Development of a Quasi-chemical Viscosity Model for Fully Liquid Slags in the Al_2O_3 – CaO – FeO – MgO – SiO_2 System. Part 1. Description of the Model and Its Application to the MgO , MgO – SiO_2 , Al_2O_3 – MgO and CaO – MgO Sub-systems

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A structurally-based quasi-chemical viscosity model for fully liquid slags in the Al_2O_3 – CaO – FeO – MgO – SiO_2 system has been developed. The model links the slag viscosities to the internal structures of the melts through the concentrations of various $\text{Si}_{0.5}\text{O}$, $\text{Me}_{2/n}^{n+}\text{O}$ and $\text{Me}_{1/n}^{n+}\text{Si}_{0.25}\text{O}$ viscous flow structural units. The concentrations of these structural units are derived from a quasi-chemical thermodynamic model of the system. The model described in this series of papers enables the viscosities of liquid slags to be predicted within experimental uncertainties over the whole range of temperatures and compositions in the Al_2O_3 – CaO – MgO – SiO_2 system.

KEY WORDS: slag viscosity; viscosity model; Al_2O_3 – CaO – MgO – SiO_2 .

1. Introduction

A new mathematical formalism has been developed to describe the viscosities of molten oxides as a function of composition and temperature.^{1,2)} The formalism, hereafter referred to as the quasi-chemical viscosity (QCV) model, enables the internal structural information of complex slags to be related to this physicochemical property. The internal structural information changes systematically with changing bulk composition and temperature and is derived from consideration of the thermodynamic equilibrium in the system. The QCV model provides a link between fundamental thermodynamic and physicochemical properties of the slags, and enables the slag viscosities for all compositions and temperatures in the chemical system to be predicted using the same set of model parameters. Application of this approach and the evaluation of QCV model parameters for the system Al_2O_3 – CaO – FeO – SiO_2 have previously been reported by the authors.²⁾

The present paper is the first in a series describing the effect of MgO on slag viscosities and extending the QCV model to the quaternary system Al_2O_3 – CaO – MgO – SiO_2 . The present paper provides descriptions of the quasi-chemical viscosity model and optimisation procedure, outlines the principles applied in the evaluation of experimental data and the resultant viscosity models for the MgO , Al_2O_3 – MgO , CaO – MgO and MgO – SiO_2 systems.

Many of the materials that are used as feedstocks for pyrometallurgical processes include MgO -containing minerals. In some cases MgO is deliberately added to these high-

temperature processes to adjust and to optimise the chemical and/or physicochemical characteristics of the systems. The influence of MgO on melt viscosity is therefore significant not only from a fundamental scientific point of view, but also because of its relevance to a wide range of industrial applications.

A number of viscosity models found in the literature on the Al_2O_3 – CaO – FeO – MgO – SiO_2 system have recently been reviewed by the authors.³⁾ It would appear that at present no viscosity model accurately describes this property over the whole range of chemical compositions. The Urbain formalism is one of the most widely used slag viscosity models and is based on the application of polynomial functions of slag composition to describe the pre-exponential and exponential terms in the Weymann–Frenkel equation.⁴⁾ Urbain reported⁴⁾ different model parameters for each ternary system Al_2O_3 – MgO – SiO_2 and Al_2O_3 – CaO – SiO_2 , and suggested a method of extrapolating model predictions to multi-component systems. However, this method does not provide close agreement between the model predictions and experimental data in the Al_2O_3 – CaO – MgO – SiO_2 systems over the whole compositional range. Several viscosity models have been developed on the basis of the Urbain formalism.^{5,6)} The Kalmanovich–Frank model⁵⁾ adopted the Urbain model for viscosity of the particular coal ash slags. Riboud *et al.*⁶⁾ corrected the Urbain formalism to describe the viscosities of some industrial mould fluxes (in the Al_2O_3 – CaO – Na_2O – SiO_2 – CaF_2 system). Viscosity predictions of these and some other models^{7,8)} for the Al_2O_3 – CaO – MgO – SiO_2 system and its sub-systems will be

analysed and compared in the third paper of the present series.

A number of structurally-based viscosity models^{9–14} have been developed for slags in the quaternary system $\text{Al}_2\text{O}_3\text{--CaO--MgO--SiO}_2$ with small additions of other oxides.¹⁵ The Iida viscosity model⁹ is based on the so called “network parameter”, which was correlated with a basicity index and temperature. The Iida model performs well for the compositions reported but not applicable for the whole compositional range in multi-component systems without further development. The NPL viscosity model¹⁰ is based on the structurally-related optical basicity concept¹⁰ and the Arrhenius equation. The NPL model provides a good estimation of the viscosities of iron blast furnace slags. The Zhang model^{11,12} is based on the Weymann–Frenkel equation and links the slag viscosity to the internal structure of the slag expressed through the concentrations of bridging, non-bridging and free oxygens derived from the cell thermodynamic model.¹⁶ This model performs well in a number of slag systems according to the reported comparison with the experimental data. The KTH viscosity model¹³ is based on the Eyring equation and Gibbs free energy of activation of viscous flow. The limited reported comparison of the model predictions and the experimental data showed a good model performance. The Tanaka viscosity model¹⁴ was developed using the Arrhenius equation. It links the slag viscosity to the so called “non-bridging space”, which is proportional to the concentration of non-bridging oxygens determined from the cell thermodynamic model.¹⁶ Good agreement between the model predictions and the experimental data was reported for a limited range of compositions.

Analysis of the various viscosity models for metallurgical and coal ash slags has shown that further work is needed to develop a general, self-consistent and reliable viscosity model that can be applied in the whole compositional range of the $\text{Al}_2\text{O}_3\text{--CaO--FeO--MgO--SiO}_2$ system, including all unary, binary, ternary and quaternary sub-systems.

2. Quasi-chemical Viscosity Model Description

The formalism for the quasi-chemical viscosity (QCV) model developed by the authors has been presented in detail in earlier publications.^{1,2} A brief description of the essential features of the model is given below for the benefit of the reader.

Frenkel’s kinetic theory of liquids¹⁷ considers a liquid to possess a solid-like structure with molecules oscillating about average positions in their energetic cells (potential wells). The oscillations result in the movement of a molecule, or more generally, of a viscous flow structural unit (SU) after a certain time from its cell into an adjacent cell, provided the latter is vacant. These vacant cells, or “holes” are distributed randomly throughout the liquid. From this point of view, the reaction of a liquid (proportional to the viscosity) to the applied shear force is determined by two factors: the ability of structural units to jump over the potential barrier and the concentration of “holes” in the liquid.

