Simulation of ferro-alloy smelting in DC arc furnaces using Pyrosim and FactSage

Rodney T. Jones *, Markus W. Erwee

Mintek, 200 Malibongwe Drive, Private Bag X3015, Randburg 2125, South Africa

ABSTRACT

Mintek has applied DC arc furnace technology to the reductive smelting of numerous materials over more than three decades. The first industrial implementation of this technology was for the smelting of chromite fines to produce ferrochromium in 1984. Since 1985, process simulation has been carried out using Pyrosim and FactSage software to study this process. Some examples are presented of the mass and energy balances and thermodynamic calculations used for the steady-state simulation of chromite smelting for the production of ferrochromium. There is a place for equilibrium calculations involving non-ideal slag and alloy solutions, as well as for empirical models that can be used in an operating plant environment.

© 2016 Elsevier Ltd. All rights reserved.

1. Introduction

1.1. Chromite Smelting

It has been over thirty years since DC arc furnace smelting technology was first implemented industrially, in 1984, for the smelting of fine chromite ores to produce ferrochromium. Since then, the size of these furnaces has expanded, and the power has increased from 12 MW to 72 MW, and this technology has been applied to the production of numerous other commodities in furnaces up to 80 MW [1].

The production of ferrochromium takes place at very high temperatures, by reacting chromite ore, together with fluxes such as lime and silica, with a carbonaceous reducing agent. Eq. (1) shows a highly simplified version of the principal reaction that takes place.

$$FeO \cdot Cr_2O_3 + 4C \rightarrow Fe + 2Cr + 4CO \qquad (1)$$

The chromite ore has a spinel crystalline structure, represented by $(Fe,Mg)O \cdot (Cr,Al)_2O_3$, that is very stable even at high temperatures. As this reacts with carbon, some small quantity of "partially altered chromite" remains. This material has the primary spinel at its core, with an outer layer of secondary spinel (essentially $MgAl_2O_4$ from which Cr and Fe was removed). Fluxes are added to

the furnace in order to decrease the melting temperature of the oxide melt where the reactions take place. Most of the reduction occurs as the reductant interacts with the slag.

Chromite ores vary considerably in composition. A selection of typical ore compositions [2] is shown in Table 1.

An important parameter in chromite smelting is the Cr/Fe ratio, as this ratio largely determines, for a given furnace type, the grade (% Cr) of the product. Ferrochromium is sold according to its Cr content, and there is usually no payment given for other elements present, such as Fe, Si, and C. In typical South African operations, where ores have Cr/Fe ratios of 1.3–1.7, the product produced will be high-carbon ferrochromium. Ores are often mixed to achieve a blend that can be processed economically. High-carbon ferrochromium contains roughly 50–52% Cr, 6–8% C, 0.5–1.5% Si, with the balance being Fe and some minor impurities (including some P). The slag contains roughly 4–6% Cr_2O_3, 0.5–2% FeO, 15–25% MgO, 30–40% Al_2O_3, 2–15% CaO, and the balance SiO_2. The metal composition is relatively fixed, but the slag composition varies based on the fluxing regime employed by the specific operation. In contrast to South African operations, ores from Kazakhstan, for example, have very high Cr/Fe ratios (~3.8), resulting in metal products of higher grades (> 70% Cr, 20% Fe, 8% C, < 1% Si).

The traditional approach to chromite smelting (more than a century old) involves the use of submerged-arc furnaces which require the use of lumpy ores and coke to provide a porous bed of solid feed material that allows the reaction gases to percolate away and escape from the reaction zone. The DC arc furnace was introduced originally to enable the direct smelting (without costly

---

* Corresponding author.
  E-mail address: rtjones@global.co.za (R.T. Jones).

Table 1
Composition (mass %) of various chromite ores that have been smelted at Mintek (from Geldenhuys [2]).

