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GTOx

Version 18

Summary & Examples

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Introduction

The GTOx database Version 18 contains thermodynamic data covering binary, ternary and quaternary sub-systems among the following components:

**Oxides-Metals-Phosphates-Sulfides-Sulfates-Carbonates-Chlorides-Fluorides
based on Al-Ca-Cr-Cu-Fe-Li-Mg-Mn-K-Na-Ni-Si-Sr-Ti-V-Zn**

with a focus on oxides. Information concerning the sub-systems already assessed in the database is given in appropriate charts in the [next chapter](#). For calculations in higher order systems the data of the subsystems are extrapolated. The database is the result of an ongoing thermochemical (Gibbs energy) and thermophysical (density, viscosity) assessment project to obtain the data for the respective phases in each system. These assessments have been carried out in the framework of past and ongoing projects sponsored by German as well as European funding agencies in close collaboration with Forschungszentrum Jülich (IEK-2)¹. A significant database advancement has been made in the last development period with respect to the unification of the thermodynamic description of the liquid state. Details are given in the chapters [Phases](#) and [What is new in version 18?](#).

Recently, the scope of the database has been expanded in order to additionally cover thermophysical properties of oxides. The most relevant properties are the viscosities of slag melts, however, some work was also devoted to modelling the density, and thus the molar volume, of such melts. The density database will also be extended to the solid phases, thus enabling the linking of the two properties viscosity and volume in the modelling of viscosities in the solid-liquid range.

For representative cases of data assessments as well as applications of the data see the Chapters [Assessment examples](#) and [Application examples](#). For users with a direct need for phase diagrams calculated using the present database, GTT additionally offers access to its GTOx Documentation, i.e. the full collection of all phases diagrams calculated during the thermodynamic assessments. Please [contact us](#). For those readers who are interested in the recent changes and additions to this version, please check the Chapter: [What is new in version 18?](#).

¹ Forschungszentrum Jülich GmbH - Institut für Energie- und Klimaforschung, Structure and Function of Materials (IEK-2), PD Dr. Michael Müller

Database content overview

The present GTOx database consists of Gibbs energies for the liquid phase (containing metals, oxides, carbonates, sulfides, sulphates, Fluorides, chlorides) as well as 166 solid solution phases and 901 stoichiometric phases. The figures (1-4) below indicate systems which have been assessed. Note that an O or R in a green square indicates that the data are mainly valid for (O)xidizing respectively (R)educing conditions. Such a distinction has to be made for metals with multiple valences (Fe, Mn, Cu, Cr, V, Ti). If neither O nor R is indicated for these metals, the systems are assessed for both conditions.

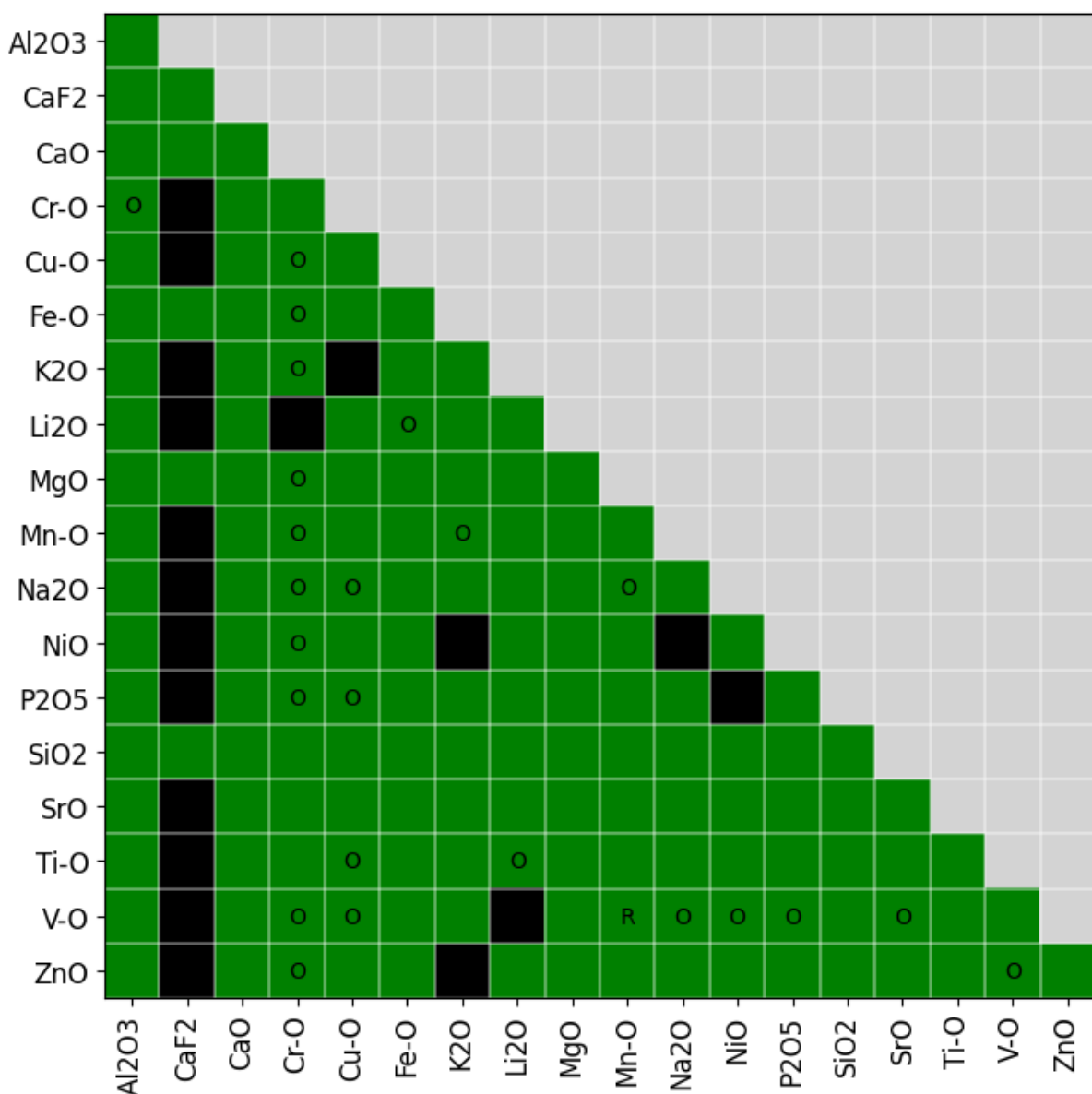


Figure 1: Assessed (green) binary oxide systems in the GTOx database. O and R denote systems for which the data is mainly valid for oxidizing and reducing conditions, respectively.