Based on the postulates of liquid state and liquid viscosity initially formulated by Frenkel¹⁷ the Eyring viscosity equation has been developed,¹⁸ which was used for the present

QCV model:

$$\eta = \frac{2RT}{\Delta E_v} \frac{(2\pi m_{\text{SU}} kT)^{1/2}}{v_{\text{SU}}^{2/3}} \exp\left(\frac{E_a}{RT}\right) \dots\dots\dots (1)$$

where R and k are the gas ($\text{J K}^{-1} \text{mol}^{-1}$) and Boltzmann (J K^{-1}) constants, respectively, $\pi \approx 3.1416$, T is the absolute temperature (K), ΔE_v and E_a are the vaporisation and activation energies (J mol^{-1}), respectively, m_{SU} and v_{SU} are the weight and volume of a structural unit of viscous flow (kg and m^3 , respectively).

The definition of the viscous flow structural unit is based on the understanding that molten slags have complex internal structures dependent on composition and temperature.^{19,20} A silicate slag may be considered to consist of nearly close-packed arrangements of oxygen anions with smaller metal cations occupying the interstitial positions; the cations are distributed through the melt maintaining electroneutrality and interacting over a short range with each other.¹⁹ The conventional description of slag structure includes the network of silica tetrahedra SiO_4^{4-} broken by metal cations.^{19,20} Fincham and Richardson²¹ further suggested that a silicate slag can schematically be considered to consist of the three different types of oxygens: “bridging” (O^0 –connected to two silicon cations), “non-bridging” (O^- –connected to only one silicon), and “free” (O^{2-} –associated with non-silicon cations). This concept has been successfully used in numerous thermodynamic models related to the silicate slag structure.

Following these concepts, the structural units of viscous flow in the present QCV model applied to the silicate slags are defined as oxygen anions with metal cations partly associated with them: $\text{Si}_{0.5}\text{O}$, $\text{Me}_{2/n}^+\text{O}$ and $\text{Me}_{1/n}^+\text{Si}_{0.25}\text{O}$. Thus, for example, in a ternary system $\text{Al}_2\text{O}_3\text{--MgO--SiO}_2$, there are six different structural units Al--O--Al , Al--O--Mg , Al--O--Si , Mg--O--Mg , Mg--O--Si and Si--O--Si , denoted by the abbreviations Al--Al , Al--Mg , Al--Si , Mg--Mg , Mg--Si and Si--Si , respectively.

The average weights m_{SU} and volumes v_{SU} of the structural units are used in conjunction with Eq. (1), and in the binary MeO--SiO_2 system they are expressed in the following form through the concentrations of different structural units present in the melt:

$$m_{\text{SU}} = m_{\text{Si--Si}} X_{\text{Si--Si}} + m_{\text{Me--Si}} X_{\text{Me--Si}} + m_{\text{Me--Me}} X_{\text{Me--Me}} \dots\dots (2)$$

$$v_{\text{SU}} = v_{\text{Si--Si}} X_{\text{Si--Si}} + v_{\text{Me--Si}} X_{\text{Me--Si}} + v_{\text{Me--Me}} X_{\text{Me--Me}} \dots\dots (3)$$

where $m_{\text{Si--Si}}$ and $v_{\text{Si--Si}}$, $m_{\text{Me--Me}}$ and $v_{\text{Me--Me}}$, and $m_{\text{Me--Si}}$ and $v_{\text{Me--Si}}$ are the volumes and masses of the $\text{Si}_{0.5}\text{O}$, $\text{Me}_{2/n}^+\text{O}$ and $\text{Me}_{1/n}^+\text{Si}_{0.25}\text{O}$ structural units, respectively, where n is the oxidation state of a metal cation Me^{n+} ; and $X_{\text{Si--Si}}$, $X_{\text{Me--Me}}$, and $X_{\text{Me--Si}}$ (here and below) are the molar fractions of respective structural units. The volumes of the corresponding structural units are calculated using the effective diameters of structural units estimated from the ionic radii of different ions (O, Si, Me) composing a particular structural unit; the ionic radii are taken from Shannon²²; the angles between different bonds within a structural unit are not taken into account. The final values of m_{SU} and v_{SU} are given in **Table 1**.

In the QCV model² for the binary system MeO--SiO_2 the

integral molar activation energy E_a is expressed as follows:

$$E_a = E_{a, \text{Si-Si}} X_{\text{Si-Si}} + E_{a, \text{Me-Si}} X_{\text{Me-Si}} + E_{a, \text{Me-Me}} X_{\text{Me-Me}} \dots (4)$$

where $E_{a, \text{Si-Si}}$, $E_{a, \text{Me-Si}}$ and $E_{a, \text{Me-Me}}$ are the partial molar activation energies of each type of structural unit.

The vaporisation energy ΔE_v is expressed as:

$$\Delta E_v = \Delta E_{v0} \exp(\epsilon_{v, \text{Si-Si}} X_{\text{Si-Si}} + \epsilon_{v, \text{Me-Si}} X_{\text{Me-Si}} + \epsilon_{v, \text{Me-Me}} X_{\text{Me-Me}}) \dots (5)$$

where E_{v0} is the unit constant (taken as 1 J/mol), $\epsilon_{v, \text{Si-Si}}$, $\epsilon_{v, \text{Me-Si}}$ and $\epsilon_{v, \text{Me-Me}}$ are the dimensionless partial vaporisation energy coefficients of each type of structural unit.

