Development of a Quasi-chemical Viscosity Model for Fully Liquid Slags in the Al_2O_3 – CaO –‘ FeO ’– MgO – SiO_2 System. Part 2. A Review of the Experimental Data and the Model Predictions for the Al_2O_3 – CaO – MgO , CaO – MgO – SiO_2 and Al_2O_3 – MgO – SiO_2 Systems

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A structurally-based quasi-chemical viscosity model has been developed for the Al_2O_3 – CaO –‘ FeO ’– MgO – SiO_2 system. The model links the slag viscosity to the internal structure of melts through the concentrations of various anion/cation $\text{Si}_{0.5}\text{O}$, $\text{Me}_{2/n}^{n+}\text{O}$ and $\text{Me}_{1/n}^{n+}\text{Si}_{0.25}\text{O}$ viscous flow structural units. The concentrations of structural units are derived from the quasi-chemical thermodynamic model.

The focus of the work described in the present paper is the analysis of experimental data and the viscosity models for fully liquid slags in the Al_2O_3 – CaO – MgO , Al_2O_3 – MgO – SiO_2 and CaO – MgO – SiO_2 systems.

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

1. Introduction

The present paper is the second in a series describing the development of the structurally-based quasi-chemical viscosity (QCV) model for the Al_2O_3 – CaO –‘ FeO ’– MgO – SiO_2 system. A structurally-based viscosity model for fully liquid silicate slags applied to the Al_2O_3 – CaO –‘ FeO ’– MgO – SiO_2 system at metallic iron saturation has previously been developed by authors.¹⁾ The present series of papers describes further extension of the model for the Al_2O_3 – CaO –‘ FeO ’– MgO – SiO_2 system to incorporate an effect of MgO . In the first of this series of papers²⁾ the QCV model was described and viscosity predictions were provided for the MgO , CaO – MgO , Al_2O_3 – MgO and MgO – SiO_2 subsystems. The present paper focuses on the viscosities in the ternary subsystems Al_2O_3 – CaO – MgO , CaO – MgO – SiO_2 and Al_2O_3 – MgO – SiO_2 .

The Al_2O_3 – MgO – SiO_2 , CaO – MgO – SiO_2 and Al_2O_3 – CaO – MgO slag systems are important as they form the basis of the quaternary Al_2O_3 – CaO – MgO – SiO_2 , which describes industrial iron-making slags. The Al_2O_3 – MgO – SiO_2 is the base system for submerged arc ferrochromium smelting slags. In these industrial smelting applications slag viscosity has a significant influence on productivity and metal recovery. In addition, CaO – MgO – SiO_2 slags can be formed as the result of reaction of dolomite ($\text{CaCO}_3 \cdot \text{MgCO}_3$) and silica (SiO_2). These combinations of materials are sometimes encountered as sub-processes in the preparation and processing of metallurgical materials, leading eventually to more complex reactions. The Al_2O_3 – CaO – MgO slag system is important for pyrometallurgical treatment of radioac-

tive wastes.³⁾

Briefly, the methodology used in developing the QCV model in the present study involves the following stages: 1) collect and carefully analyse all the experimental data available for the slag systems under investigation; 2) exclude unreliable experimental datasets from the model optimisation (using analysis of phase equilibria and 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 structural units 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 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 data variability over the whole range of conditions.

2. Comparisons between QCV Model Predictions and Experimental Data

2.1. Al_2O_3 – CaO – MgO

The viscosities of liquid slags in the Al_2O_3 – CaO – MgO system have not been systematically investigated experimentally to date: only two experimental studies have been found in the literature. Bakhvalov *et al.*³⁾ used a “vibra-

Fig. 1. Predicted liquidus (FactSage) and experimental data in the Al_2O_3 -CaO-MgO system.

Fig. 2. Selected viscosity measurements by Bakhvalov *et al.*³⁾ in the Al_2O_3 -CaO-MgO system.

tional" or oscillating-type of the rheometer and did not report any additional information on the technique/materials used. Shalimov and co-workers^{4,5)} reported viscosity measurements undertaken using the rotational bob method, which is believed⁶⁾ to be not as accurate as the oscillating (or vibrational) rheometer for relatively low viscosities in the range of 0.01–0.1 Pa·s.