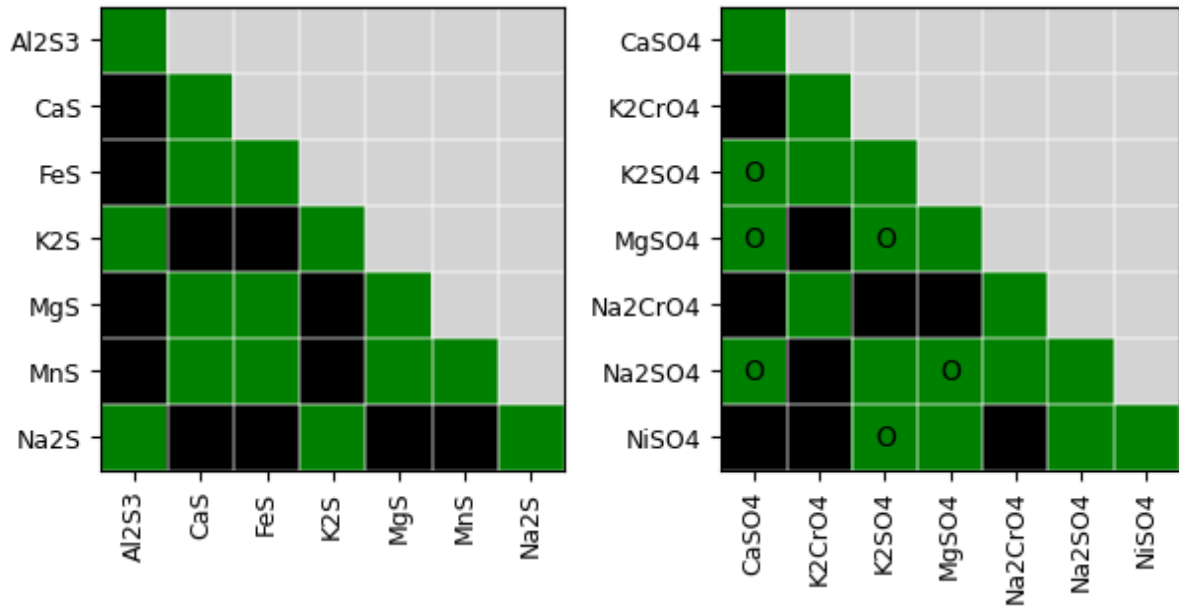


Figure 2: Assessed (green) sulfide-containing (left) or sulphate-containing (right) binary systems in the GTOx database. O denotes systems for which the data is mainly valid for oxidizing conditions.

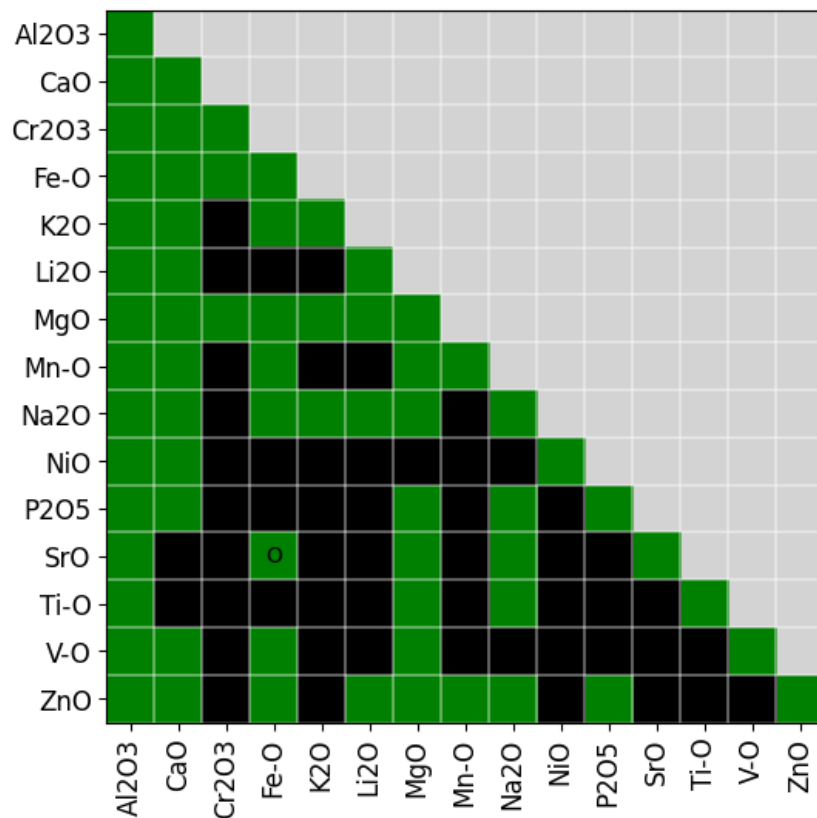


Figure 3: Assessed (green) SiO₂-containing ternary systems in the GTOx database. O denotes systems for which the data is mainly valid for oxidizing conditions.