The partial activation energies and vaporisation energy coefficients of a given structural unit depend strongly on the interactions with surrounding structural units. In the QCV model, based on the analysis of the experimental viscosity data, only the interactions between the nearest neighbouring structural units are considered. Moreover, the Si-Si partial activation energy $E_{a, \text{Si-Si}}$ and the Si-Si vaporisation energy coefficient $\epsilon_{v, \text{Si-Si}}$ were found to be the only variable

parameters in the binary silicate systems:

$$E_{a, \text{Si-Si}} = E_{a, \text{Si-Si}}^0 + E_{a, \text{Si-Si}}^{\text{Si-Si}, 1} X_{\text{Si-Si}} + E_{a, \text{Si-Si}}^{\text{Si-Si}, 2} X_{\text{Si-Si}}^2 + E_{a, \text{Si-Si}}^{\text{Me-Si}} X_{\text{Me-Si}},$$

$$E_{a, \text{Me-Si}} = E_{a, \text{Me-Si}}^0, \quad E_{a, \text{Me-Me}} = E_{a, \text{Me-Me}}^0 \dots (6)$$

$$\epsilon_{v, \text{Si-Si}} = \epsilon_{v, \text{Si-Si}}^0 + \epsilon_{v, \text{Si-Si}}^{\text{Si-Si}, 1} X_{\text{Si-Si}} + \epsilon_{v, \text{Si-Si}}^{\text{Si-Si}, 2} X_{\text{Si-Si}}^2 + \epsilon_{v, \text{Si-Si}}^{\text{Me-Si}} X_{\text{Me-Si}},$$

$$\epsilon_{v, \text{Me-Me}} = \epsilon_{v, \text{Me-Me}}^0, \quad \epsilon_{v, \text{Me-Si}} = \epsilon_{v, \text{Me-Si}}^0 \dots (7)$$

where $E_{a, \text{Si-Si}}^0$, $\epsilon_{v, \text{Si-Si}}^0$, $E_{a, \text{Me-Si}}^0$, $\epsilon_{v, \text{Me-Si}}^0$, $E_{a, \text{Me-Me}}^0$, $\epsilon_{v, \text{Me-Me}}^0$, $E_{a, \text{Si-Si}}^{\text{Si-Si}, 1}$, $\epsilon_{v, \text{Si-Si}}^{\text{Si-Si}, 1}$, $E_{a, \text{Si-Si}}^{\text{Si-Si}, 2}$, $\epsilon_{v, \text{Si-Si}}^{\text{Si-Si}, 2}$, $E_{a, \text{Me-Si}}^{\text{Me-Si}}$ and $\epsilon_{v, \text{Me-Si}}^{\text{Me-Si}}$ are adjustable parameters describing influence of neighbouring structural units on the given SU. The final set of the model coefficients is given in Table 2.

The concentrations of the structural units $X_{\text{Si-Si}}$, $X_{\text{Me-Si}}$ and $X_{\text{Me-Me}}$ are equal to and derived from the corresponding concentrations of the second nearest neighbouring bonds (SNNB) calculated using the quasi-chemical thermodynamic model.^{23,24} The quasi-chemical thermodynamic model has been developed by Guggenheim²⁵ and then modified by Blander and Pelton.²⁶ The model takes into account short-range ordering in the ionic melt by considering, for example, in the binary slag system MeO-SiO₂, the formation of two nearest-neighbour pairs (Me-Si) from a (Me-Me) and a (Si-Si) pair.²⁶ Since its development the quasi-chemical model as part of the FactSage (earlier F**A***C***T*) computer package²³ has been successfully applied to describe experimental phase equilibria, thermodynamic and other types of data in many slag systems, from binary to multi-component systems.²⁷ The quasi-chemical formalism is assumed to accurately describe the internal structural ordering in the

Table 1. Average weight and volume of structural units.

Average weight of structural unit ($\cdot 10^{-26}$ kg):
$m_{\text{SU}} = 4.99X_{\text{Si-Si}} + 5.64X_{\text{Al-Al}} + 9.31X_{\text{Ca-Ca}} + 11.93X_{\text{Fe-Fe}} + 6.69X_{\text{Mg-Mg}}$
$+ 5.32X_{\text{Al-Si}} + 7.15X_{\text{Ca-Si}} + 8.46X_{\text{Fe-Si}} + 5.84X_{\text{Mg-Si}} + 7.48X_{\text{Al-Ca}}$
$+ 8.79X_{\text{Al-Fe}} + 6.17X_{\text{Al-Mg}} + 10.62X_{\text{Ca-Fe}} + 8.00X_{\text{Ca-Mg}} + 9.31X_{\text{Fe-Mg}}$
Average volume of structural unit ($\cdot 10^{-29}$ m ³):
$v_{\text{SU}} = 1.92X_{\text{Si-Si}} + 3.04X_{\text{Al-Al}} + 5.79X_{\text{Ca-Ca}} + 4.34X_{\text{Fe-Fe}} + 3.99X_{\text{Mg-Mg}}$
$+ 2.43X_{\text{Al-Si}} + 3.50X_{\text{Ca-Si}} + 2.96X_{\text{Fe-Si}} + 2.83X_{\text{Mg-Si}} + 4.27X_{\text{Al-Ca}}$
$+ 3.65X_{\text{Al-Fe}} + 3.49X_{\text{Al-Mg}} + 5.03X_{\text{Ca-Fe}} + 4.84X_{\text{Ca-Mg}} + 4.16X_{\text{Fe-Mg}}$

Table 2. Parameters of the quasi-chemical viscosity model for fully liquid slags in the system Al₂O₃-CaO-FeO-MgO-SiO₂.

Activation energy ($\cdot 10^2$ kJ/mol):

$$E_a = E_{a, \text{Si-Si}} X_{\text{Si-Si}} + E_{a, \text{Al-Al}} X_{\text{Al-Al}} + E_{a, \text{Ca-Ca}} X_{\text{Ca-Ca}} + E_{a, \text{Fe-Fe}} X_{\text{Fe-Fe}} + E_{a, \text{Mg-Mg}} X_{\text{Mg-Mg}} + E_{a, \text{Al-Si}} X_{\text{Al-Si}} + E_{a, \text{Ca-Si}} X_{\text{Ca-Si}} + E_{a, \text{Fe-Si}} X_{\text{Fe-Si}} + E_{a, \text{Mg-Si}} X_{\text{Mg-Si}} + E_{a, \text{Al-Ca}} X_{\text{Al-Ca}}$$

$$+ E_{a, \text{Al-Fe}} X_{\text{Al-Fe}} + E_{a, \text{Al-Mg}} X_{\text{Al-Mg}} + E_{a, \text{Ca-Fe}} X_{\text{Ca-Fe}} + E_{a, \text{Ca-Mg}} X_{\text{Ca-Mg}} + E_{a, \text{Fe-Mg}} X_{\text{Fe-Mg}}$$

$$+ \frac{\left(\sum_i X_{\text{Al-i}} \right)^\alpha \left(E_{a, \text{AlCa}}^{\text{ch/c}} \left(\sum_i X_{\text{Ca-i}} \right)^\beta + E_{a, \text{AlFe}}^{\text{ch/c}} \left(\sum_i X_{\text{Fe-i}} \right)^\beta + E_{a, \text{AlMg}}^{\text{ch/c}} \left(\sum_i X_{\text{Mg-i}} \right)^\beta \right)}{\left(\sum_i X_{\text{Al-i}} + \sum_i X_{\text{Ca-i}} + \sum_i X_{\text{Fe-i}} + \sum_i X_{\text{Mg-i}} \right)^{\alpha+\beta}} X_{\text{Si-Si}}$$