Origin	Cr$_2$O$_3$	FeO	MgO	Al$_2$O$_3$	SiO$_2$	Cr/Fe
Kazakhstan	51.2	11.9	19.8	6.5	6.9	3.8
Zimbabwe	50.8	13.3	17.9	12.7	3.9	3.4
India A	53.5	16.9	11.4	11.4	1.3	2.8
India B	50.9	17.9	10.9	12.7	1.2	2.5
North America	44.0	18.2	12.8	12.5	5.9	2.1
South Africa LG	46.6	25.0	10.8	15.1	0.6	1.6
South Africa UG2	42.6	27.4	9.3	14.9	1.2	1.4
South Africa MG	42.9	28.5	8.8	15.7	3.0	1.3

agglomeration) of chromite fines that emanated from the highly friable 'Transvaal chromite' ores.

1.2. Features of DC arc furnaces

In order to accommodate the feeding of fine feed materials (without clogging up the exit path for the gases produced by the chemical reactions), an open molten slag bath (at least partially uncovered by feed material) is required. The fine feed material is dropped onto the molten bath, into which it almost immediately assimilates, melting and dissolving into the slag phase where the reactions take place. The absence of a heaped burden of solid feed material means that coke (relatively scarce and expensive) is not required, and cheaper reductants may be used instead. The energy for the process is supplied by means of an open plasma arc that is generated between the bottom tip of the cathode and the upper surface of the molten slag. The open arc provides an additional degree of freedom with respect to the electrical conductivity of the slag, in that the power is not principally determined by the resistive heating of the slag, but can be adjusted by varying the arc. This additional degree of freedom allows the slag composition to be chosen (unconstrained by electrical properties) based on the metallurgical benefit that may arise from a favourable chemical activity regime, and it is usual for the recovery of chromium to be significantly higher in a DC arc furnace than in an AC submerged-arc furnace, and for the composition of the alloy to be more adjustable. The use of a DC arc furnace avoids the arc repulsion that occurs in AC furnaces where the arcs flare toward the walls, leading to hot spots on the areas of the side-walls in closest proximity to the electrodes. DC furnaces also experience lower electrode consumption. In large DC furnaces, a higher current can be carried per electrode (or smaller electrodes can be used for the same current), because in AC furnaces there is a 'skin effect' where current is concentrated in the outer periphery of the electrodes. DC arc furnaces can treat feed materials with a wide range of composition (because of the extra degree of freedom coming from power being supplied by an open arc). Table 2 shows some typical recovery figures and specific energy requirements for various furnace types. DC arc furnace technology is regarded as one of the lowest-cost options for the production of ferrochromium.

1.3. Industrial installations

The first industrial application of a DC arc furnace for smelting came about when Middelburg Steel & Alloys converted an existing AC furnace at Palmiet Ferrochrome (now Mogale Alloys) in Krugersdorp to a 12 MW (16 MVA) DC arc furnace in 1984. This furnace was upgraded to 40 MVA (~33 MW) in 1988. An additional 10 MW furnace was later built on the same site (Fig. 1).

Based on the successful operation of the DC arc furnace for chromite smelting at Krugersdorp, Middelburg Ferrochrome (now part of Samancor Chrome) built a 44 MW (62 MVA) DC arc furnace, the largest of its type, in Middelburg in 1997. This was followed, in 2009, by an additional 60 MW furnace in Middelburg, currently the largest DC arc furnace in South Africa [4]. The 44 MW furnace was subsequently upgraded to 60 MW.

Kazchrome (a ferrochromium producer in Kazakhstan) contracted with Mintek in 2007 to undertake smelting testwork. Based on this, and on other design inputs provided by Mintek in 2009, SMS Siemag built four 72 MW DC arc furnaces in Aktobe, Kazakhstan, and commissioning began around 2013.

2. Process simulation

Fig. 2 schematically presents the inputs and outputs of a generic chromite smelting process. It is sufficient for any process simulator to be able to carry out a calculation of products from any specified set of input conditions; as a design calculation (which calculates the required inputs for a desired set of products) can be carried out using an iterative series of simulations.

