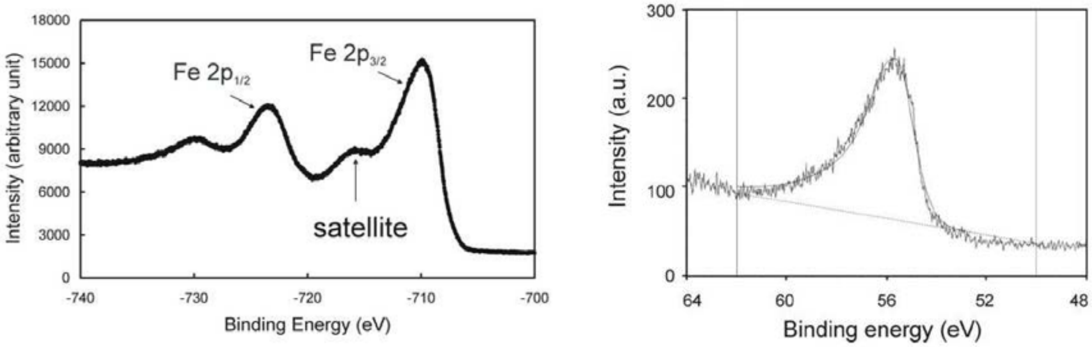


Figure 2 XPS spectra from a fractured $2FeO.SiO_2$ standard sample a) 2p, and b) 3p [6]

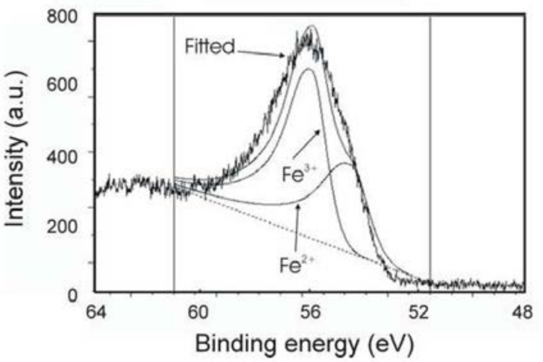


Figure 3 XPS spectrum for stoichiometric solid Fe_3O_4 ($FeO.Fe_2O_3$) fitted using independently determined parameters for Fe^{2+} and Fe^{3+}; predicted FeO/Fe_2O_3 ratio = 0.49 (0.35/0.65) [6]

4. **Modeling tools**

A range of thermodynamic modeling tools are available to support and enable the rigorous analysis of these experimentally determined data. The increasing computer speed and memory now available has made it possible to integrate the whole range of fundamental thermodynamic properties of individual components with measured properties in multi-component, multi-phase systems in ways that are thermodynamically consistent [7, 8]. Commercial software packages such as FactSage, MTdata, SGTE, ThermoCalc, CSIRO-MPE [9-14] can now be routinely used by professional engineers in process design and development. An important feature of mathematical descriptions of Gibbs free energy data and free energy minimization routines is the ability to select infinite combinations of process variables at will without the restrictions imposed by the relatively limited experimentally determined conditions and data available. The ability to extrapolate and interpolate into compositional space has been one of the major steps forward in the field in the past several decades. Further discussion on these tools and their use is given in a later section of the paper.

5. Phase equilibria

Most industrially important processing systems are multi-phase rather than single phase systems. From a practical point of view, therefore, when examining the chemical equilibrium in a system, the first consideration is to determine the phases present under the composition, temperature and pressure conditions. Once the operating window within this phase assemblage is clearly established, the distribution of elements between these phases can be examined and quantified.

5.1 Representation of phase equilibria

Unary

One of the exciting aspects of chemical thermodynamics is its universality and applicability to a wide range of disciplines. There are many contributions to the knowledge of phase equilibria from earth sciences, including examples of unary systems demonstrating phase equilibria in single component systems as polymorphic changes that can take place as functions of temperature and pressure. This is a reminder that our descriptions of these systems should extend beyond the process conditions of interest to immediate metallurgical operations, a point that becomes more poignant when considering more generic descriptions of the thermodynamic behaviour of individual components.

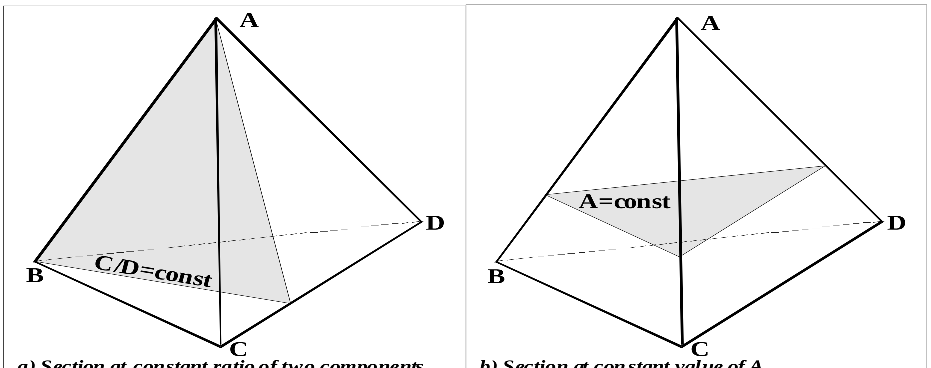
Binary and Ternary Systems

The use and description of binary, pseudo-binary and ternary phase diagrams by metallurgical and materials engineers is now taken as routine and key component of the skills set in these disciplines. Over recent years we have been fortunate that compilations, such as, Phase Diagrams for Ceramists [15] and Slag Atlas [16] have been prepared since these have proven to be valuable resources.