where

$$\sum_i X_{\text{Al-i}} = 2X_{\text{Al-Al}} + X_{\text{Al-Si}} + X_{\text{Al-Ca}} + X_{\text{Al-Fe}} + X_{\text{Al-Mg}}, \quad \sum_i X_{\text{Ca-i}} = 2X_{\text{Ca-Ca}} + X_{\text{Ca-Si}} + X_{\text{Al-Ca}} + X_{\text{Ca-Fe}} + X_{\text{Ca-Mg}},$$

$$\sum_i X_{\text{Fe-i}} = 2X_{\text{Fe-Fe}} + X_{\text{Fe-Si}} + X_{\text{Ca-Fe}} + X_{\text{Al-Fe}} + X_{\text{Fe-Mg}}, \quad \sum_i X_{\text{Mg-i}} = 2X_{\text{Mg-Mg}} + X_{\text{Mg-Si}} + X_{\text{Al-Mg}} + X_{\text{Ca-Mg}} + X_{\text{Fe-Mg}}; \quad \alpha=3, \beta=1$$

and

$$E_{a, \text{Si-Si}} = 0.79 + 4.65X_{\text{Si-Si}}^2 + 4.98X_{\text{Al-Si}} + 2.34X_{\text{Ca-Si}} + 2.17X_{\text{Fe-Si}} + 2.77X_{\text{Mg-Si}}, \quad E_{a, \text{Al-Al}} = 1.30, \quad E_{a, \text{Ca-Ca}} = 0.82, \quad E_{a, \text{Fe-Fe}} = 0.50, \quad E_{a, \text{Mg-Mg}} = 1.16,$$

$$E_{a, \text{Al-Si}} = 2.78 - 0.96X_{\text{Ca-Si}} - 3.11X_{\text{Fe-Si}} - 0.38X_{\text{Mg-Si}} + 5.63X_{\text{Al-Ca}} + 7.48X_{\text{Al-Fe}}, \quad E_{a, \text{Ca-Si}} = 1.20 - 0.07X_{\text{Fe-Si}} + 0.22X_{\text{Mg-Si}} + 0.29X_{\text{Al-Ca}} + 0.37X_{\text{Ca-Fe}} + 2.00X_{\text{Ca-Mg}},$$

$$E_{a, \text{Fe-Si}} = 0.28 + 0.95X_{\text{Mg-Si}} + 1.20X_{\text{Al-Fe}} - 7.53X_{\text{Ca-Fe}} - 1.80X_{\text{Fe-Mg}}, \quad E_{a, \text{Mg-Si}} = 1.00 + 1.5X_{\text{Al-Mg}} + 1.00X_{\text{Ca-Mg}} + 2.70X_{\text{Fe-Mg}},$$

$$E_{a, \text{Al-Ca}} = 1.83 - 0.02X_{\text{Al-Fe}} + 0.56X_{\text{Al-Mg}}, \quad E_{a, \text{Al-Fe}} = (1/2)(E_{a, \text{Al-Al}} + E_{a, \text{Fe-Fe}}), \quad E_{a, \text{Al-Mg}} = 1.33, \quad E_{a, \text{Ca-Fe}} = (1/2)(E_{a, \text{Ca-Ca}} + E_{a, \text{Fe-Fe}}),$$

$$E_{a, \text{Ca-Mg}} = (1/2)(E_{a, \text{Ca-Ca}} + E_{a, \text{Mg-Mg}}), \quad E_{a, \text{Fe-Mg}} = (1/2)(E_{a, \text{Fe-Fe}} + E_{a, \text{Mg-Mg}}), \quad E_{a, \text{AlCa}}^{\text{ch/c}} = 1.90, \quad E_{a, \text{AlFe}}^{\text{ch/c}} = 1.20, \quad E_{a, \text{AlMg}}^{\text{ch/c}} = 1.29.$$

Vaporisation energy (J/mol):

$$\Delta E_v = \exp(\epsilon_{v, \text{Si-Si}} X_{\text{Si-Si}} + \epsilon_{v, \text{Al-Al}} X_{\text{Al-Al}} + \epsilon_{v, \text{Ca-Ca}} X_{\text{Ca-Ca}} + \epsilon_{v, \text{Fe-Fe}} X_{\text{Fe-Fe}} + \epsilon_{v, \text{Mg-Mg}} X_{\text{Mg-Mg}} + \epsilon_{v, \text{Al-Si}} X_{\text{Al-Si}} + \epsilon_{v, \text{Ca-Si}} X_{\text{Ca-Si}} + \epsilon_{v, \text{Fe-Si}} X_{\text{Fe-Si}} + \epsilon_{v, \text{Mg-Si}} X_{\text{Mg-Si}}$$

$$+ \epsilon_{v, \text{Al-Ca}} X_{\text{Al-Ca}} + \epsilon_{v, \text{Al-Fe}} X_{\text{Al-Fe}} + \epsilon_{v, \text{Al-Mg}} X_{\text{Al-Mg}} + \epsilon_{v, \text{Ca-Fe}} X_{\text{Ca-Fe}} + \epsilon_{v, \text{Ca-Mg}} X_{\text{Ca-Mg}} + \epsilon_{v, \text{Fe-Mg}} X_{\text{Fe-Mg}})$$

where

$$\epsilon_{v, \text{Si-Si}} = 17.3 + 11.12X_{\text{Si-Si}} - 6.22X_{\text{Si-Si}}^2 + 1.60X_{\text{Al-Si}} + 0.04X_{\text{Ca-Si}} + 0.06X_{\text{Fe-Si}} + 0.05X_{\text{Mg-Si}}, \quad \epsilon_{v, \text{Al-Al}} = 13.59, \quad \epsilon_{v, \text{Ca-Ca}} = 13.02, \quad \epsilon_{v, \text{Fe-Fe}} = 11.25,$$