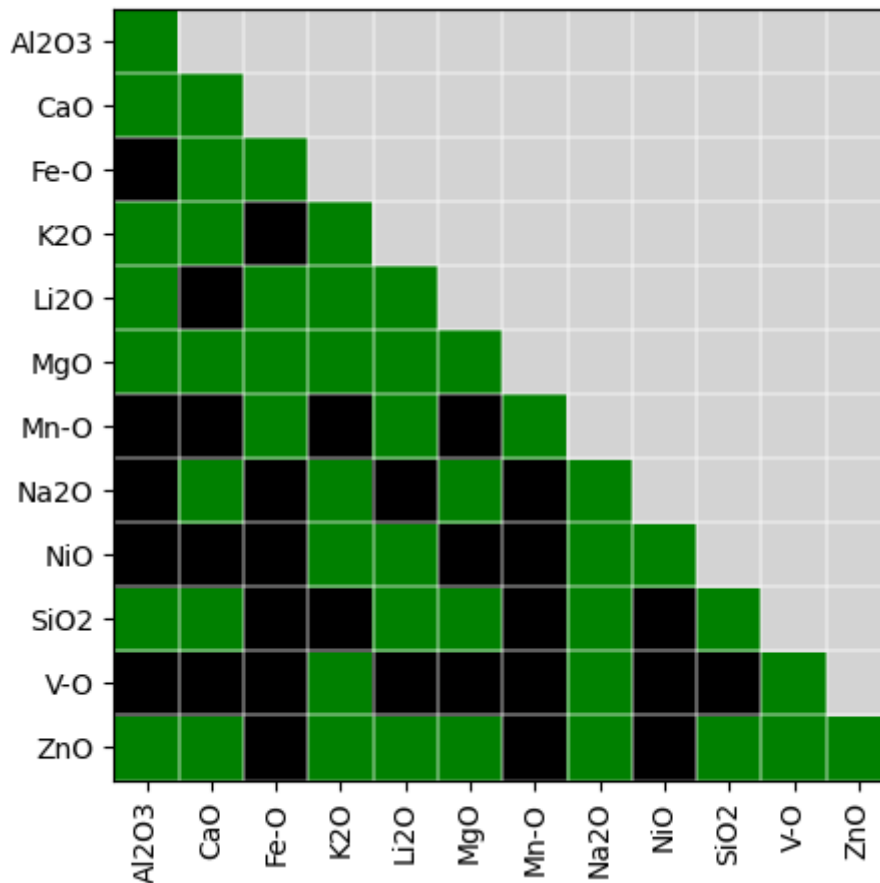


Figure 4: Assessed (green) P_2O_5 -containing ternary systems in the GTOx database.

Figure 3 shows the ternary systems containing SiO_2 . As can be seen, most combinations usually observed in ferrous and non-ferrous metallurgy, cement making and combustion ashes (systems with main components from SiO_2 - Al_2O_3 - CaO - FeO_x - MgO - MnO_x) are covered.

Figure 4 shows the ternary systems containing P_2O_5 . Recently, there has been strong interest in P_2O_5 -containing systems because of the focus on Phosphorous recovery from, for instance, sewage sludge, but also because many iron ores processed in East Asia in particular contain large amounts of P_2O_5 . Furthermore, P_2O_5 is an important component of biomass ashes. To describe these applications, most combinations usually observed – such as systems with main components from SiO_2 - Al_2O_3 - CaO - FeO_x - K_2O - MgO - Na_2O – are covered.

Thermophysical modelling

Viscosity

A viscosity model for fully liquid (i.e. also supercooled) melts has been developed, where the viscosity is directly correlated to the structure of oxide melts, and the melt structure in turn is described based on the thermodynamic description applied, i.e. using the modified non-ideal associate species model. The present viscosity model covers the system **SiO₂-Al₂O₃-CaO-MgO-Na₂O-K₂O-FeO_x** using a set of model parameters for the viscosity which all have a clear physical meaning.

A corresponding *viscosity calculator* has been developed based on [ChemSheet](#). A screenshot of the user interface is shown below in Figure 5. Note that a valid ChemSheet license is required to use the viscosity calculator.

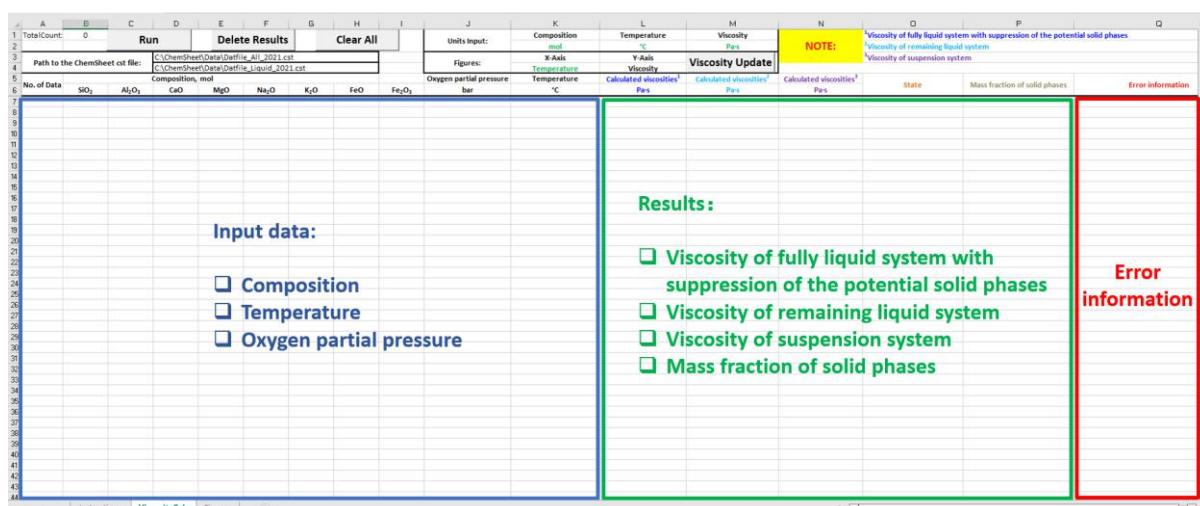


Figure 5: Screenshot of the GTTox-based viscosity calculator in ChemSheet.