3. Pyrosim

Back in the 1980s, there were no readily available pyrometallurgical flowsheet simulation programs for personal computers. Pyrosim was developed at Mintek, as a sequential modular simulator based on a thermodynamic database, originally to simulate the production of raw stainless steel, but the structure was kept general enough to allow it to be used to calculate predictive steady-state mass and energy balances for a very wide range of processes. Programming started in 1985, on a 64 kB Apple II computer (1 MHz). Pyrosim was first presented at the APCOM 87 conference in 1987 [5]. In 1988, the program migrated to IBM-compatible PCs using the MS-DOS operating system, and a structured and compiled version of BASIC (the PowerBASIC DLL compiler), and was used for the first time in industry. Since then, there have been 95 installed sites in 22 countries on 6 continents. Rapid advancements in personal computing have taken place since then. For example, there was a 1500 fold increase in speed and storage capacity, from the Apple II to a fast Pentium personal computer of twenty years ago (rated at 100 MIPS – a great deal slower than today's machines). A typical Pyrosim simulation would have taken over an hour on an Apple II, but just over three seconds on a 33 MHz i486 computer (1200 times faster)(Fig. 3).

Table 2
Chrome recovery and specific energy consumption for different furnace types (partially reproduced from [3]).

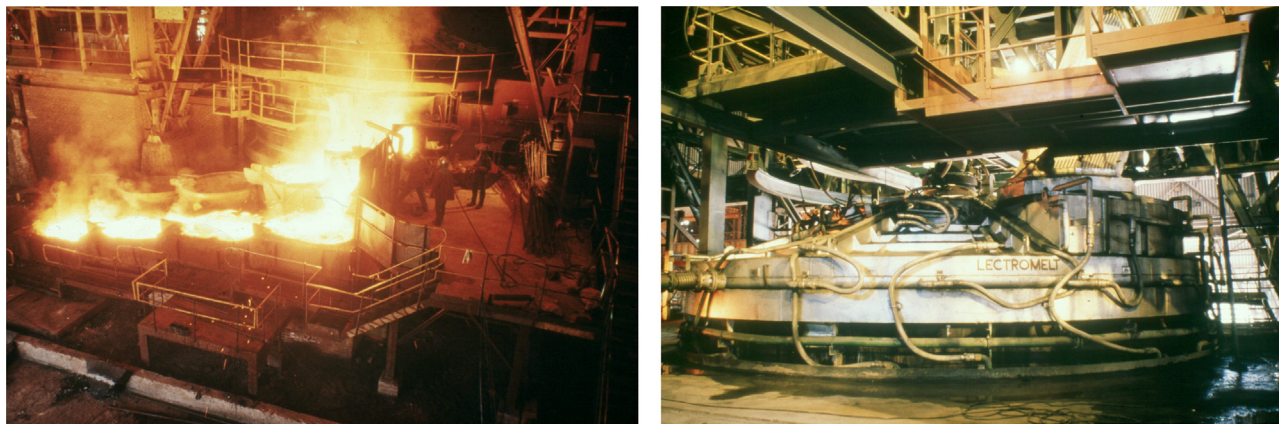| Type of furnace	Chromium recovery	Specific energy requirement, SER (kW h/t)
Open AC furnace (without raw material screening)	70–75%	4300
Closed AC furnace (with pelletized feed and pre-heating)	83–88%	3200
Pre-reduction followed by closed AC furnace	88–92%	2400 (electrical energy consumed, *i.e.*, excluding energy required from burning fuel in the pre-reduction kiln)
Closed DC furnace	88–92%	4200

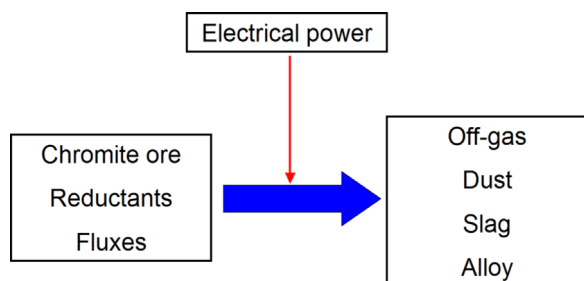Fig. 1. Chromite smelting at Palmiet Ferrochrome (now Mogale Alloys).

Fig. 2. Typical inputs and outputs of a chromite smelting process.

Pyrosim included models based on chemical equilibrium (for example, metal, slag, and gas) using the free energy minimisation algorithm pioneered by Gunnar Eriksson [6]. Before the ready availability of sophisticated non-ideal solution models for slag and metal systems, the 'Ideal Mixing of Complex Components' approach [7] was included as an option in Pyrosim.