Higher order

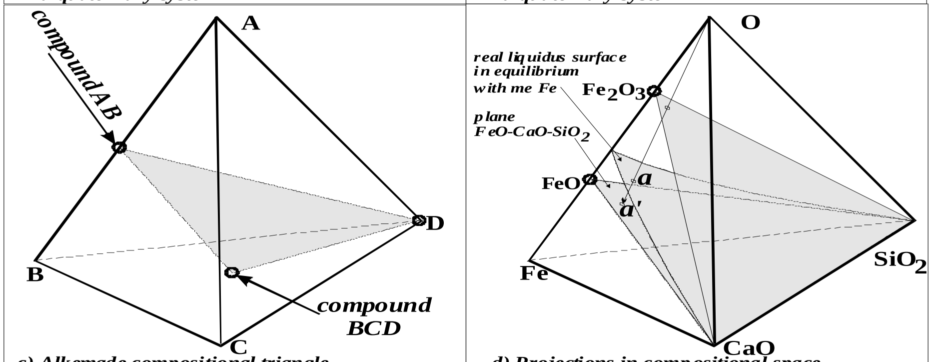
When it comes to extending descriptions to higher order systems we encounter two major sets of hurdles a) a lack of experimental data in these higher order systems, this stems directly from the increased number of experimental points required to accurately define these systems, and b) the difficulties in visualisation and representation of the relative chemical stabilities of phases, which becomes more problematical as the number of components is increased.

There are different ways in which to describe and navigate through compositional space in multi-component systems, some of these options are illustrated in Figure 4. These approaches make it possible to reduce the 4-component and higher order systems to pseudo-ternary systems as long as the restrictions on the chemistry of the system are acknowledged by the user.



a) Section at constant ratio of two components in a quaternary system

b) Section at constant value of A in a quaternary system



c) Alkemade compositional triangle in a quaternary system

d) Projections in compositional space

Figure 4 Examples of the use of projections in compositional space [2]

An important feature of the construction of the pseudo-ternary sections is selection of the compositions of the apices. It is conventional in construction of most phase diagrams to select “end members” to be pure components or stoichiometric compounds. This partly stems from the ability to use the phase rules and Alkemade rules to advantage to enable interpretation of the changes occurring in the system. This is, however, not completely satisfactory when it comes to interpreting a series of phase transformations in multi-component higher order systems.

The selection of the compositions for the corners of the pseudo-ternary should not be arbitrary, they should be selected based on the process variables, or changes in chemical composition during reaction, in the system of interest. In this way the implications of changes in chemistry that occur during processing can be tracked and explained. In addition it is possible to understand the transition from one pseudo-ternary system to another.

These points are best illustrated by example. Consider the series of reaction steps that occur during the processing of lead/zinc slags during oxidation smelting, reduction smelting and subsequent cooling. The chemistry of the system can be described by the components FeO-Fe_2O_3-ZnO-PbO-CaO-SiO_2. An example of a slag microstructure in this system formed as a result of oxidation smelting at high temperature is shown in Figure 5 [17]. It can be seen that there are three solid phases coexisting with the liquid at the processing temperature. In addition initial phase analysis demonstrates that compounds having extensive solid solutions exist at all stages of processing. In this case it is not possible to describe industrial slags in this six component system using any combination of stoichiometric compounds.

The problem is overcome through careful analysis of the phases present and sequence of changes that take place during processing. In the example under consideration the liquidus surfaces of the slag under the initial oxidation smelting conditions are described by the pseudo-ternary section Fe_2O_3-ZnO-$(PbO+CaO+SiO_2)$ in air, where the CaO/SiO_2 and $PbO/(CaO + SiO_2)$ ratios present in the liquid phase are constant. This is deduced from recognition of a number of factors, a) the great a majority of the iron present in the system is in the ferric rather than the ferrous state, b) that both iron and zinc species are present in high melting temperature compounds exhibiting solid solutions, and c) that the lead, calcium and silicon species are not present to a significant extent in any of the iron and zinc-containing compounds in the composition ranges of interest. Zincite solid solution $(Zn,Fe)O$, spinel solid solution $(Zn,Fe,Mg)O.(Fe,Al)_2O_3$, melilite solid solution, $2(Zn,Fe)O.CaO.2SiO_2$, and liquid can be present at process temperatures.