Figure 1 shows the liquidus isotherms in the Al_2O_3 -CaO-MgO system predicted by FactSage^{7,8)} and the experimental compositions studied in Bakhvalov *et al.*³⁾ and Shalimov *et al.*^{4,5)} Experimental information^{3–5)} is available only for low-MgO compositions (below ~12 wt%) close to the Al_2O_3 -CaO binary. Comparison of the reported temperatures and compositions with the phase equilibria information predicted with FactSage indicates that some of experimental data were obtained at conditions below the liquidus.

Figure 2 shows selected results of Bakhvalov *et al.*³⁾ and liquidus temperatures calculated by FactSage.^{7,8)} It can be seen that in all cases a sharp increase of slag viscosity (resulting in inflection points in the logarithm viscosity vs. reciprocal temperature line) is observed at temperatures corresponding to the predicted liquidus. This figure clearly

Fig. 3. Comparison of the experimental^{3–5)} and predicted (QCV model) viscosities in the Al_2O_3 -CaO-MgO system at $\text{Al}_2\text{O}_3/\text{CaO}/\text{MgO}=41/53/6$ wt%.

demonstrates that careful analysis of phase equilibria (for example, using such software as the FactSage computer package) should be used for the experimental data in order to exclude possible heterogeneous viscosity measurements.

Comparison between Bakhvalov's³⁾ and Shalimov's^{4,5)} results at the same composition ($\text{Al}_2\text{O}_3/\text{CaO}/\text{MgO}=41/53/6$ wt%) is presented in Fig. 3. The temperatures of the liquidus and phase field boundaries predicted by FactSage are also indicated in this graph by small arrows. It can be seen that there is a correlation between these temperatures and inflection points on the viscosity–temperature curves. Again rapid increases of the viscosity measurements with decreasing temperature are believed to be directly related to the crystallisation of the slag. According to Fig. 3 solidification of the slag sample in Shalimov's work^{4,5)} appeared to occur at a higher temperature (~1450°C) compared to that reported by Bakhvalov³⁾ (~1300°C). The difference in these temperatures could be related to temperature measurements, thermal history, slag composition and/or experimental design and procedure.

Figures 4(a)–4(f) show the predicted iso-SNNB (second-nearest-neighbour bonds²⁾) concentrations in the Al_2O_3 -CaO-MgO system at 1600°C for real and metastable liquid slag; these concentrations were predicted using the optimised thermodynamic database for this system and the FactSage computer package.^{7,8)} It can be seen from the concentration lines from this figure that Al^{3+} cation in this system preferentially forms (Al-Mg) and (Al-Ca) SNNB from (Al-Al), (Ca-Ca) and (Mg-Mg) SNNB (similar to the behaviour of the Si^{4+} cation in SiO_2 -containing systems). At intermediate composition ranges the concentrations of the (Al-Ca) and (Al-Mg) are significant, and only at high Al_2O_3 , CaO or MgO compositions over ~70 wt% the sum of the (Al-Ca) and (Al-Mg) concentrations is less than 0.7 mol fraction.

The optimised values of the molar activation and vaporisation energies for all corresponding unary and binary subsystems have been given in previous publications.^{1,2)} The corresponding partial activation energies/vaporisation energy coefficients in this ternary system have been extrapolated from the corresponding unary and binary systems. Only one small ternary parameter expressing effect of the (Al-Mg) concentrations on the activation energy of viscous

Fig. 4. Predicted (FactSage) SNNB iso-concentrations in the Al_2O_3 -MgO-CaO system at 1600°C.

flow²⁾ was required to better describe viscosities in the Al_2O_3 -CaO-MgO system and higher-order SiO_2 -containing systems.

Figure 5 shows iso-viscosity lines [$\text{Pa}\cdot\text{s}$] predicted by the present QCV model for liquid slags at 1600°C. The viscosities of the slags in this Al_2O_3 -CaO-MgO system are low ($\sim 0.2 \text{ Pa}\cdot\text{s}$) and are significantly smaller than the viscosities observed in SiO_2 -containing ternary slag systems (e.g. see Figs. 9 and 17).