Another powerful capability of Pyrosim is its general Empirical model. The program is able to calculate the number of degrees of freedom from the number of chemical elements in the feed and the number of phases present in the furnace. The program then allows the user to specify the appropriate number of pieces of information in one of two ways. It is possible for the user to specify the content (in mass %) of any species in any phase, or ratios between any pair of species in any combination of phases. This internally generates a set of linear equations that can be solved directly (with a warning given if a non-independent set of variables

is inadvertently selected).

Of particular relevance to chromite smelting is an empirical model, called Pyrobal, where the percentages of Cr_2O_3 and FeO in the slag, and Si and C in the alloy are specified, along with the distribution ratios for P and S between alloy and slag. This information is sufficient to specify the composition and flowrates of all product streams, and to allow for the calculation of the required mass and energy balance. Many industrial chromite smelting plants prefer to use these empirical models with known plant-specific parameters, as they are more accurate than generic equilibrium models (as the furnaces are not perfect equilibrium devices). Some plants have developed spreadsheet versions of these empirical models.

4. F*A*C*T and FactSage

F*A*C*T (Facility for the Analysis of Chemical Thermodynamics) was established in the late 1970s as a means to carry out thermodynamic calculations. Until the mid 1980s, the use of this large thermodynamic database involved remote access of a mainframe computer at McGill University via the rather slow telecommunication networks of that time (the Saponet satellite link in Mintek's case). At that time, calculations were expensive to run, and very limited in the number of elements that could be accommodated. In the 1990s, the software moved over to personal computers that had become sufficiently powerful. The great strength of this system, now known as FactSage [8], is that it integrated assessed thermodynamic data, including multi-
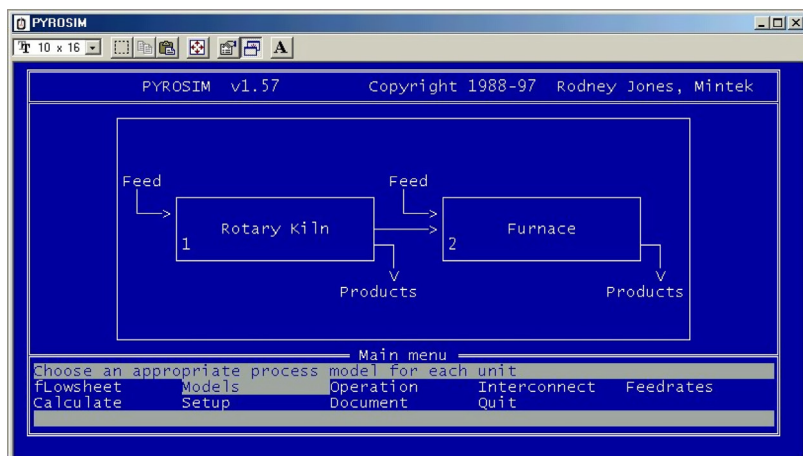

Fig. 3. Pyrosim was originally developed on an Apple II computer, then under MS-DOS.

component non-ideal solution models, together with the leading algorithm for free-energy minimization, namely Solgasmix [6], now ChemSage.

5. Plant simulation methodology

When designing a smelting strategy for chromite smelting, the basic steps (shown in Fig. 4) begin with a mass balance. An empirical mass balance, together with an energy balance, is typically carried out using a package such as Pyrosim, or a spreadsheet. In addition to this, FactSage [8] provides additional benefit by generating more appropriate values for slag and metal enthalpy when calculating energy balances. The basic steps involved in designing a slag appropriate for chromite smelting are shown in Fig. 4.

5.1. Metal liquidus temperature

For a given Cr/Fe ratio in the ore, and a specified recovery of both Cr and Fe to the metal product, it is possible to estimate the carbon requirement and the alloy composition. The amount of Si in the metal is usually fixed based on the experience on the plant involved. Once the composition of the metal is known, an estimate is made of the liquidus temperature of the metal alloy.

It is very common amongst South African furnace operators to estimate the metal liquidus temperature based on regression models of measured data. One such dataset is that published by Wethmar et al. [9], a subset of which is shown in Fig. 5. Another more modern approach adopted recently is the use of tools such as FactSage, in combination with the SGTE solution database, to estimate the liquidus temperature of the metal (see two examples in Table 3). This helps to avoid the significant error that can be incurred in reading off a set of diagrams, and also avoids excessive abuse of extrapolation of regression models based on experimental data.