Density

A density model for fully liquid (i.e. also supercooled) melts has been developed covering the system **SiO₂-Al₂O₃-CaO-MgO-Na₂O-K₂O**. Note that densities of solid phases are not yet part of the release but already under development.

Application examples

De-phosphorisation of steels in the BOF process

In the basic oxygen steelmaking (BOF) process, the accurate control of phosphorous removal up to ultra-low values is very important to ensure a high quality of the end product. This has proven to be associated with several challenges, leading to a preferred usage of high-priced low-P iron ores. Thus, in the scope of the European RFCS project BOFdePhos (RFSR-CT-2014-00005), important thermodynamic and kinetic aspects of the dephosphorisation reaction such as the effect of solid phases on phosphorous distribution and lime dissolution in a foamy slag were investigated.

It was found that BOF slags contain solid oxides during a large period of the blow and, in most cases, also at the end of blow. The type and amount of solid phases is strongly affected by temperature and minor oxides content such as MgO-, MnO- and Al₂O₃-content. The consideration of solid phases formation in the slag, especially the P-dissolving C₂S-C₃P solid solution, is crucial for a successful modelling and control of de-phosphorisation. However, most of the phosphorous distribution equations available in the literature were developed for homogeneous slags. Thus, a new approach for the thermodynamic modelling of the P-distribution between a heterogeneous slag and liquid iron covering the total blowing period in the converter was developed and incorporated in a kinetic de-phosphorisation model using [SimuSage](#). The two phase diagrams below show the most relevant phase relationships pertaining to the de-phosphorisation as calculated from the GT_{Ox} database:

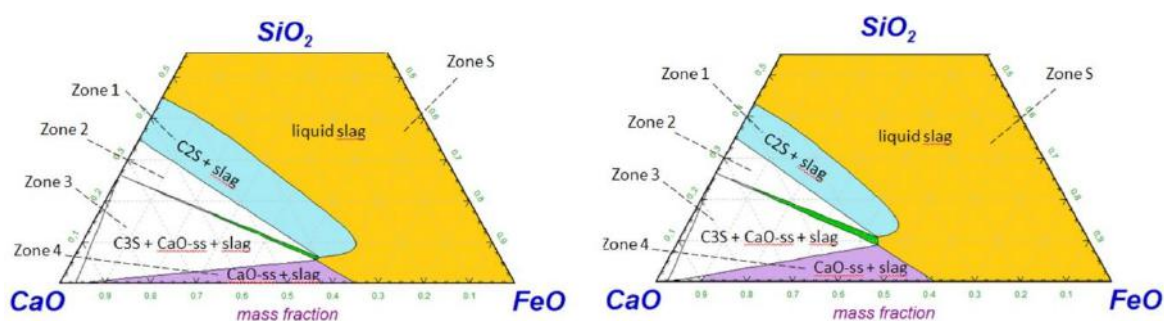


Figure 6: Liquidus isothermals of the system CaO-FeO_x-SiO₂ in equilibrium with liquid Fe at 1550 °C (left) and 1700 °C (right).

Figure 6 shows two isothermal sections of the CaO-FeO_x-SiO₂ system. Depending on processing conditions (lime addition, temperature, blow rate, stirring etc.), the actual slag composition mostly varies between the yellow (fully liquid) and light blue (liquid plus C₂S-C₃P) regions. The ranges marked in the diagram are discussed in further detail in the paper [Khadhraoui2018].

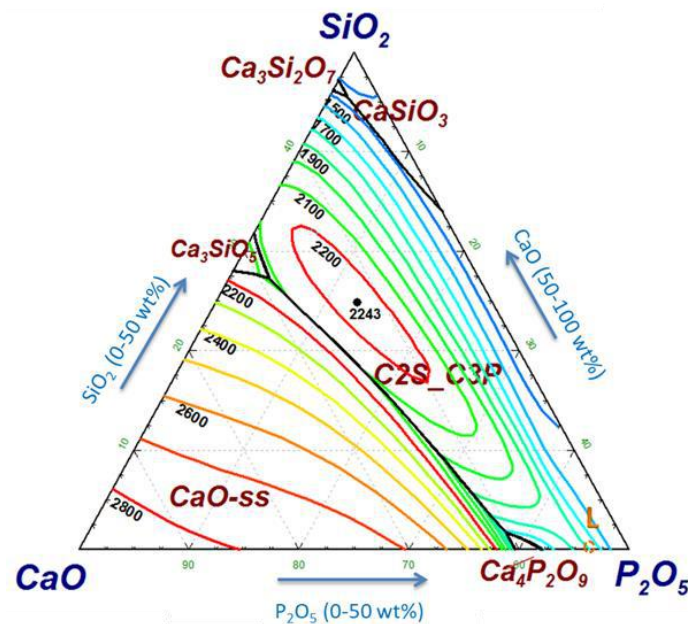


Figure 7: The CaO-rich corner of the CaO-P₂O₅-SiO₂ system. Note the primary precipitation range of the C₂S-C₃P phase.

Figure 7 shows the liquidus surface in the CaO-rich corner of the CaO-P₂O₅-SiO₂ system. It becomes obvious that the very complex pseudo-binary solution phase between the compositions 2CaO·SiO₂ and 3CaO·P₂O₅ called C₂S-C₃P is very stable with a congruent melting point at 2243 K. In the BOF process, this behavior leads to the above-mentioned heterogeneous slags, i.e. slags containing both solid and liquid phase contributions. The partitioning of phosphorous between the heterogeneous slag and the steel bath is heavily affected by the presence of the solid silicate phosphate. Using GT_{Ox} as the basis of a BOF model enables consideration of this complex interdependence.