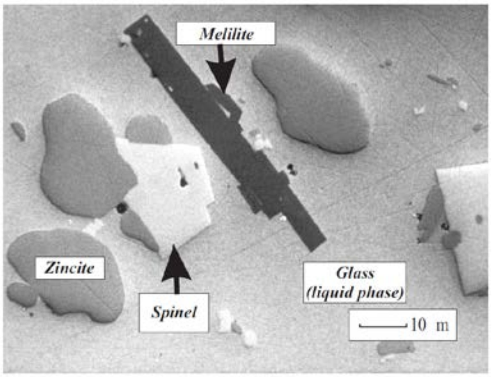


Figure 5 Phases observed in a lead-zinc primary smelting slag under oxidizing conditions [17]

The relationship between the six component system and the pseudo-ternary section is illustrated in Figure 6 [18].

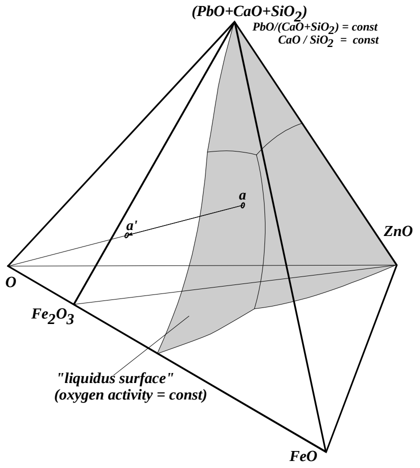


Figure 6 Compositional tetrahedron with constant CaO/SiO_2 and $PbO/(CaO+SiO_2)$ ratios [18]

An example of the liquidus surface of the pseudo-ternary Fe_2O_3-ZnO-$(PbO+CaO+SiO_2)$ in air for fixed CaO/SiO_2 and $PbO/(CaO+SiO_2)$ is shown in Figures 7a and b [18]. The system consists of primary phase fields of spinel, zincite, melilite, hematite, magneto-plumbite and pseudo-wollastonite; the spinel, zincite and melilite phases exhibit extensive solid solutions. Both spinel, $ZnO.Fe_2O_3$, and zincite, (Zn,Fe)O, form very high melting temperature phases and it can be seen that the liquidus is dominated by the spinel and zincite phase fields. The eutectic valley runs from the Fe_2O_3-ZnO binary almost directly towards the third apex representing $(PbO + CaO + SiO_2)$, this binary reaction meets the ternary eutectic point E at which the spinel, zincite and melilite phases coexist.

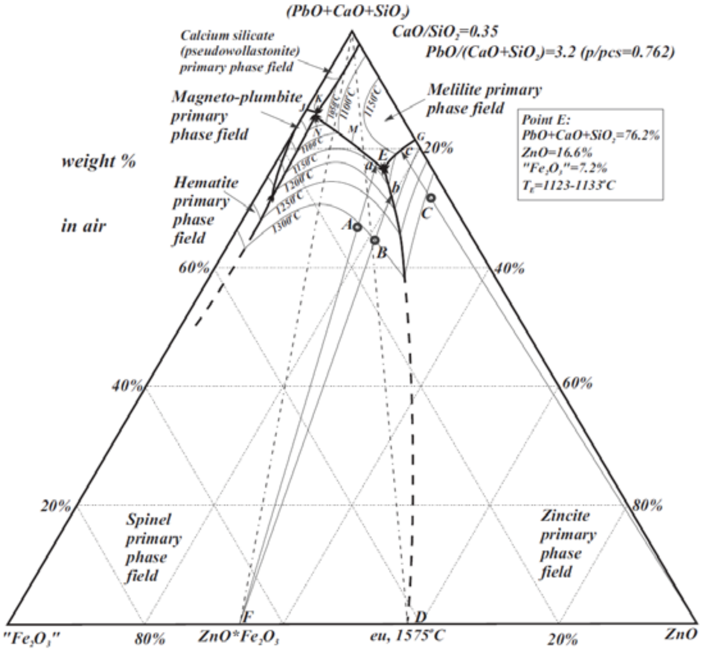


Figure 7a Fe_2O_3-ZnO-$(PbO+CaO+SiO_2)$ in air for CaO/SiO_2 = 0.35 and $PbO/(CaO + SiO_2)$ =3.2 [18]