5.2. Slag liquidus temperature and viscosity

The slag composition needs to be fixed to achieve a certain liquidus temperature that is suitable for effecting separation
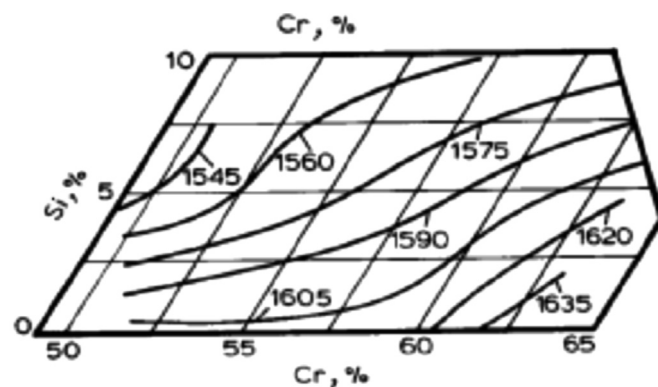
Fig. 5. Liquidus isotherms in °C at 8% C for a Fe–Cr–Si–C alloy.

Table 3
Typical metal product compositions (mass %) with their respective liquidus temperatures (calculated using FactSage 7.0).

	Cr	Fe	C	Si	Liquidus (°C)
HC FeCr from SA operation	50.0	40.5	8.0	1.5	1528 (SGTE)
HC FeCr from Kazakhstan operation	71.0	20.0	8.0	1.0	1644 (SGTE)

between slag and metal. In practice, this is often done using the 'bulk' liquidus temperature of the $MgO–Al_2O_3–SiO_2–CaO$ content, ignoring the relatively small (less than 10%) amount of undissolved chromite (nominally $FeCr_2O_4$) that remains in the slag after smelting. The true liquidus temperature would be a function of the relevant partial pressure of O_2 in the system, which would define the ratios of Cr^{3+}/Cr^{2+} and Fe^{3+}/Fe^{2+} ions in the slag.

Once the metal liquidus temperature is known, the next step is to design a slag with a composition that yields a slag with a 'bulk' liquidus temperature that is roughly 100–150 °C above that of the metal. The reason for this is that the metal that forms by reaction is to be kept molten through heating by the slag, i.e., the metal is heated indirectly by the arc through the electrically resistive slag.

To choose the relevant slag composition to yield an appropriate slag liquidus temperature, furnace operators use a combination of phase diagrams for the $MgO–Al_2O_3–SiO_2$ and $MgO–Al_2O_3–SiO_2–CaO$ systems. A more popular method is to use the regression correlations constructed by Pesta [10]. However, the correlations are limited to a small composition range, and error in extrapolation often occurs. For this reason, FactSage is gaining popularity in the local chromite smelting industry.

The bulk of the slag that forms after reduction of CrO_x and FeO_x from chromite consists of $MgO–Al_2O_3$ and SiO_2 (with some CaO present as well). This slag, if left unfluxed, would have a high melting point (since the ore itself has a high melting point). Fig. 6 shows a liquidus projection of the $MgO–SiO_2–Al_2O_3$ system.

As an example, two extreme cases are contrasted here: fluxing of South African ores versus fluxing of ore that originates from Kazakhstan. The normalised (to three components, based on the compositions in Table 1) compositions of four ores are shown: one ore from Kazakhstan ("Kaz"), and three ores from South Africa ("MG", "UG2", and "LG"). The aim is to add a flux, such as SiO_2, to lower the melting point of the slag to temperatures around 1650–1800 °C, depending on the liquidus temperature of the metal.