$$\epsilon_{v, \text{Mg-Mg}} = 14.25, \quad \epsilon_{v, \text{Al-Si}} = 20.28 + 9.00X_{\text{Ca-Si}}, \quad \epsilon_{v, \text{Ca-Si}} = 14.46, \quad \epsilon_{v, \text{Fe-Si}} = 9.60, \quad \epsilon_{v, \text{Mg-Si}} = 13.33, \quad \epsilon_{v, \text{Al-Ca}} = 16.88,$$

$$\epsilon_{v, \text{Al-Fe}} = (1/2)(\epsilon_{v, \text{Al-Al}} + \epsilon_{v, \text{Fe-Fe}}), \quad \epsilon_{v, \text{Al-Mg}} = (1/2)(\epsilon_{v, \text{Al-Al}} + \epsilon_{v, \text{Mg-Mg}}), \quad \epsilon_{v, \text{Ca-Fe}} = (1/2)(\epsilon_{v, \text{Ca-Ca}} + \epsilon_{v, \text{Fe-Fe}}), \quad \epsilon_{v, \text{Ca-Mg}} = (1/2)(\epsilon_{v, \text{Ca-Ca}} + \epsilon_{v, \text{Mg-Mg}}),$$

$$\epsilon_{v, \text{Fe-Mg}} = (1/2)(\epsilon_{v, \text{Fe-Fe}} + \epsilon_{v, \text{Mg-Mg}}).$$

slags.

It has been found experimentally¹⁹⁾ that Al^{3+} can occupy tetrahedral coordination positions and participate in a network-type structure, in a similar way to Si^{4+} ions, if the excess negative charge for Al^{3+} is compensated by the presence of alkali or alkaline earth cations. This is commonly referred to as the “charge compensation effect”.¹⁹⁾ As a result, the experimental viscosities in the Al-containing silicate slag systems $\text{Al}_2\text{O}_3-(\text{Me}^+, \text{Me}^{2+})_x\text{O}-\text{SiO}_2$ at constant SiO_2 molar concentrations have maxima at $\text{Al}_2\text{O}_3/(\text{Me}_2, \text{Me})\text{O}$ ratios close to 1.²⁸⁾ To describe the slag viscosity in these Al-containing systems the following charge compensation term was added to the activation energy of viscous flow (written for the $\text{Al}_2\text{O}_3-\text{CaO}-\text{MgO}-\text{SiO}_2$ system):

$$E_a^{\text{ch/c}} = \frac{\left(\sum_i X_{\text{Al}-i} \right)^\alpha \left(E_{a,\text{AlCa}}^{\text{ch/c}} \left(\sum_i X_{\text{Ca}-i} \right)^\beta + E_{a,\text{AlMg}}^{\text{ch/c}} \left(\sum_i X_{\text{Mg}-i} \right)^\beta \right)}{\left(\sum_i X_{\text{Al}-i} + \sum_i X_{\text{Ca}-i} + \sum_i X_{\text{Mg}-i} \right)^{\alpha+\beta}} X_{\text{Si-Si}} \quad (8)$$

where

$$\begin{aligned} \sum_i X_{\text{Al}-i} &= 2X_{\text{Al-Al}} + X_{\text{Al-Si}} + X_{\text{Al-Ca}} + X_{\text{Al-Mg}} \\ \sum_i X_{\text{Ca}-i} &= 2X_{\text{Ca-Ca}} + X_{\text{Ca-Si}} + X_{\text{Al-Ca}} + X_{\text{Ca-Mg}} \\ \sum_i X_{\text{Mg}-i} &= 2X_{\text{Mg-Mg}} + X_{\text{Mg-Si}} + X_{\text{Al-Mg}} + X_{\text{Ca-Mg}} \end{aligned}$$

and $E_{a,\text{AlMe}}^{\text{ch/c}}$, α , and β are adjustable parameters. The charge compensation term $E_a^{\text{ch/c}}$ (Eq. (8)) is a function of the concentrations of Al^{3+} , Ca^{2+} and Mg^{2+} cations in the melt. In the present study the values of α and β were selected to achieve the maximum of the charge compensation term, and therefore of the viscosity, at $X_{(\text{Ca}, \text{Mg})\text{O}}/X_{\text{Al}_2\text{O}_3} \approx 1$, ensuring the best agreement with the experimental data.

In summary, the QCV model links the slag viscosity to the internal structure of melts through the concentrations of various anion/cation structural units that are present in the melt. In the present study the concentrations of these structural units are derived from the quasi-chemical thermodynamic model of the system $\text{Al}_2\text{O}_3-\text{CaO}-\text{MgO}-\text{SiO}_2$ using the FactSage computer package.^{23,24)}

3. Principles of Viscosity Model Development

During the development of the viscosity model a particular methodology was adopted to ensure consistent treatment of the data. The resulting viscosity model parameters provide accurate and reliable predictions of the slag viscosities over a wide range of compositions and temperatures using the existing data sets.

The methodology used in developing the QCV model in the present study involves the following steps: 1) collect all the experimental data available for the slag systems under investigation and carefully analyse the experimental procedures, apparatus and results reported from different studies;

2) exclude unreliable experimental datasets from further model optimisation (2.1. perform analysis of phase equilibria using existing phase diagrams and computer packages such as FactSage²³⁾ and exclude viscosity data obtained at temperatures below liquidus, 2.2. derive and analyse the trends in the activation and vaporisation energies obtained from experimental viscosity data); 3) evaluate the variability (internal scatter) of experimental data; 4) analyse the trends in the concentrations of SU obtained from the quasi-chemical thermodynamic model; 5) calculate the masses and volumes of the structural units using mass balance and available ionic radii data; 6) optimise the model coefficients for the whole compositional range of the slag systems considered including all unary, binary, ternary *etc.* sub-systems by repeating optimisation cycles from low- to high-order systems; 7) analyse the model parameters obtained during optimisation to understand general trends and dependencies; 8) repeat steps 6 and 7 until the agreement between model predictions and experimental data is comparable to the variability over the whole range of conditions.

3.1. Evaluation of Experimental Data

Experimental measurements of slag viscosities at high temperatures are subject to a number of possible error sources. A careful and systematic analysis of the experimental results is therefore important to be able to identify inaccurate and erroneous measurements, and exclude them from consideration when undertaking the optimisation of model parameters.

One of the major sources of the experimental errors is the contamination of the melt by dissolving container or/and sensor materials. This normally results in changes of slag composition and of container/sensor geometry. Post-experimental analysis of the slag compositions reduces these potential errors. Experimental data that exhibit clear evidence of contamination are either eliminated from the optimisation or given low weights in determining the model parameters.