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Refractory applications

To improve the lifetime of refractory materials, the potential corrosion by slags needs to be minimized. For this purpose, a counter-cross calculation for the refractory/slag interface is often used [Udagawa1993] [Carlborg2018]. In such a calculation two well specified end compositions are treated like two “components” of a pseudo-binary system. The overall composition of the system is given by the fraction of one of the end compositions. This fraction is changed from 0 to 1 and the resulting equilibrium phase distribution is generated (see below).

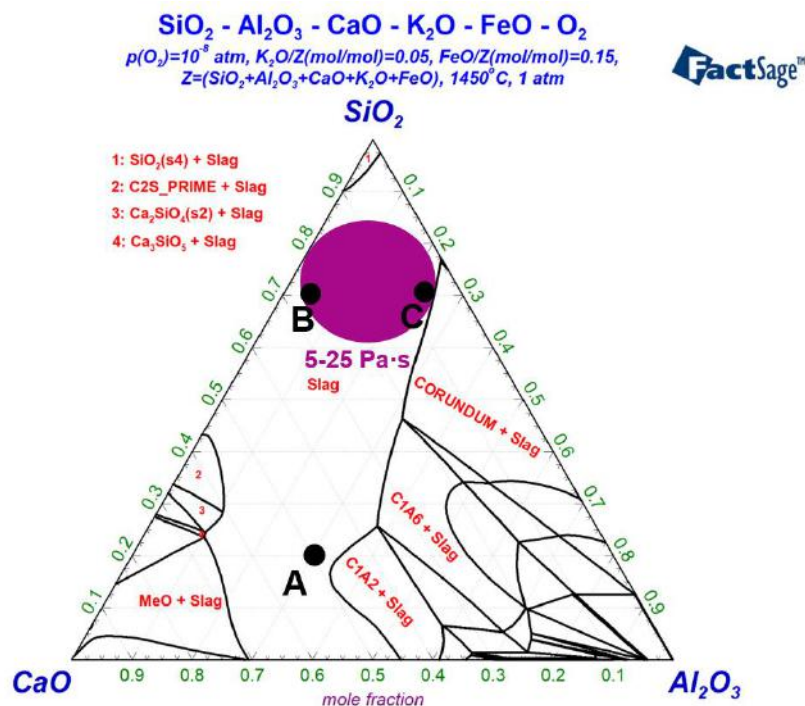


Figure 8: Phase diagram of the system SiO₂-Al₂O₃-CaO-K₂O-FeO at 1450 °C and reducing atmosphere with indicated target viscosity range of 5-25 Pa·s.

The phase diagram of a typical gasifier slag system SiO₂-Al₂O₃-CaO-K₂O-FeO at 1450 °C and under a reducing atmosphere is shown in Figure 8. As an example, a counter-cross reaction between an Al₂O₃-based refractory material (for simplicity pure alumina is used) and a slag A is illustrated in Figure 9. Although the refractory can react with the slag A, the formation of three solid solution phases, i.e. CaO·6Al₂O₃, Kaliophilite-HT, and CaO·2Al₂O₃ results in the formation of a protective layer on the surface of the refractory. It should be mentioned that in a counter-cross calculation the diffusion rate of each species in both slag and refractory phases is assumed to be the same.

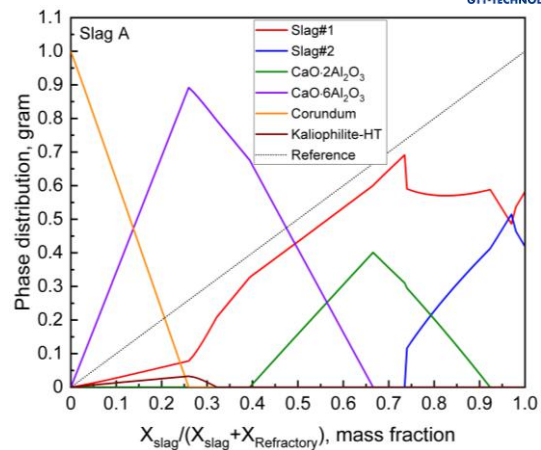


Figure 9: Potential reactions between refractory and slag using a counter-cross calculation.

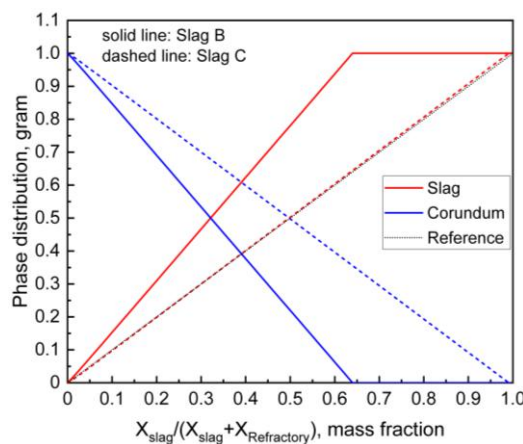


Figure 10: Comparison of the corroding effect of two slags B and C on an Al_2O_3 -based refractory material.

Under the constraint that the viscosity range for slags in entrained flow gasifiers is recommended to be in the range of 5 - 25 Pa·s, the corrosion of the two slag candidates B and C on the Al_2O_3 -based refractory material is compared, as shown in Figure 10. Compared to the dotted line as reference (i.e. without any reaction between the slag and the refractory material), an obvious increase in slag mass is noticed for the slag B, which indicates the dissolution of the refractory material into the slag. It will cause a decrease in lifetime of the refractory material. An adjustment of the slag composition from slag B to C can almost eliminate the dissolution.

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Distribution of Vanadium

Vanadium oxides were added to the GTTox database because of their important role in ferro-titanium metallurgy as well as in petroleum coke gasification. With the knowledge about the complex behavior of vanadium in slags as well as in liquid metal alloys it is possible to calculate the vanadium distribution ratios $(V)/[V]$, called L_v , between iron melts and slags in a wide range of temperatures and compositions, corroborating the validity of the model under reducing conditions. An example is shown in Figure 11.