Fluxing of chromite ore is focused largely on fluxing MgO and Al_2O_3. Each ore has a distinct MgO/Al_2O_3 ratio, for which an appropriate amount of SiO_2 is added to lower the liquidus temperature of the melt. For example, there is a substantial difference between South African ores (composition in the M_3O_4/Spinel primary phase field, with $MgO/Al_2O_3\sim0.56–0.72$) and Kazakhstan ores (composition in the Monoxide/Periclase primary phase field,
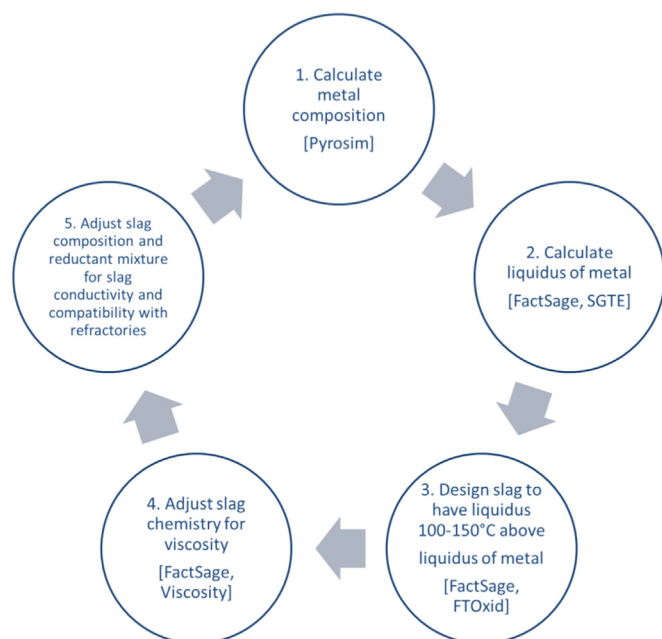
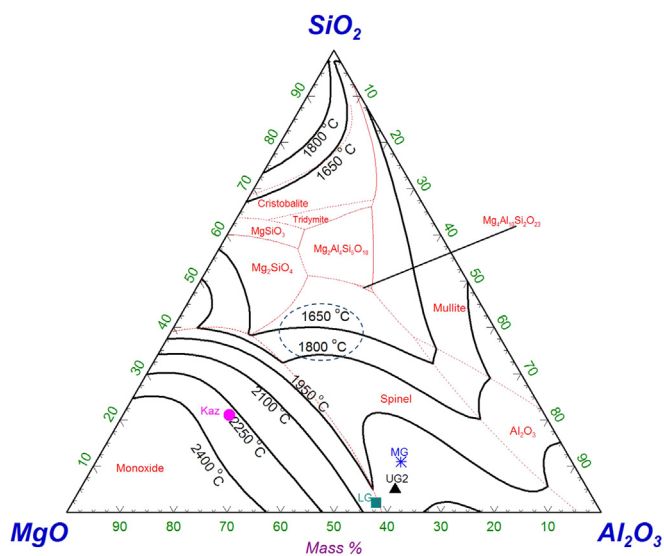**Fig. 4.** Basic steps involved in designing a slag appropriate for chromite smelting.

Fig. 6. Liquidus projection of the MgO–Al$_2$O$_3$–SiO$_2$ system at 1 atm. pressure (calculated using FactSage 7.0, FTOxid database). The four points shown on the diagram indicate the normalised composition of four different ore types. The circled area indicates the typical slag compositions where chromite smelters aim to operate.
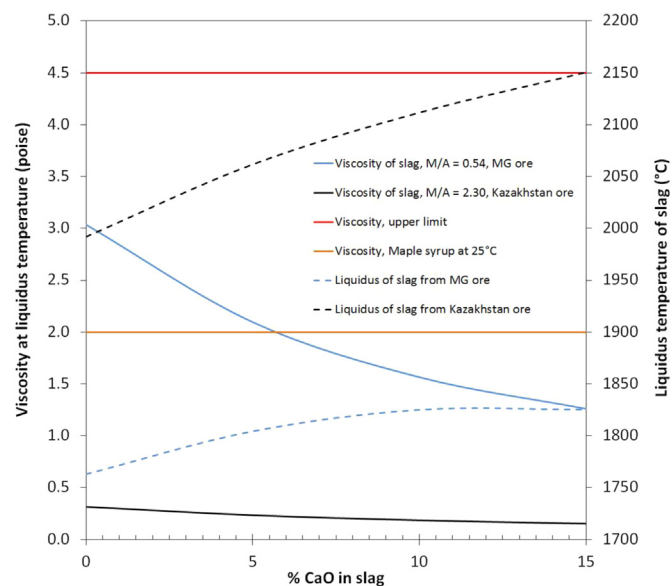

Fig. 8. The effect of CaO on the viscosity and liquidus temperature of two different slag systems, calculated using FactSage 7.0, with the FTOxid database.

with MgO/Al$_2$O$_3$~3.05), which means that the fluxing requirement is quite different.