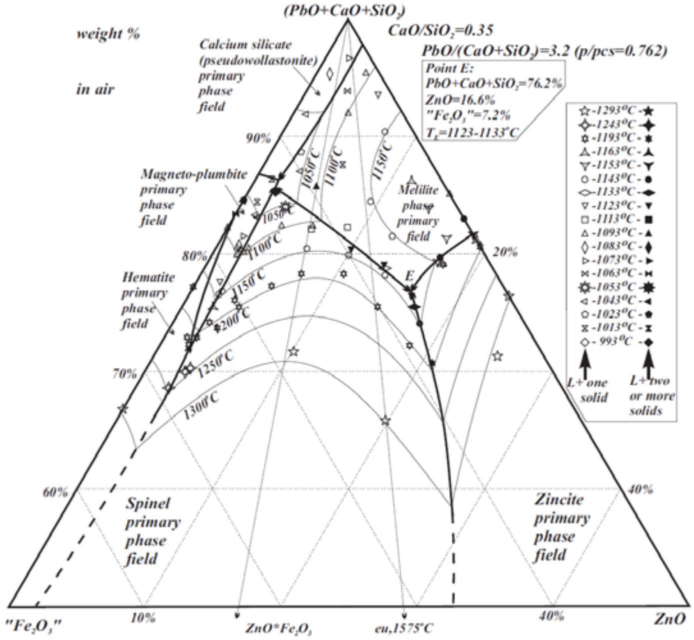


Figure 7b Fe_2O_3-ZnO-(PbO+CaO+SiO_2) in air for CaO/SiO_2 = 0.35 and PbO/(CaO + SiO_2) =3.2 with experimental liquidus points [18]

For the smelting of lead-rich mixed lead/zinc sulphide concentrates the spinel ZnO.Fe_2O_3 is the primary phase formed; the bulk slag compositions for smelting of zinc concentrates lead to the formation of zincite solid solutions (Zn,Fe)O. When spinel or zincite precipitate from the melt only iron and zinc are removed from the liquid phase, so that the ratios of all other chemical species (PbO, CaO, SiO_2) in the liquid are unchanged. The composition of the remaining liquid therefore remains in the pseudo-ternary section for the selected CaO/SiO_2 and PbO/(CaO + SiO_2) ratios. By selecting both iron and zinc as apices in the pseudo-ternary section the proportions of spinel and zincite in the slags in these primary phase fields at a fixed temperature can be predicted using the conventional lever (mass balance) rules. The phase assemblage at the third apex can be deduced from consideration of the PbO-CaO-SiO_2 ternary [19]. At lower temperatures these lead and zinc smelting slags form eutectic mixtures of spinel and melilite, or spinel and zincite, or zincite and melilite, phases together with a low-iron liquid phase that contains progressively less iron as the temperature is lowered. The liquid compositions resulting from the bulk slag compositions A, B and C approach the ternary point E on the pseudo-ternary.

This type of representation can be used to systematically examine the effect of CaO/SiO_2 and PbO/(CaO + SiO_2) ratio on the liquidus and phase equilibria in these systems, figure 8 [20]. On cooling the crystallization of the remaining liquid can be approximated by reference to the PbO-ZnO-(CaO + SiO_2) subsystem [21].

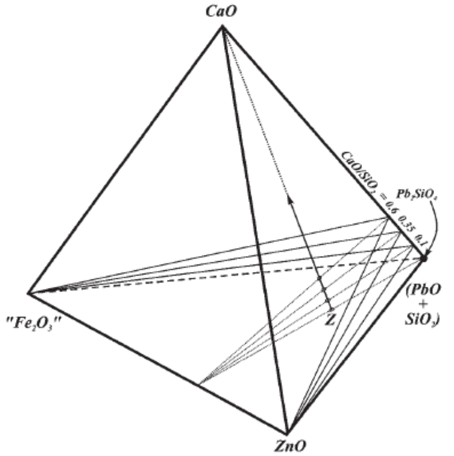


Figure 8 Compositional tetrahedron CaO-ZnO-Fe_2O_3-(PbO+SiO_2) showing the pseudo-ternary sections for weight ratios CaO/SiO_2 = 0, 0.1, 0.35 and 0.6 at PbO/SiO_2 in air. [20]

The analysis and description of these systems does not stop here, however, since in practice these slags undergo further stages of treatment to recover metal values or to satisfy environmental storage criteria.

The smelting of the slags at low oxygen pressures results in the reduction of lead to the metallic form and hence removal from the slag, during these processes the ferric iron is also reduced to predominantly ferrous iron; the resulting slag can then be represented by the FeO-ZnO-(CaO+SiO_2) pseudo-ternary (see Figure 9). The system consists of primary phase fields of wustite, zincite, melilite, fayalite and pseudo-wollastonite, all except the latter exhibit extensive solid solutions. The pseudo-ternary representation, however, makes it possible to accurately characterize the behavior of the system, and systematically investigate the effect of changes in slag chemistry, e.g. CaO/SiO_2 ratio as illustrated in Figures 9b [22] and 10 [23]. The effects of minor elements, such as, MgO and Al_2O_3 can also be readily incorporated in the descriptions of the sub-systems. Figure 11 summarises the wide range of compositions and processes that can be analysed and more clearly understood starting from the slag that is initially generated from the smelting of lead/zinc concentrates in oxidising atmospheres to final reduction and removal of the last traces of lead and zinc from the system.