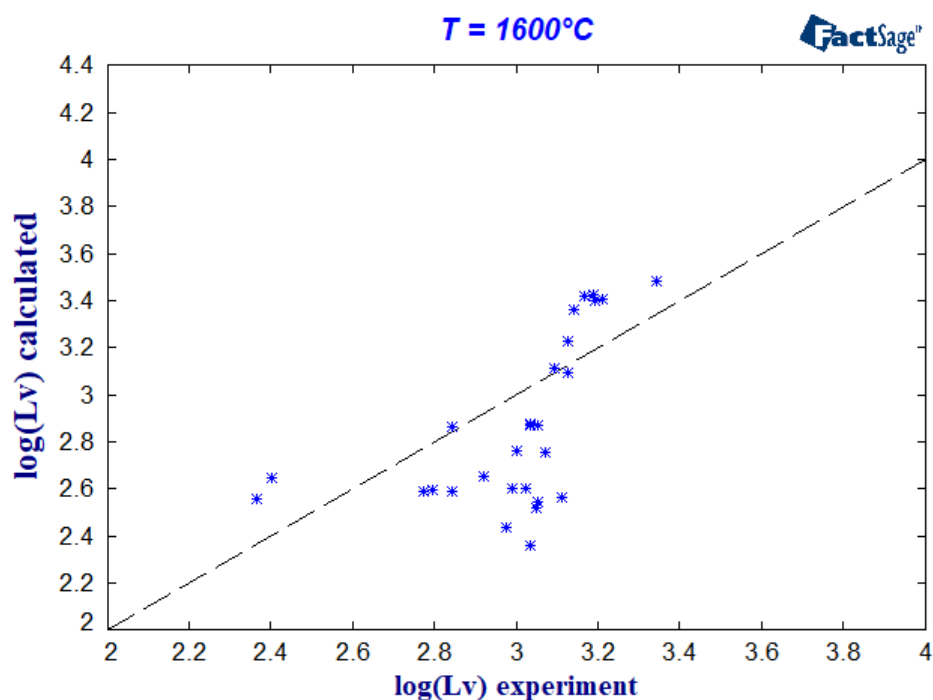


Figure 11: Relationship between the calculated and experimentally determined vanadium distribution at 1600 °C [Inoue1982].

The additionally developed viscosity model shows good agreement between the calculated and experimental values in vanadium-containing slags. More details can be found in the publication by Jantzen et al. [Jantzen2021].

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Slag formation, fouling, and condensation from coal/biomass/waste gasification and combustion

During gasification and combustion, the majority of the inorganic species are converted to slag, whereas other inorganic species behave as fly ash entrained in the syngas or flue gas. To understand the slag formation process, ash fusion temperatures (AFTs) are often used in practice. Thermochemical calculations provide insight on AFTs of different fuel ashes with respect to temperature, composition, and atmosphere. Three ash samples from the literature were taken as examples, their compositions and flow temperatures are given in Table 1.

Sample	Composition of ashes, wt%								AFT, °C
	SiO ₂	Al ₂ O ₃	CaO	MgO	Na ₂ O	Fe ₂ O ₃	TiO ₂	SO ₃	
Ash 1	30.7	27.8	9.21	1.06	0.42	20.6	0.82	8.04	1340
Ash 2	41.5	36.5	7.12	0.56	0.18	8.32	1.33	2.67	1465
Ash 3	44.8	36.3	5.49	0.85	0.34	4.96	1.98	2.9	1520

Table 1: Composition and ash fusion temperatures (AFT) of three selected ash samples [Wang2021].

The phase distribution of Ash 1 as function of temperature significantly differs for different atmospheres, as shown in Figure 12, where the reducing atmosphere is defined as a gas mixture of 60%CO-40%CO₂ while the oxidizing atmosphere is a gas mixture of 21%O₂-79%N₂, i.e. air.

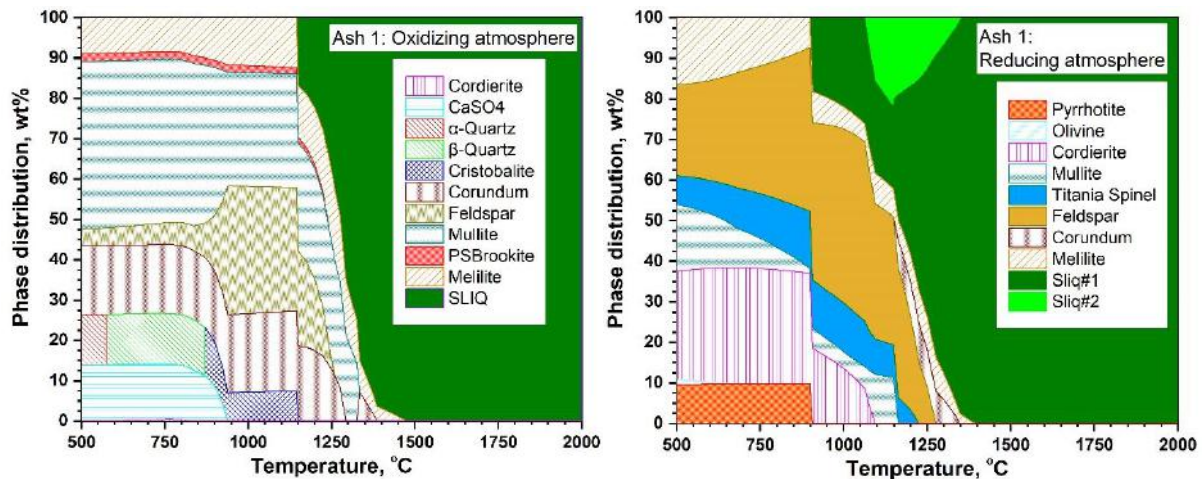


Figure 12: Phase distribution of Ash 1 at oxidizing (left) and reducing (right) atmosphere.