It is very easy to visualise (see Fig. 7) this requirement, using the Equilib module in FactSage rather than trying to deduce it from a phase diagram. In Fig. 7, it is clear that lower amounts of SiO$_2$ are required to flux ores from Kazakhstan, compared to ores from South Africa. This is due largely to the fact that the liquidus temperatures of metal produced (see Table 3) from Kazakhstan ores are inherently higher than those of products produced from South African ores, i.e., to achieve a slag 'liquidus' temperature of 100–150 °C above the liquidus of the metal, more SiO$_2$ is required in South African systems than Kazakh systems.

Once the bulk liquidus temperature of the slag is established, the viscosity of the slag must be adjusted to make the slag 'tappable'. The slag viscosity is usually adjusted slightly by adding CaO as a flux, but this depends highly on the MgO/Al$_2$O$_3$ ratio in the slag, as well as the MgO/SiO$_2$ ratio of the slag. There is a trade-off between adding CaO to the slag to lower the viscosity, without increasing the liquidus temperature too much, as shown in Fig. 8. In some cases, such as the smelting of Kazakh ores, there is no reason to add CaO to the slag, since the MgO/Al$_2$O$_3$ ratio is quite

high, i.e., sufficient basic cations are present to maintain a low slag viscosity.

FactSage has a very useful viscosity module, which is often used to calculate the viscosity of a melt at the liquidus temperature of the slag. The result is often compared to current operations, to see whether the change in slag composition would have a negative effect on slag viscosity. Many plant operators still, however, prefer using the model developed by Urbain [11] to estimate slag viscosity if they do not have access to FactSage. In Fig. 8, the viscosity of a slag produced from a typical MG-type ore is contrasted to that of a slag produced from Kazakhstan ores (the detailed compositions of these slags and their respective metal products are given in the paper by Geldenhuys [2]) as a function of the amount of CaO that can be added to the slag. From this diagram, it is quite easy to deduce how much CaO is required to lower the viscosity of a slag to such an extent that it can be tapped easily from a furnace. Operators aim for a viscosity lower than 2.0 poise (when the calculation is done in FactSage), which is roughly the same as the viscosity of maple syrup at room temperature. Anecdotally, the reported upper limit to tap slag from a furnace seems to be roughly 4.5 poise for industrial operations. From this, it is easy to see why South African operators would intentionally add CaO to their slag, but this is not required for operations that process ores from Kazakhstan.

Notably, there is a trade-off between the viscosity of the slag and the liquidus temperature of the slag, as the amount of CaO is increased. Fortunately, in most cases, the effect of CaO on viscosity is substantially stronger than the marginal increase in the liquidus temperature of the slag. FactSage makes calculations such as these possible and also substantially faster than estimating the parameters otherwise.

Finally, once the slag composition has been adjusted to achieve the required liquidus temperature and viscosity, the slag is tweaked for compatibility with the refractories as well as for electrical conductivity. There is some complexity to choosing an appropriate refractory material for the slag involved, as there are many factors that need to be taken into account that fall beyond the scope of this paper. That said, FactSage is often used to calculate whether a particular refractory material would be more suitable than another, using the Equilib module.
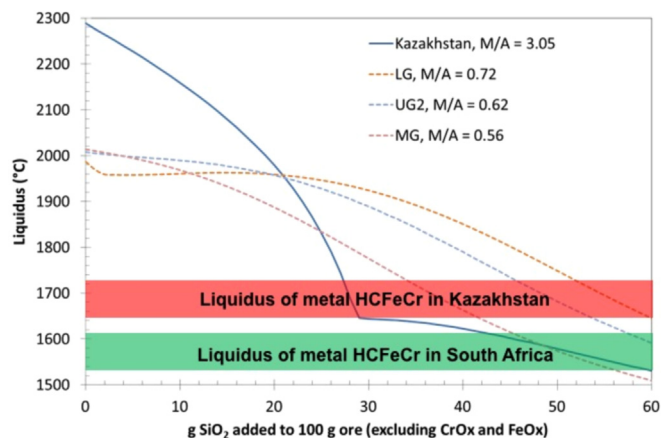

Fig. 7. The liquidus temperature of melts that originate from ores when SiO$_2$ is added as a flux. Note M/A refers to the mass ratio of MgO/Al$_2$O$_3$ in the ore. Calculations were done using FactSage 7.0, with the FTOxid database.