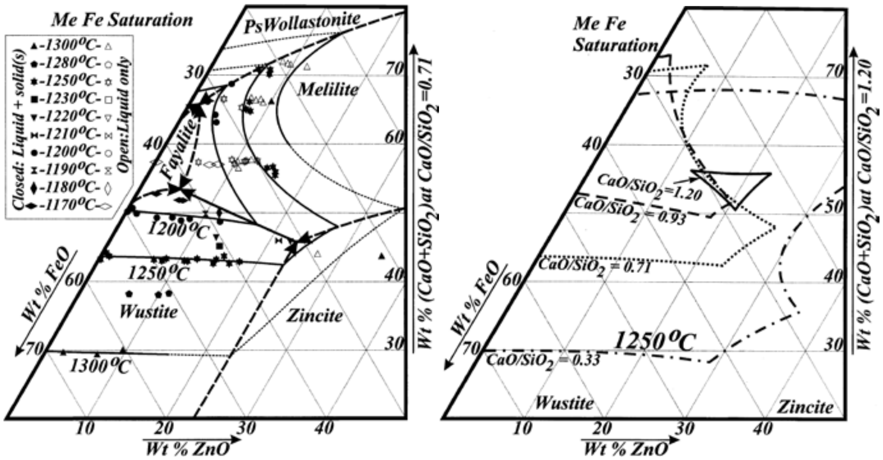


Figure 9 The liquidus of the iron-rich FeO-ZnO-(CaO+SiO_2) pseudo-ternary section a) CaO/SiO_2 = 0.7[22]. and b) effect of CaO/SiO_2 ratio at 1250°C[23]

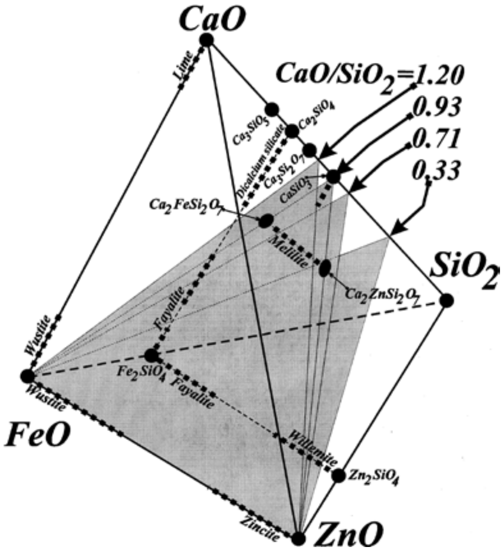


Figure 10 Representation of the FeO-ZnO-(CaO+SiO_2) system through the use of pseudo-ternary sections [23]

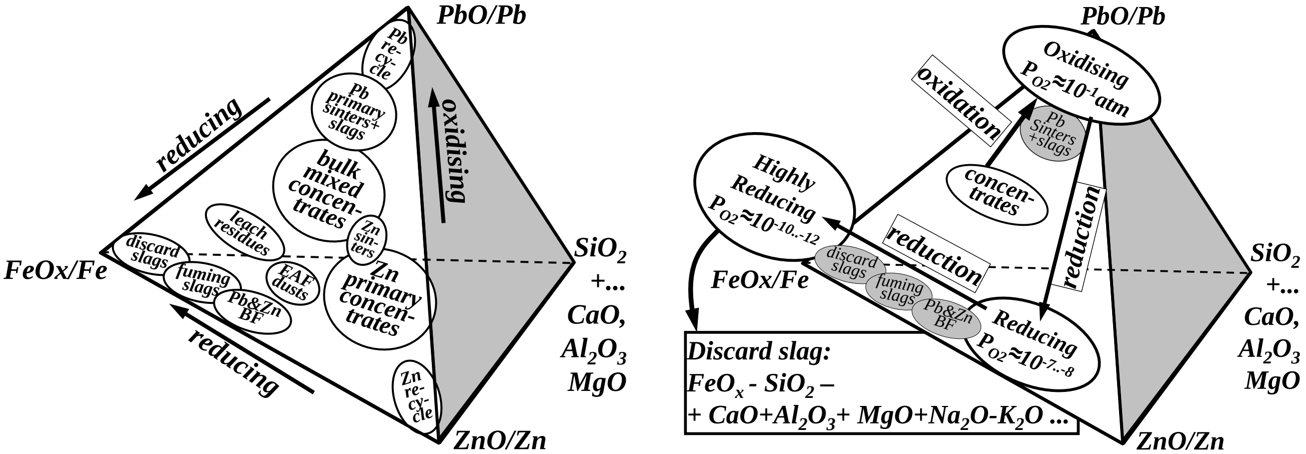


Figure 11 The sequence and range of conditions experienced by lead/zinc smelting slags and high temperature processing [24].

Using the pseudo-ternary approach it is therefore possible to analyse, and more clearly understand, the implications of changes to process chemistry on individual processing operations and the implications for up and downstream processing.