Comparing the experimentally measured AFT of Ash 1 of 1340 °C (see Table 1) with the temperature at which the ash is fully liquid under reducing conditions (1375 °C) in Figure 12 (left) it can be seen that the liquidus temperature is an excellent predictor for the experimentally measured flow temperature.

The mass fraction of a slag (between solidus and liquidus temperature) can also be used to evaluate the fouling behavior of fly ashes on surfaces of the downstream units of a gasifier or combustion chamber, and the description is reported elsewhere in detail [Kleinhans2018]. In addition to fly ash, trace elements released from fuels will also condense on these surfaces. The condensation mechanism of Zn vapor, taken as an example, can be illustrated using the Scheil-Gulliver cooling model [Zhao2021]. Figure 14 implies a supercooling of the condensate ZnO (a pure solid phase). The difference between the experimental and calculated ZnCl₂ condensate has been discussed in detail elsewhere [Zhao2021].

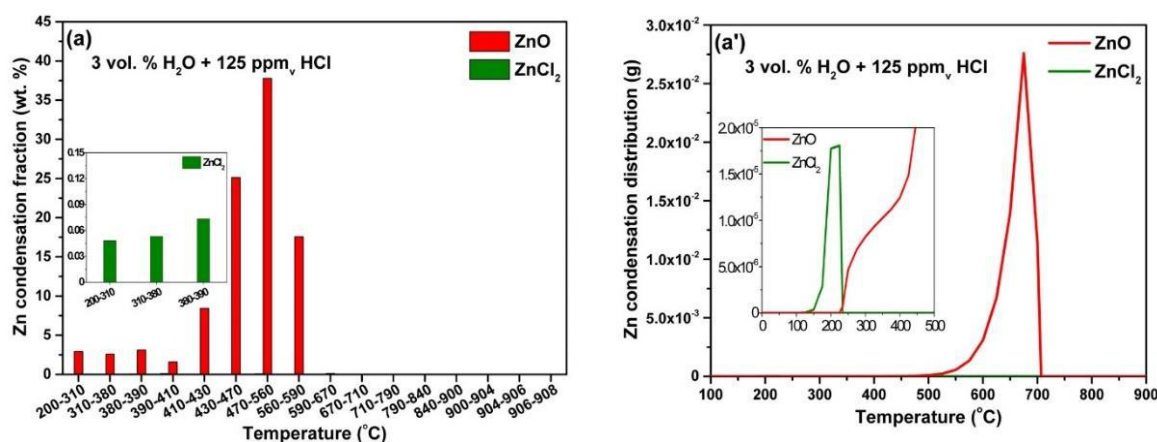


Figure 13: (a) IC and ICP-OES measurements for zinc-containing species under atmosphere containing HCl with 3 vol% steam compared to (a') the predictions with FactSage using the Scheil-Gulliver cooling model [Zhao2021] (Reprinted with permission by Elsevier).

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Optimization of slag mobility in entrained flow gasifiers

In order to achieve smooth slag flow and tapping during the operation of entrained flow slagging gasifiers, a viscosity range $\ln(\eta, \text{Pa}\cdot\text{s})$ of 1.6–3.2 at 1400–1550 °C is desirable. Typically, blended feedstocks with the addition of fluxing agents are used to adjust the slag viscosity. As shown in Figure 14(a), the viscosity of the model gasifier slags (for the composition see Table 2), taken as examples, is outside of the desirable viscosity range.

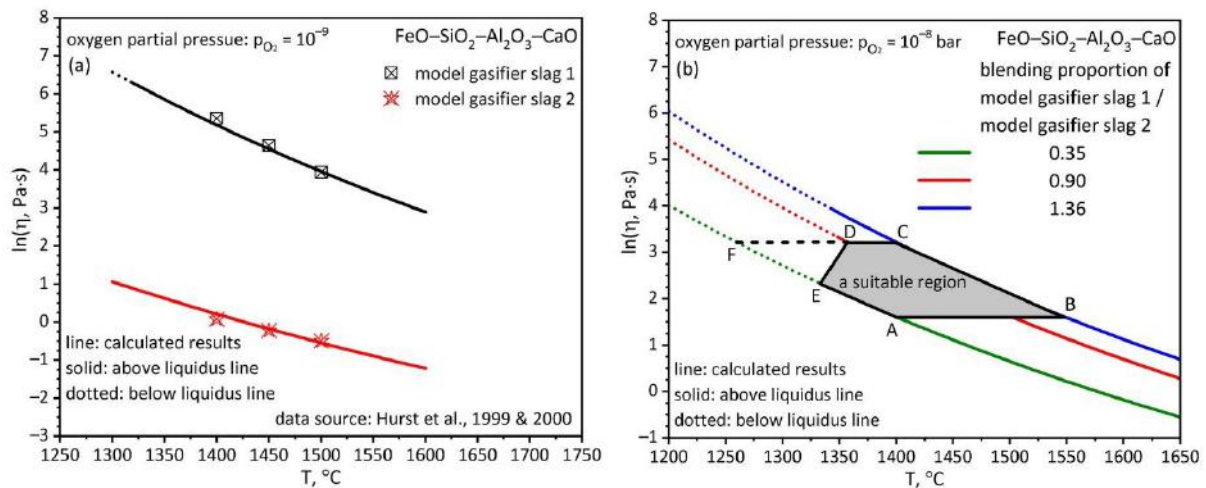


Figure 14: (a) Viscosity predictions compared to the experimental data [Hurst1999] [Hurst2000] of model gasifier slags at an oxygen partial pressure of 10^{-9} bar, (b) Selection of a suitable blending proportion of slags [Wu2021] (Reprinted with permission by Elsevier).