2.2. CaO-MgO-SiO₂

Eleven experimental studies⁹⁻¹⁹⁾ of slag viscosities are reported for the CaO-MgO-SiO₂ system. Sipp¹⁶⁾ reported viscosity measurements for low temperatures ($\leq 1050 \text{ K}$) using the uni-axial compression method described elsewhere.¹⁶⁾ These results are related to the “metastable” glasses and were not included in the current model optimisation.

Most of the researchers^{12-17,19)} have used Pt or Pt/Rh materials for both the container and sensor, which is the most suitable in the temperature range investigated (1523–1873 K). However, Kawai¹⁰⁾ used the graphite crucibles and bobs for viscosity measurements up to 1700°C. According to the analysis by Gul'tyai,⁹⁾ who also used graphite, this material starts reacting with SiO_2 in the slag at temperatures higher than 1500°C (intensive reaction occurs for $T \geq 1650^\circ\text{C}$) and therefore during experiments temperatures should not exceed 1600–1650°C. This condition was not satisfied in the experiments carried out by Kawai¹⁰⁾ and might be the reason for a systematic deviation of his results from others. Kozu and Kani¹¹⁾ reported neither materials of crucible and bob used nor other details of experiments; it is

Fig. 5. Predicted (QCV model) liquid iso-viscosities [$\text{Pa}\cdot\text{s}$] at 1600°C in the Al_2O_3 -CaO-MgO system.

not possible therefore to evaluate reasons for the deviation of their results from others.

The rotational cylinder viscometry technique was used in a number of studies^{9-11,15,17-19)}; this method is considered to be one of the most accurate in the investigated range of viscosities (~ 0.1 – $10 \text{ Pa}\cdot\text{s}$). Some researchers¹²⁻¹⁴⁾ used the oscillating bob method, which is also suitable for these viscosities. Gul'tyai⁹⁾ did not publish a full description of the apparatus used, except it was reported to be a rotational viscometer.

Since the composition and state of the slag can change during viscosity experiments it is important to carry out the post-experimental analysis of the quenched slag samples to verify the composition and to ensure that samples are homogeneous and bubble-free. Only a few researchers reported that such an analysis was carried out: Scarfe *et al.*,¹⁵⁾ Sykes *et al.*,¹⁷⁾ and Urbain *et al.*¹⁸⁾; these results were therefore given a higher weight in the model optimisation.

The widest compositional range in the CaO-MgO-SiO₂ system was investigated by Gul'tyai,⁹⁾ while a number of researchers reported only one composition measured (usually the composition of diopside— $\text{CaMgSi}_2\text{O}_6$, which is of geological interest). The widest investigated temperature range was reported by Urbain and co-workers¹⁸⁾ for the composition close to diopside.

Figure 6 shows the liquidus isotherms calculated by FactSage and experimental compositions investigated by a number of researchers.⁹⁻¹⁸⁾ Most of the experimental measurements were undertaken in the compositional areas in which the liquidus temperatures are predicted to be below 1600°C. Careful analysis of the experimental data showed that some of the results by Gul'tyai⁹⁾ at lower SiO_2 concentrations, and by Kawai,¹⁰⁾ were carried out below the liquidus.

Agreement between the experimental^{9,11,12,15,17)} and predicted viscosities as a function of reciprocal temperature at or close to the composition of diopside ($\text{CaMgSi}_2\text{O}_6$) is shown in Fig. 7. All the cited researchers except Licko¹²⁾ used the rotational viscometry technique; the experimental procedures were similar, except in the studies by Gul'tyai.⁹⁾ Most of the data are consistent with each other, except the

Fig. 6. Predicted liquidus (FactSage) and compositions of experimental viscosity measurements in the CaO–MgO–SiO₂ system.