The oxidation states of transition metal elements, such as iron or chromium in the slag, can vary during viscosity experiments depending on atmosphere, temperature and bulk composition, and these changes can lead to significant changes in phase equilibria and to variation of the slag viscosity. In order to avoid this uncertainty it is important to maintain such experimental conditions that ensure the system is uniquely characterised, *e.g.* through the use of the controlled oxygen partial pressure or metal saturation. Experimental data obtained in uncontrolled or undefined oxygen partial pressures are not used in the optimisation.

The appearance of solid phases is another source of the experimental uncertainty that can dramatically alter the viscous behaviour of the slag. Thus, it is always necessary to ensure that viscosity measurements were carried out in homogeneous, fully molten slags. One of the reasons of the presence of solid phases is the crystallisation that normally occurs when the system temperature is lowered below the liquidus. In order to estimate liquidus temperatures in multi-component slag systems it is possible to use a thermodynamic computer program such as FactSage²³⁾ or MTDATA.²⁹⁾ It is also important to avoid the presence of other heterogeneities (gas bubbles, liquid metal droplets) in

the melt, since these can also influence the overall viscous behaviour. Only data that has been obtained in fully liquid slags are used in the viscosity model optimisation.

Temperature measurements obtained using a thermocouple adjacent to the sample have better precision compared to those obtained using an optical pyrometer. The above considerations are important in the critical evaluation of the experimental viscosity data of slag systems in general.

3.2. Variability

A scatter (which is normally referred to as “variability”) is always present within a particular experimental dataset and between different experimental sources. A particular dataset can sometimes be neglected because of the inaccuracies of the experimental technique used, but in many cases the variability of the available experimental data determines the limits of the best agreement achievable by a given viscosity model. In order to evaluate the variability, in the present study all experimental data for each sub-system have been sub-divided into small compositional ranges (within 5 mol%) and the best fits for each small compositional range for pre-exponential term and apparent activation energy were found using the Eyring-type equation. Since the selected compositional ranges were small, the experimental data should be described with very high precision.

The variabilities of the experimental data within these compositional areas, and the differences between predictions and experimental data have been calculated using the formula used by Mills *et al.*³⁰⁾:

$$\Delta = \frac{1}{N} \sum \left| \frac{(\eta_n)_{\text{calc}} - (\eta_n)_{\text{ex}}}{(\eta_n)_{\text{ex}}} \right| \dots\dots\dots (9)$$

where N is a number of points and n is a particular slag system, the subscripts “calc” and “ex” refer to the calculated and experimental viscosities at a given composition and set of process conditions.

3.3. Model Parameters Optimisation

The optimisation of the present model was performed in accordance with the principles formulated above. First, the masses and volumes of the structural units were fixed using mass balance and available ionic radii data.²²⁾ At a given composition it is assumed that the viscosity is expressed through the Eyring equation (see Eq. (1)) and depends only on two parameters—the activation and vaporisation energies E_a and ΔE_v . The “experimental” activation and vaporisation energies can then be found by adjusting the values of E_a and ΔE_v to fit the experimental viscosities at each particular composition. These “experimental” values of E_a and ΔE_v were used in the model optimisation. Finally, the calculated viscosities were then fitted into all accepted experimental values of the slag viscosities over the whole composition range including all unary, binary, ternary, quaternary and higher-order systems. For the compositional and temperature ranges where no experimental data were found, the activation and vaporisation energies and viscosity trends were analysed to ensure that they were consistent with data available and trends in closely related compositions.

3.4. Analysis of the Trends in Structural Unit Concentrations

Since the present model is based on the internal structure of the slag melt, the examination of trends in the concentrations of structural units obtained from the thermodynamic quasi-chemical model^{23,24)} is an important part of the viscosity model development. These SU concentrations rather than bulk composition reflect the internal structure of the slags and form the basis for the viscosity predictions. An analysis of the trends in SU concentrations provides a more general understanding of possible ways in which model parameters can be used to describe higher-order systems (ternary, quaternary *etc.*). Examples of this trend analysis will be given in the various papers of this series.

3.5. Analysis of the Activation and Vaporisation Energies

Systematic analysis of the activation and vaporisation energies obtained from the model enables improved understanding of the relationship between the slag viscosity and internal structure and, ensures self-consistent and reliable predictions of slag viscosity.

Based on the analysis of general trends in viscosity and physical meaning of the model parameters, a number of restrictions were introduced in the model development. For example, the values of E_a and ΔE_v were set to be positive over the whole compositional range. It was found that the data could be described by assuming that only the partial activation energy and vaporisation energy coefficient of (Si–O–Si) structural unit were variable; the values of the other partial activation energies and vaporisation energy coefficients were assumed to be constant. For binary slag systems in which no experimental data are available the corresponding partial activation energies and vaporisation energy coefficients were linearly interpolated from the unary data. Viscosities were assumed to rise monotonically with increasing SiO₂ concentration.

3.6. Analysis of Model Parameters

There are a number of features of the quasi-chemical viscosity model presented in this series of papers that can be highlighted. a) The model has a physical basis and the model parameters bear some physicochemical meaning. b) The values of the molar partial activation energies and vaporisation energy coefficients obtained using the experimental data in the binary and ternary systems are extrapolated into higher order systems in which no experimental data are available, enabling predictions to be performed and, in some cases, discrepancies between experimental data to be identified. c) Restrictions are introduced on the model parameters—for example, the sign (positive) and the magnitude of the molar partial and integral activation energies, and molar integral vaporisation energies. d) The trends in the changes of the model parameters can be analysed in the experimentally well-characterised systems; these trends can then be used for interpolations and extrapolations in other systems in which experimental data is lacking. e) The model is flexible enough to reflect major structural changes, but “rigid” for composition ranges with similar structural units distributions. f) The molar activation

and vaporisation energies have been “de-convoluted” and can be analysed and used for other applications.

Importantly it should be pointed out that the optimisation procedures carried out in the present study did not simply start with identifying parameters in binary systems and then gradually add correction factors for behaviour observed in more complex systems. Rather the parameters were evaluated by an iterative process in which the interpolation of data from multi-component slags towards binary and ternary systems was taken into account to obtain the optimum values. This then accounts for the structure of the present set of papers describing the slag viscosities of the Al_2O_3 – CaO –“ FeO ”– MgO – SiO_2 system—all parameters and interactions have been taken into account right from the start. The viscosity models, although described and explained for the various MgO -containing binary, ternary and quaternary subsystems in turn, they are produced from consideration of all of the available data in the quinary system. Using this approach, the optimised model parameters describing the experimental viscosities as well as the experimental activation and vaporisation energies are applicable for the complete range of compositions and temperatures for fully liquid slags in the Al_2O_3 – CaO – MgO – SiO_2 system.