6. Conclusions

The past three decades have seen the introduction of an effective new smelting technology for ferro-alloys, as well as increasingly capable process simulation tools. Flowsheet simulators based on chemical thermodynamic databases running on personal computers were introduced to the pyrometallurgical industry in the 1980s and have become rather ubiquitous since then. There is a place for equilibrium calculations involving non-ideal slag and alloy solutions, as well as for empirical models that can be used in an operating plant environment.

Acknowledgements

References

[1] R.T. Jones, DC arc furnaces – Past, present, and future, Celebrating the Mega-scale, in: Proceedings of the Extraction and Processing Division Symposium on Pyrometallurgy in Honor of David G.C. Robertson, TMS 2014, 16–20 February 2014, San Diego, California, USA, pp. 129–139. ⟨http://www.mintek.co.za/Pyromet/Files/2014Jones-DCArcFurnaces.pdf⟩.

[2] I.J. Geldenhuys, Aspects of DC chromite smelting at Mintek – an overview, Infacon XIII, Almaty, Kazakhstan, 9–12 June 2013, pp. 31–47. ⟨http://www.pyrometallurgy.co.za/InfaconXIII/0031-Geldenhuys.pdf⟩.

[3] J. Basson, J. Daavittilia, High carbon ferrochrome technology, in: M. Gasik (Ed.), Handbook of Ferroalloys: Theory and Technology, Butterworth-Heineman, United Kingdom, 2013, p. 332.

[4] D. Sager, D. Grant, R. Stadler, T. Schreiter, Low cost ferroalloy extraction in DC-arc furnace at Middelburg Ferrochrome, Infacon 12, Helsinki, 6–9 June 2010, JSAIMM J., vol. 110, no. 12, December 2010, pp. 717–724. ⟨http://www.saimm.co.za/Journal/v110n12p717.pdf⟩, ⟨http://www.pyrometallurgy.co.za/InfaconXII/803-Sager.pdf⟩.

[5] R.T. Jones, Computer simulation of pyrometallurgical processes, APCOM 87, in: Proceedings of the Twentieth International Symposium on the Application of Mathematics and Computers in the Minerals Industries, vol. 2: Metallurgy, Johannesburg, SAIMM, October 1987, pp. 265–279. ⟨http://www.mintek.co.za/Pyromet/Files/Apcom87.pdf⟩.

[6] G. Eriksson, Thermodynamic studies of high temperature equilibria. XII. SOL-GASMIX, a computer program for calculation of equilibrium compositions in multi-phase systems, Chem. Scr. 8 (1975) 100–103.

[7] R.T. Jones, B.D. Botes, Description of non-ideal slag and metal systems by the intermediate-compound method, in: Proceedings of Colloquium on Ferrous Pyrometallurgy, SAIMM, Vanderbijlpark, South Africa, 18 April 1989. ⟨http://www.mintek.co.za/Pyromet/Files/IMCC.pdf⟩.

[8] FactSage software, CRCT, ThermFact Inc., and GTT-Technologies. ⟨http://www.factsage.com⟩.

[9] J.C.M. Wethmar, P.R. Jochens, D.D. Howat, Phase equilibria in the Cr–Fe–Si–C system in the composition range representative of high–carbon ferrochromium present in South Africa, Metal. Sci. 9 (1975) 291–296.

[10] M. Pesta, F.M. Majoribanks, G.A. Oosthuizen, G. Salgado, Regression Formulae for the Calculation of the Liquidus Temperature, Viscosity, and Conductivity of Slag in the Production of High-Carbon Ferrochromiu, Mintek Report 2120, Randburg, South Africa, 1981.

[11] K.C. Mills, Viscosities of Molten Slags Chapter 9, Slag Atlas, Verein Deutscher Eisenhuttenleutte, Verlag Stahleisen GmbH, Dusseldorf, Germany, 1995.