Similar approaches have been taken to describe other complex industrial slag systems for Imperial Smelting Furnace (ISF) slags FeO-ZnO-(CaO-Al_2O_3-SiO_2) [25], and ferro-manganese and silico-manganese MnO-(CaO+MgO)-(Al_2O_3+SiO_2) [26] slags.

6. New experimental techniques

Conventional approaches to the liquidus determination have involved the use of synthetic oxide mixtures equilibrated, where possible, in inert crucible materials followed by quenching and optical metallography; for slag metal equilibria following quenching the compositions of the respective phases have been determined using wet chemical analysis. These approaches whilst relatively simple to undertake experimentally have their limitations in that it is not always possible to obtain inert crucible materials and contamination of the melts can have significant effects on the liquidus determination and partitioning.

The issue of contamination is overcome through the use of crucibles manufactured from the primary phase. This approach followed by physical separation of the phases and wet chemical analysis of the quenched liquid has been used to determine liquidus isotherms. However, the presence or otherwise of additional solid phases suspended in the liquid phase cannot be verified if bulk chemical analysis is the method used. The use of large samples, required for bulk wet chemical analysis, means that the maximum cooling rate on quenching is limited by thermal diffusion; this limits the range of chemical systems and chemical compositions that can be investigated.

In systems in which the one or more components have a significant vapour pressure there is a continuous change in bulk composition and it is therefore not possible to obtain accurate phase equilibrium data using conventional bulk analysis techniques.

To overcome these limitations modified approaches have been developed involving very small slag masses (0.1g) and the use of electron probe X-ray microanalysis (EPMA) techniques to determine the compositions of the phases present in the samples [2]. There are a number of important advantages of these new approaches; since the compositions of the phases are measured following equilibration the results are not influenced by any change in bulk composition provided local equilibrium can be achieved; the presence of additional solid or liquid phases can be detected; the compositions of solid solutions can be measured; any compositional variation with the individual phases, indications that equilibrium has not been achieved, can be detected; equilibrium can be achieved in relatively short times; the very small slag mass means that rapid quenching is achieved extending the range of compositions that can be investigated. In summary, multiphase equilibria can be investigated using the primary phase substrate support technique thus avoiding contamination of the melts; liquidus isotherms can be readily and accurately determined; the accuracy of the analysis is in most cases comparable to that achievable in wet chemical analysis.

This approach has been used to successfully determine liquidus isotherms in the systems FeO_x-CaO-SiO_2 under controlled oxygen partial pressures using platinum metal support, and FeO_x-CuO_y-CaO-SiO_2 using primary phase substrate support also under controlled oxygen partial pressures at copper metal saturation. The data obtained for these systems are shown in Figures 12-16. In these cases a decision must be made as to how best represent the system Ca-Si-Fe-O for the range of oxygen pressures of interest since iron may be present in the slag in the ferric and ferrous states. For reducing conditions the iron can be approximated by projecting onto the FeO-CaO-SiO_2 plane (Figure 12).

Examples of the multiphase equilibria obtained in the FeO_x-CaO-SiO_2 system using the substrate support techniques are shown in Figure 13, and the liquidus at $PO_2 = 10^{-6}$ atm for a range of temperatures in Figure 14.

The approach can be further extended to include not only control of oxygen partial pressure and primary phase saturation at a fixed temperature but also the presence of metal phase, as in the system “Cu_2O”-“FeO”-CaO-SiO_2 system at copper metal saturation. Examples of representation and data obtained for these systems are illustrated in Figures 15 and 16 respectively [28].

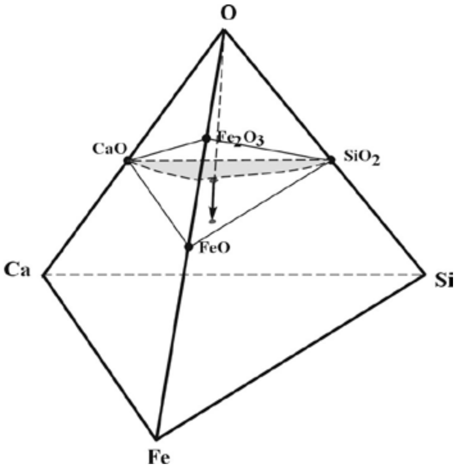
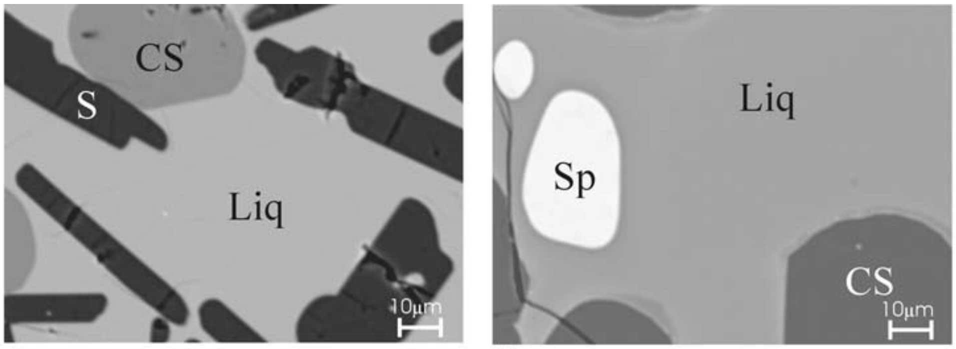


Figure 12. Compositional space in the system Ca-Si-Fe-O and projection onto the FeO-CaO-SiO_2 plane.