4. Comparison between QCV Model Predictions and Experimental Data

This section provides QCV model predictions for the MgO , Al_2O_3 – MgO and CaO – MgO sub-systems, in which no experimental data are available in the literature. Evaluation of slag viscosities in these systems is important for the further model development. The QCV model predictions for the MgO , Al_2O_3 – MgO and CaO – MgO systems were obtained using the methodology described above (see Sec. 3), *i.e.* optimising all available experimental data in binary, ternary and quaternary MgO -systems (discussed in next papers of the series) and analysing general trends in viscosities for close or similar slag systems. It is an advantage of the model that viscosities in the systems without experimental data can be evaluated from available experimental information in the compositional areas located not far from the region of interest. A comparison of the QCV model predictions and experimental data for the MgO – SiO_2 system is also given in this section. The phase equilibria and internal structures of the slags have been predicted using an optimised thermodynamic database for the system Al_2O_3 – CaO –“ FeO ”– MgO – SiO_2 .^{24,27} This database includes a quasi-chemical thermodynamic model describing the liquid slag phase, and has been used in conjunction with the FactSage computer program.²³⁾

4.1. MgO

The melting temperature of the pure magnesium oxide is approximately 3 098 K.²³⁾ Only some estimates of viscosity and no experimental data were found in literature on pure MgO .

Figure 1(a) gives the viscosities of pure MgO as a function of reciprocal temperature predicted by the present model (solid line). Estimations of MgO viscosities derived by the significant structures theory of the liquid state³¹⁾ (dashed line) and by extrapolation from the MgO – SiO_2 by

Fig. 1. (a) Predicted (QCV model) and estimated viscosities of pure MgO , Al_2O_3 , CaO and “ FeO ”; (b) predicted (QCV model) viscosities of pure oxides at 1 200°C–3 500°C.

the Urbain model⁴⁾ (dot-dashed line) are also given. In the present model the activation energy and vaporisation energy coefficient for the pure MgO ($E_{a,\text{Mg-Mg}}$ and $\epsilon_{v,\text{Mg-Mg}}$, respectively) have been chosen to better reproduce binary experimental data in the system MgO – SiO_2 , and give viscosity values close to those of the Urbain model estimates.

A comparison of the predicted viscosities of pure liquid Al_2O_3 , “ FeO ”, CaO ¹⁾ and MgO oxides extrapolated by the QCV model to a large temperature range (1 200–3 500°C) are given in Fig. 1(b). The viscosities of MgO are close to those of CaO , but the value of the activation energy (the slope of the curve in Fig. 1) is slightly greater. “ FeO ” viscosity at these temperatures is greater than that for CaO and MgO . This figure also indicates that activation energy of viscous flow (slope) for the pure “ FeO ” is less than those for other oxides. The slope and absolute values of the Al_2O_3 viscosity are greater than those of CaO , “ FeO ”, and MgO .

4.2. Al_2O_3 – MgO

No experimental data for the Al_2O_3 – MgO system has been found in the literature. The system is characterised by high liquidus (above 2 000°C) and low viscosities.

Figure 2 gives the SNNB concentrations at 2 100°C calculated using FactSage.^{23,24)} As Al_2O_3 mole fraction is increased from 0 to approximately 0.25, the concentrations of Al–Mg SNNBs increase rapidly to approximately 0.72 at

Fig. 2. Predicted SNNB (FactSage) in the liquid phase for the Al_2O_3 -MgO system at 2100°C.

Fig. 3. Predicted liquid viscosities (QCV model) in the Al_2O_3 -MgO, Al_2O_3 -CaO and Al_2O_3 -FeO systems.

the expense of the rapidly decreasing Mg-Mg SNNBs. Further Al_2O_3 mole fraction increase over 0.25 results in the gradual decrease of the Al-Mg and the increase of Al-Al SNNB concentrations.

Due to the absence of the experimental data, the viscosity model parameters for this system were selected using the following assumptions. The partial molar activation energies ($E_{\text{Al-Al}}$ and $E_{\text{Al-Mg}}$) and partial vaporisation energy coefficients ($\epsilon_{\text{vAl-Al}}$ and $\epsilon_{\text{vAl-Mg}}$) were selected to be independent of composition. Initial values of $E_{\text{Al-Mg}}$ and $\epsilon_{\text{vAl-Mg}}$ were assumed to have average values of the corresponding values for Al-Al and Mg-Mg partial energies/coefficients. Analysis of the experimental data, the viscosities and $E_{\text{Al-Mg}}$ values in the ternary Al_2O_3 -MgO-SiO₂ system were used to estimate values in the Al_2O_3 -MgO system and trends similar to those in the Al_2O_3 -CaO-SiO₂ and Al_2O_3 -CaO systems²⁾ were employed.

Predicted viscosities for the Al_2O_3 -MgO system at $T=2100, 2200, 2300^\circ\text{C}$ as a function of Al_2O_3 concentration are present in Fig. 3; the viscosities of the Al_2O_3 -CaO and Al_2O_3 -FeO systems predicted by the present model at 2300°C are given for comparison. It can be seen from this figure that the viscosity of the Al_2O_3 -MgO system is close to that of the Al_2O_3 -FeO system.

4.3. CaO-MgO

The liquidus and solidus temperatures are very high in

Fig. 4. Predicted SNNB (FactSage) in the liquid phase for the CaO-MgO, CaO-FeO and Al_2O_3 -CaO systems.

this system—predictions by FactSage^{23,24)} indicated the solidus to be above 2300°C. No experimental data on viscosities were found in the literature.

Figure 4(a) shows the SNNB concentrations in the CaO-MgO system at 2400°C calculated with FactSage (here and further in the text, a metastable liquid is considered at temperatures below the liquidus). The (Ca-Mg) bond concentrations have maximum of only ~0.33 mol fraction that indicates there is no preferential tendency to form Ca-Mg bonds from the Ca-Ca and Mg-Mg bonds and the system therefore is “not ordered”. The trends in the CaO-MgO system are compared to the $\text{AlO}_{1.5}$ -CaO or CaO-FeO systems (see Figs. 4(b)–4(c) where “ordering” is more pronounced).