Fig. 7. Comparison of the experimental and predicted (QCV model) viscosities at the composition of diopside (CaMgSi₂O₆).

data by Kozu and Kani.¹¹⁾ The latter authors did not report experimental details, and it is not possible to evaluate reasons for such deviation from the rest of the results. The present model agrees well with the measurements reported by most of the authors.^{9,12,15,17)}

The iso-concentrations (0.1, 0.2, ..., 0.9 mol fr) of the SNNB in the CaO–MgO–SiO₂ system at 1500°C are shown in Figs. 8(a)–8(f). The concentrations of the Si–Si SNNB (Fig. 8(a)) are not sensitive to the CaO/MgO weight ratio but decreases rapidly towards values close to zero with a decrease of SiO₂ concentration below 40 wt%. Both $X_{\text{Ca-Si}}$ (Fig. 8(d)) and $X_{\text{Mg-Si}}$ (Fig. 8(e)) have maximum values at orthosilicate compositions (2MgO·SiO₂ and 2CaO·SiO₂, respectively) and similar distributions across the ternary system: the “maxima” extended towards opposite binary joins (the CaO–SiO₂ for Mg–Si and the MgO–SiO₂ for Ca–Si SNNB, respectively). The concentrations of non-silicate SNNB $X_{\text{Ca-Ca}}$, $X_{\text{Mg-Mg}}$ and $X_{\text{Ca-Mg}}$ (see Fig. 8(b), 8(c),

Fig. 8. Predicted SNNB iso-concentrations in the CaO–MgO–SiO₂ system (FactSage) at 1500°C.

Fig. 9. Predicted (QCV model) iso-viscosities [Pa·s] at 1500°C in the CaO–MgO–SiO₂ system.

8(f)) approach values that have a significant effect on the viscosity trends only at low SiO₂ concentrations (less than 30 wt%).

Figure 9 shows iso-viscosity curves [Pa·s] and liquidus calculated by FactSage at $T=1500^\circ\text{C}$. It can be seen that viscosities slightly increase with increasing of the CaO concentration along iso-SiO₂ lines. Slag viscosities increase rapidly with increasing SiO₂ concentration.

The experimental^{9,10,12,13)} and calculated slag viscosities as a function of CaO/(CaO+MgO) weight ratio at 50 wt% SiO₂ for different temperatures are shown in Fig. 10. The

Fig. 10. Liquid slag viscosities as a function of wt CaO/(CaO+MgO) at 50 wt% SiO₂ for a range of temperatures in the system CaO–MgO–SiO₂.

Fig. 11. Liquid slag viscosities as a function of wt SiO₂ at wt CaO/(CaO+MgO)=0.6 for a range of temperatures in the system CaO–MgO–SiO₂.

dashed lines connecting the experimental points are plotted to guide the reader to results reported by the different authors and different temperatures. The viscosities calculated by the present QCV model agree well with the experimental points. It can be seen from this figure that several points by Kawai¹⁰) have obvious deviation from the other results. Two points at weight ratio CaO/CaO+MgO $\approx$ 0.34 at 1500 and 1600°C were obtained below or close to the liquidus predicted by FactSage and were not included in the model optimisation. This is also the case for one point by Gul'tyai⁹) at 1400°C. Again, this point is not used in the optimisation. Data by Machin,^{13,14}) Licko,¹²) Scarfe¹⁵) and Urbain¹⁸) were given preference during selection of model parameters.

Figure 11 shows the experimental^{9,12–15,18}) and calculated slag viscosities as a function of wt SiO₂ at weight ratio CaO/(CaO+MgO)=0.6 for different temperatures (1400, 1500, 1600 and 1700°C). The data point by Gul'tyai⁹) at 1500°C corresponds to the sub-liquidus measurements and was not used in the model optimisation. Good agreement between calculated and experimental viscosities can be achieved with the present viscosity model.

2.3. Al₂O₃–MgO–SiO₂

The Al₂O₃–MgO–SiO₂ system is another example of a well-investigated slag system: there are viscosity data from

Fig. 12. Predicted liquidus (FactSage) and compositions of experimental viscosity measurements in the Al₂O₃–MgO–SiO₂ system.

11 experimental studies^{14,18,20–28}) available in the literature.

Most of the researchers employed the rotational cylinders method and Pt (or Pt/Rh alloys)^{14,22,24–26}) or Mo^{18,21,23,27,28}) materials for the sensor and container. The use of molybdenum implies the use of neutral atmosphere (Ar, N₂), whilst Pt (or Pt/Rh alloys) can be used in air. The “torsional” rheometer used by Ermolaeva²⁰) might not be suitable for the viscosities and temperatures investigated; as will be pointed out below these results have an obvious deviation from the other studies.