(a) Liquid(Liq), tridymite (S) and pseudowollastonite (CS) at 1200°C **(b)** Liquid(Liq) spinel (Sp) and pseudowollastonite (CS) at 1250°C

Figure 13 Backscattered SEM micrographs typical of equilibrated FeO-Fe_2O_3-CaO-SiO_2 slag samples [27].

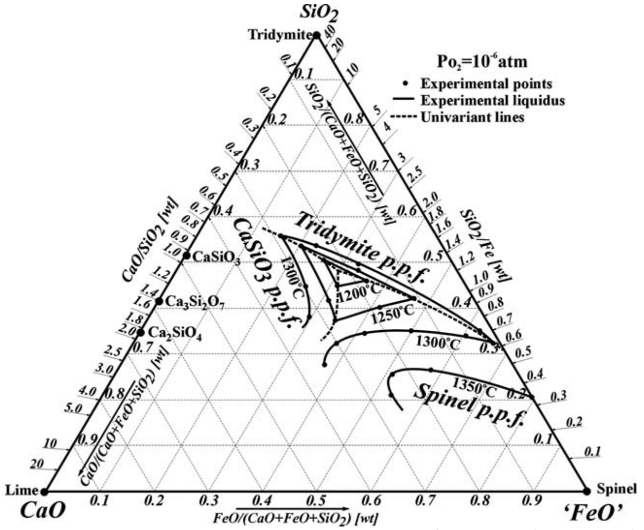


Figure 14 Liquidus isotherms in the ‘‘FeO’’-CaO-SiO_2 system at 1200°C, 1250 °C, 1300 °C, and 1350 °C at a $PO_2 = 10^{-6}$ atm. [27].

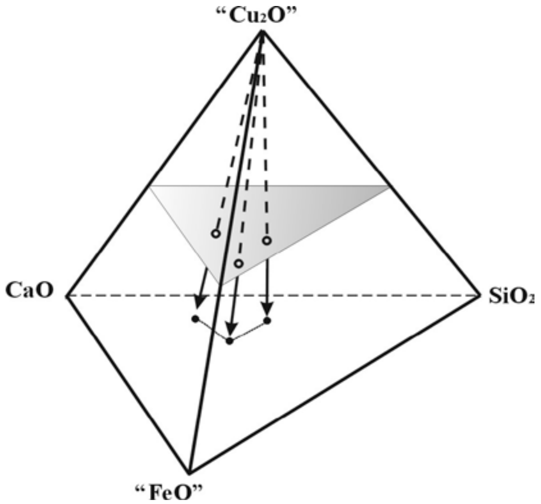


Figure 15 "Cu_2O"-"FeO"-CaO-SiO_2 system and projection onto the "FeO"-CaO-SiO_2 plane [28].

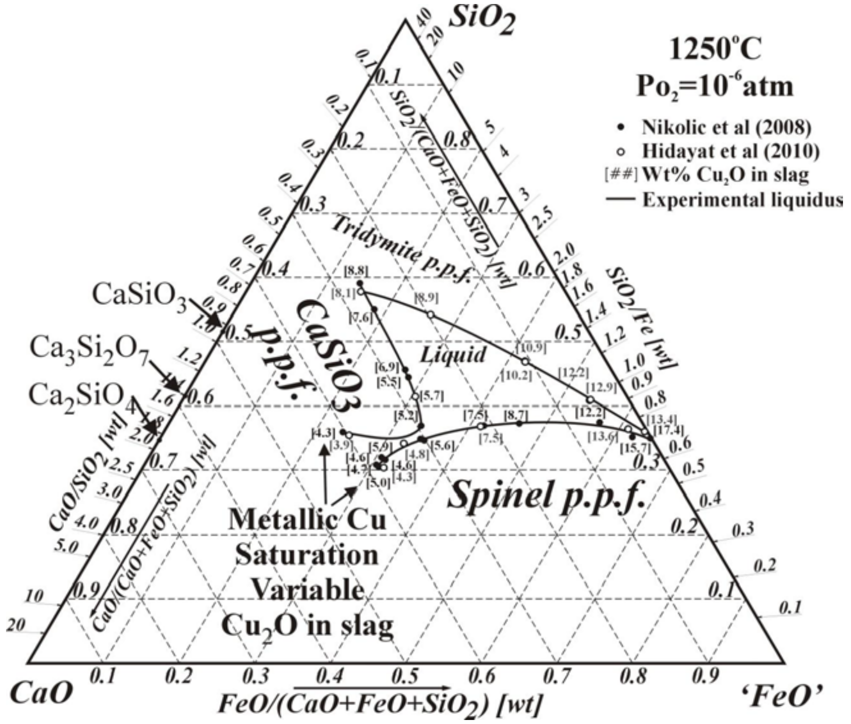


Figure 16 FeO_x-CuO_y-CaO-SiO_2 system at metallic copper saturation at 1250°C and 1300 °C at an oxygen partial pressure of 10^{-6} atm. [28].