Due to the absence of the experimental data, the viscosity model parameters for this system were selected using the following assumptions. The partial molar activation energies ($E_{\text{Ca-Ca}}$ and $E_{\text{Ca-Mg}}$) and partial vaporisation energy coefficients ($\epsilon_{\text{vCa-Ca}}$ and $\epsilon_{\text{vCa-Mg}}$) were taken to be independent of composition. Values of the $E_{\text{Ca-Ca}}$ and $\epsilon_{\text{vCa-Ca}}$ have been described previously.²⁾ The values of $E_{\text{Ca-Mg}}$ and $\epsilon_{\text{vCa-Mg}}$ were taken to be averages of the corresponding values for Ca-Ca and Mg-Mg partial activation energies/vaporisation energy coefficients.

Figure 5 shows the predicted viscosities for the CaO-MgO binary system at $T=2400, 2500, 2600^\circ\text{C}$; viscosity values are very low (between 0.003 and 0.006 Pa·s). The predicted viscosities of the Al_2O_3 -CaO and CaO-FeO at metallic iron saturation at 2400°C are given in Fig. 6 for

Fig. 5. Predicted slag viscosities in the fully liquid CaO-MgO, CaO-FeO and Al_2O_3 -CaO systems.

Fig. 6. Phase equilibria (FactSage) and range of viscosity measurements in the MgO-SiO_2 system.

comparison. Trends in the CaO-MgO system are similar to those in the CaO-FeO system at metallic iron saturation. Viscosities in the Al_2O_3 -CaO system are higher than those in the CaO-MgO and CaO-FeO systems.

4.4. MgO-SiO_2

The ranges of compositions and temperatures over which viscosity measurements³²⁻³⁵ have been carried out in the MgO-SiO_2 system are plotted on the phase diagram calculated by FactSage^{23,24} (see Fig. 6). Most of the measurements are located in a relatively narrow compositional region from 50 to 60 mol% of SiO_2 . Figure 6 indicates that all viscosity measurements by Bockris,³² Hofmaier³³ and Urbain³⁵ have been undertaken at temperatures above liquidus, while the measurements by Licko³⁴ were reported to be performed at temperatures lower in some cases than even the solidus, indicating discrepancy between the MgO-SiO_2 phase diagram and the temperature range for viscosity measurements reported by Licko.³⁴

Figure 7 shows the predicted SNNB concentrations for the MgO-SiO_2 system at 1800°C calculated by FactSage^{23,24} (a metastable liquid is assumed for temperatures below the liquidus). It can be seen that the MgO-SiO_2 system is a highly ordered system with the maximum concentration of the Mg-Si SNNB $X_{\text{Mg-Si}}$ approaching 0.9 mol fraction at the orthosilicate composition $X_{\text{SiO}_2}=0.33$. This maximum $X_{\text{Mg-Si}}$ concentration, however is less than corresponding $X_{\text{Ca-Si}}$ maximum concentration of 0.98 in the CaO-SiO₂ system indicating that the MgO-SiO_2 system is “less ordered” than CaO-SiO₂.

Slag viscosities calculated by the present model as a function of SiO_2 concentration at $T=1600$, 1700, and 1800°C for the MgO-SiO_2 , Al_2O_3 -SiO₂, CaO-SiO₂ and FeO-SiO₂ are shown in Fig. 8; experimental viscosities³²⁻³⁵ and liquidus are also indicated on this figure. In those cases³²⁻³⁵ in which experimental data are available at temperatures other than those selected on this figure the data were interpolated using the Eyring equation $\eta=AT^{1.5}\exp(B/T)$ and the values A and B obtained from the experimental data. The model parameters for the MgO-SiO_2 system were derived using the data by Bockris,³²

Fig. 7. Predicted SNNB (FactSage) in the liquid phase for the MgO-SiO_2 system at 1800°C.

Fig. 8. Experimental and predicted viscosities in the systems MgO-SiO_2 , Al_2O_3 -SiO₂, CaO-SiO₂ and FeO-SiO₂ as a function of SiO_2 concentration.

Hofmaier,³³ and Urbain.³⁵ There is a little scatter between experimental results reported by different authors.³²⁻³⁵

The viscosities in the CaO-SiO₂, FeO-SiO₂ and Al_2O_3 -SiO₂ systems predicted by the present model at $T=1800^\circ\text{C}$ are also given in Fig. 8 for comparison. It can be seen that

Fig. 9. Comparison between the experimental and predicted (QCV model) viscosities in the system MgO–SiO₂ at MgO : SiO₂ = 1 : 1 molar.

viscosities of the MgO–SiO₂ system are between those in the Al₂O₃–SiO₂ and CaO–SiO₂ systems. The predicted viscosities in the ‘FeO’–SiO₂ system are the lowest of these systems at SiO₂ < 0.58 mol fraction, but then increase faster than those of other systems with increasing the SiO₂ concentration.

Careful analysis of the experimental data is essential for development of a reliable and accurate viscosity model. Inconsistent experimental measurements, heterogeneous viscosity data or inappropriate conditions of the experiments can lead to large inaccuracies in the model predictions. Figure 9 shows comparisons between the experimental^{32–35} and calculated (QCV model) viscosities [Pa·s] as a function of reciprocal temperature [K^{–1}] at the composition of metasilicate MgO·SiO₂ (59.85 wt% SiO₂). It can be seen from this figure that experimental data by Licko³⁴ do not agree well with the other experimental sources.^{32,33,35} The discrepancy between the reported experimental temperatures³⁴ and the phase equilibrium data has been illustrated with reference to Fig. 7 (see above). The experimental data by Licko³⁴ therefore have been excluded from the optimisation.

5. Conclusions

A general structurally-based quasi-chemical viscosity (QCV) model has been developed for the Al₂O₃–CaO–‘FeO’–MgO–SiO₂ system and its sub-systems. The model provides a link between the slag viscosities and the internal structures of the liquid slags. The internal structures are expressed in terms of the second nearest neighbouring bonds derived using a modified quasi-chemical model and optimised database of system in conjunction with the FactSage computer package.^{23,24}

The methodology and assumptions used in the development of the slag viscosity model have been described. The experimental data have been analysed and the present model has been optimised according to these principles.

The predicted (QCV model) viscosities for fully liquid slags in the systems MgO, CaO–MgO, Al₂O₃–MgO and MgO–SiO₂ have been presented. Where experimental data

are available comparisons between these measurements and model predictions have been made and discussed.

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