The majority of experimental viscosity measurements in the Al₂O₃–MgO–SiO₂ were obtained by Lyutikov²³) (for 50 slag compositions investigated), Toplis and Dingwell²⁶) (22 compositions) and Zhilo²⁷) (40 compositions). A large proportion of these results were used in the model optimisation.

Toplis and Dingwell²⁶) also reported measurements of the viscosity at lower temperatures (1094–1147 K) using the techniques only designed for measuring very high viscosities ($\geq 0^9$ Pa·s). These results are related to the glassy state and were therefore not included into the model optimisation.

The highest temperatures achieved during viscosity measurements of fully liquid slags in the Al₂O₃–MgO–SiO₂ system were reported by Urbain¹⁸) and Hofmaier²¹) to be approximately 2400 K. For such temperatures it is necessary to use a pyrometer for temperature measurements, which has a greater experimental uncertainty than the used of a thermocouple.

Figure 12 shows the liquid isotherms calculated by FactSage^{7,8}) and compositions at which experimental viscosity measurements^{14,18,20–28}) have been carried out in this system. Comparison of reported temperatures and phase equilibrium data clearly indicate that either some of the viscosity measurements by Zhilo and co-workers,^{27,28}) Ermolaeva²⁰) and Lyutikov *et al.*²³) have been carried out under liquidus temperatures or uncertainties exist for the temperature measurements. Figure 13 illustrates further analysis of the experimental data indicating that most likely the measurements reported by these three authors^{20,23,27,28})

Fig. 13. Examples of viscosity measurements in the Al_2O_3 - MgO - SiO_2 system. (Dashed lines indicate the trend.)

were performed for partly crystallised slags. The arrows on this figure indicate the liquidus temperatures for each composition calculated by FactSage. It can be seen that in each case the liquidus predicted with FactSage approximately coincides with the inflection points on the viscosity-temperature curves ($\log \eta$ vs. $1/T$) indicating that solid phases precipitated out of liquid slag were present during the experiments and had affected the viscosity measurements. The data reported by Ermolaeva²⁰ have two notable inflection points on the $\log \eta$ vs. $1/T$ plot: the first higher temperature inflection point could be related to the beginning of crystallisation (primary phase field is mullite, $\text{Al}_6\text{Si}_2\text{O}_{13}$); the second one can be related to the temperature when another solid phase (spinel solid solution) starts to precipitate out. The points reported for temperatures below the liquidus were excluded from the optimisation.

The SNNB concentrations predicted with FactSage^{7,8} in the Al_2O_3 - MgO - SiO_2 system at 1700°C are presented in Figs. 14(a)-14(f). The SNNB concentrations in the regions below the liquidus temperatures are given for homogeneous metastable liquids. Concentrations of the Si-Si SNNB are not sensitive to the changing $\text{CaO}/\text{Al}_2\text{O}_3$ ratio but decreases rapidly to less than 0.5 mol fraction as the SiO_2 concentration decreases below 70 wt%. Both $X_{\text{Al-Si}}$ (Fig. 14(d)) and $X_{\text{Mg-Si}}$ (Fig. 14(e)) have maxima at orthosilicate ($\text{Al}_2\text{O}_3 \cdot \text{SiO}_2$ and $2\text{MgO} \cdot \text{SiO}_2$, respectively) compositions, but the maximum values are significantly different being ~ 0.41 mol fraction of $X_{\text{Al-Si}}$ and ~ 0.9 mol fraction of $X_{\text{Mg-Si}}$. These “maxima” are extended across the ternary systems. Only at low SiO_2 concentrations of ~ 30 wt% the concentrations of non-silicate SNNB $X_{\text{Al-Al}}$, $X_{\text{Mg-Mg}}$ and $X_{\text{Al-Mg}}$ (Figs. 14(b), 14(c), 14(f), respectively) approach significant values that affect the viscosity trends.