The use of microanalytical techniques is being increasingly adopted for phase equilibrium determination as access and the availability of electron microprobe instruments is further improved. Other recent examples of the use of this research tool for phase analysis are given in the references in the Appendix.

7. Chemical thermodynamic modeling

The CALPHAD approach to phase diagram prediction, and the development of accurate models and databases, is one of the success stories of the past two decades [7]. Building on the extensive archive of experimental studies that have been carried out over the years the use of thermodynamic modeling has made it possible to analyse these data, to rigorously test the results for consistency in a thermodynamically consistent manner and to identify the those data that best describe the properties of the system. The models and the approach have been well described in the literature.

Whilst the focus of the present meeting MOLTEN12 is on molten slag and flux systems, however, it is important to appreciate that obtaining data on liquid systems alone is necessary but not sufficient to be able to construct accurate thermodynamic models. Just as there needs to be standards to be able to accurate experimentally measure the absolute values of physical and chemical phenomena there needs to be a set of reference points upon which to build these models; these reference points are the solid phases. By analogy it is difficult to accurately position the roof on a house without adequate walls and support structures; the same is true for thermodynamic models of the liquid phase.

These solids are not only stoichiometric in composition but are also frequently in the form of extensive solid solutions that are formed, for example, in the spinels and a wide range of solid silicate phases. These solutions occur when chemically and physically similar elements or ions are present in the system. The presence of these solid solutions although not directly relevant to fully liquid phase conditions indirectly determines the position of the liquidus and therefore has important implications for thermodynamic modelling of the system as a whole.

Perhaps surprisingly to those starting out research in this field there are still many chemical systems that have not been characterized experimentally and therefore there remain some uncertainties in the thermodynamic models. This is not to fault the modeler it should be recognized that these models are not equally accurate in all regions of compositional space. On most occasions the computer will give you an answer; importantly the precautionary principle should be exercised before decisions are made on the basis of these predictions. The models should be tested for its accuracy on experimental data nearest in the system and in the composition range of interest.

8. The future

So what is the future of phase equilibria studies of metallurgical systems? There is now an extensive library of phase diagrams and thermodynamic data. Has it all been done? Do we stop here? We believe the answer is firmly NO on both counts. Just as long as the technologies for metal production and the range of manufactured products continue to be developed there will be an ongoing need for research in phase equilibria and phase chemistry. As long as there is a driving force to improve process efficiencies and technical performance there will be a need to educate the workforce on the importance of process chemistry.

Whilst from purely a scientific point of view it ideal to know all we can about the fundamental science underlying the chemistry of our Universe, the reality is that the main driver of research is support for the development and improvement of the industrial processes necessary to sustain our respective societies. What is necessary and what are the opportunities for further development in this field?

Chemical Systems –

Even within the chemical systems currently used for metal production there continue to be changes in the technologies employed driven by the need to improve environmental performance, energy and cost efficiencies. Since in the main these are large scale industrial processes small changes to process chemistry can result in significant savings in reagent use, improved energy and metal recovery, and reduced operating costs, hence the need to carefully review phase equilibria that are assumed to be accurate, and undertake more accurate measurements in critical composition and temperature ranges.

The new combinations of elements that will be encountered from recycling of the man-made components of the future will challenge the abilities of practitioners to efficiently separate and recover valuable component elements and phases. This will require further experimental studies on partitioning in slag/metal/matte/gas systems.

Methodologies

Whilst the thermodynamic models provide the framework for extrapolation and interpolation into regions that have not been experimentally characterized it should be recognized that they do so with some measure of uncertainty; this uncertainty depends on the availability of suitable experimental data to support these predictions. What is required in the future then is a partnership between experimental and modelling studies to identify those regions of compositional space in which the descriptions need to be upgraded or added. In this way our knowledgebase can be developed more rapidly and more efficiently.

Capabilities

As technologies and practices change there is a need to maintain and further develop research capability/expertise in slag chemistry, which is a critical area of process development. Financial support from industry, who are the principal beneficiaries of this, is essential, as is the need for industry university collaboration to ensure the focus of research addresses industry needs.

Dedication: Paul Grieveson, formerly Professor of Extractive Metallurgy, Imperial College, London and Strathclyde University, Glasgow, Scotland; University of Newcastle on Tyne, England; US Steel labs, USA; Newcastle United football supporter; for his inspiration as a teacher and for revealing the challenges to be found in the exciting world of extractive metallurgy.

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