Figure 15 presents the experimental^{20,23-25,28} and calculated viscosities as a function of the $\text{Al}_2\text{O}_3/(\text{Al}_2\text{O}_3 + \text{MgO})$ weight ratio at constant SiO_2 concentration of 50 wt% and different temperatures (1500, 1600, 1700, 1800, 1900°C). Dashed lines indicate metastable liquid under the liquidus calculated by FactSage. It can be seen that significant deviation of the experimental results^{20,23-25,28} from the model predictions is observed at compositions below the liquidus. Figure 15 also illustrates the fact that the slag viscosities as

Fig. 14. Predicted SNNB iso-concentrations (FactSage) in the Al_2O_3 - MgO - SiO_2 system at 1700°C.

Fig. 15. Liquid viscosities in the Al_2O_3 - MgO - SiO_2 system as a function of $\text{wt Al}_2\text{O}_3/(\text{Al}_2\text{O}_3 + \text{MeO})$ ($\text{Me} = \text{Mg, Ca, Fe}$) at 50 wt% SiO_2 .

a function of the $\text{Al}_2\text{O}_3/(\text{Al}_2\text{O}_3 + \text{MgO})$ weight ratio have slight non-linearity that could have resulted from the charge compensation effect. The deviation from the linearity towards maximum is less pronounced in this system compared to the Al_2O_3 - CaO - SiO_2 (the value of the charge compensation term $E_{\text{a,AlCa}}^{\text{ch/c}}$ of 1.90 is larger than the $E_{\text{a,AlMg}}^{\text{ch/c}}$ value of 1.29). The viscosities of the Al_2O_3 - CaO - SiO_2 (dashed line) and Al_2O_3 - FeO - SiO_2 (dot-dashed line) systems at 1900°C are given in Fig. 15 for comparison. It can be seen that in all systems the trends of viscosity as a function of $\text{Al}_2\text{O}_3/(\text{Al}_2\text{O}_3 + \text{MeO})$ ratio ($\text{Me} = \text{Ca, Fe, Mg}$) are in general similar. The charge compensation effect is more pronounced in the Al_2O_3 - CaO - SiO_2 system. In the

Fig. 16. Experimental and predicted viscosities in the Al_2O_3 - MgO - SiO_2 system as a function of SiO_2 concentration at $\text{wt Al}_2\text{O}_3/(\text{Al}_2\text{O}_3+\text{MgO})=0.7$.

Fig. 17. Predicted iso-viscosities (QCV model) and experimental viscosities [Pa.s] in the Al_2O_3 - MgO - SiO_2 system at 1700°C.

Al_2O_3 - FeO - SiO_2 this effect is predicted to be the least.

Figure 16 shows the experimental^{14,18,20,21,23,25,26} and predicted slag viscosities as a function of wt% SiO_2 at $\text{Al}_2\text{O}_3/(\text{Al}_2\text{O}_3+\text{MgO})=0.7$ by weight (molar $A/(A+M)\approx 0.5$) for different temperatures (1500, 1600, 1700, 1800, and 1900°C); the liquidus calculated by FactSage is also indicated. Slag viscosities increase with an increase of wt pct SiO_2 . Figure 16 also illustrates the importance of the careful analysis of the experimental data. It can be seen from this figure that some experimental measurements (e.g. by Lyutikov²³) and by Ermolaeva²⁰) deviate from the general viscosity trends confirmed by other researchers (e.g. Riebling,²⁵ Urbain,¹⁸ Hofmaier²¹). Revealing such uncertainties in the experimental data is very important for model optimisation.

Figure 17 presents the iso-viscosity lines calculated for the Al_2O_3 - MgO - SiO_2 by the present model at 1700°C and liquidus predicted by FactSage. It can be seen from comparison of Fig. 14 and Fig. 17 that iso-viscosity curves follow the trends of the iso-SNNB curves and provide an ac-

curate description of the experimental data for fully liquid slags.

3. Conclusions

A general structurally-based quasi-chemical viscosity model has been developed, which accurately describes slag viscosity in the Al_2O_3 - CaO - MgO , CaO - MgO - SiO_2 and Al_2O_3 - MgO - SiO_2 systems. The model links the slag viscosity to the structure of the liquid slag expressed in terms of the second nearest neighbouring bonds; the latter are extracted from the thermodynamic quasi-chemical model available in the FactSage package.

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