Model gasifier slag	Composition, mol%				$T_{\text{liquidus}}, ^\circ\text{C}$
	SiO ₂	Al ₂ O ₃	CaO	FeO	
1	68.61	13.84	12.59	4.96	1318
2	42.55	11.42	33.18	12.86	1245

Table 2: Composition of the model gasifier slags in Figure 14 [Wu2019] (Reprinted with permission by Elsevier).

Figure 14(b) demonstrates desirable blending proportions of the selected slags as determined by the present viscosity model, where the oxygen partial pressure is assumed to be 10^{-8} bar, corresponding to a typical value during the operation of an entrained flow slagging gasifier. As a result, the gray area ABCDE in the figure indicates a suitable region of blending selected slags in combination with the liquidus information, i.e. the point E refers to a melting temperature of 1333 °C. It can be seen that the operating temperature can vary from 1333 °C to 1548 °C, and the blending proportion can vary from 0.35 to 1.36, where the blending proportion of 0.9 should result in an optimum viscosity of 15 Pa·s (i.e. $\ln(\eta, \text{Pa}\cdot\text{s})$ of 2.7) at 1400 °C. Information regarding fluctuations of the operating temperature, slag composition, and atmosphere

can be used to further determine an optimum blending proportion. For the determination of blending proportions of three or more slags, please see [Wu2019].

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Assessment examples

In this section, a selected number of cases for characteristic thermodynamic assessments which form part of the GTT database is presented.

ZnO-P₂O₅

Available experimental data was used for the generation of thermodynamic data for the system ZnO-P₂O₅. The model of non-ideal associated solutions was used to describe the liquid phase containing the following associates: ZnO·P₂O₅, 2ZnO·P₂O₅ and 3ZnO·P₂O₅. Seven literature sources concerning phase equilibria and five references dealing with the internal structure of the liquid phase have been used to generate a consistent thermodynamic dataset for the system. Figure 15 shows the phase diagram and Figure 16 the phase-internal species distribution in the liquid phase as function of the mole fraction of ZnO calculated with the Gibbs energy dataset. Calculated associate species distribution in the liquid phase ZnO-P₂O₅ at 1000 °C is compared with available experimental data (NMR, EMF, Raman). The calculation is done for the middle temperature of the experimental ones which cover 900 °C, 1000 °C and 1100 °C. The calculated results show a very good representation for all temperatures. Also the agreement between experimental and calculated phase boundaries in Figure 16 is very good.

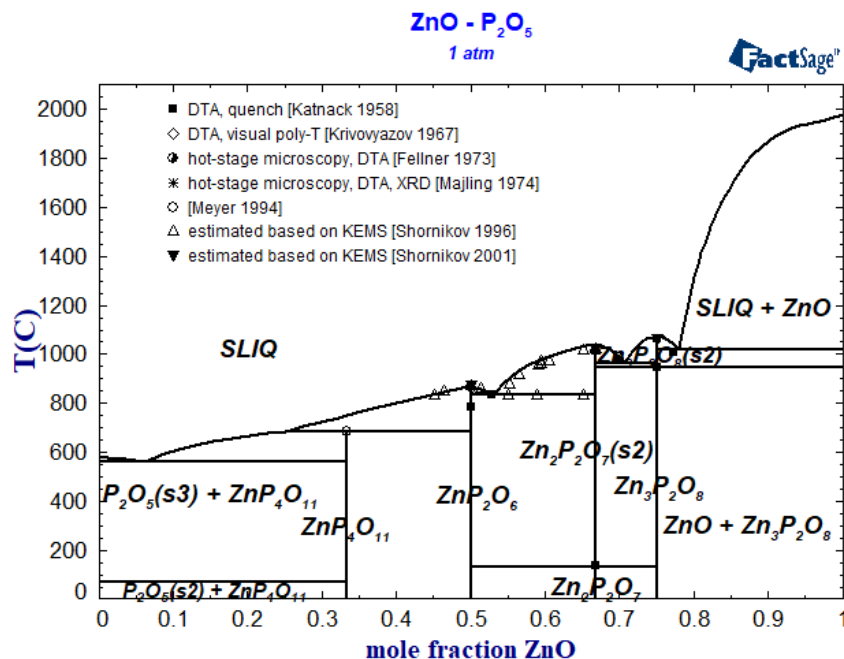


Figure 15: Calculated phase diagram of the system P₂O₅-ZnO compared with experimental data.

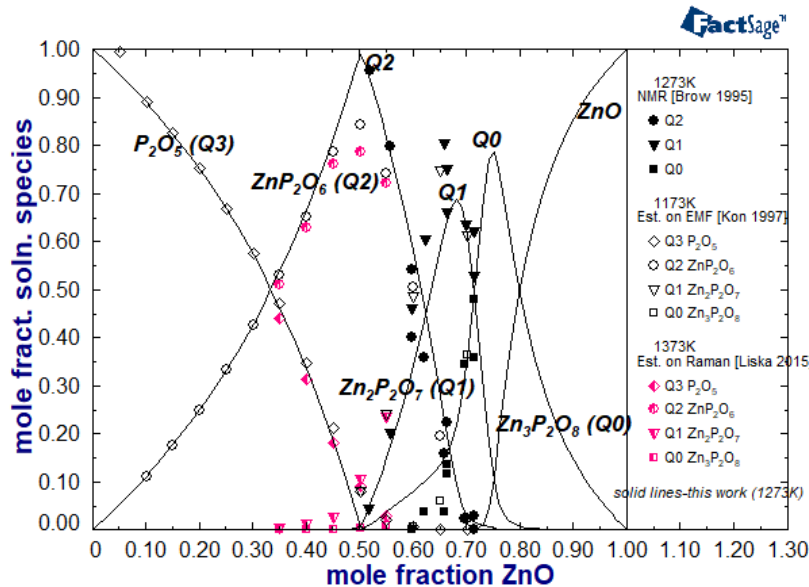


Figure 16: Calculated associate species distribution in the liquid phase P_2O_5 -ZnO at 1000 °C compared with experimental data (NMR, Raman).

The experimentally observed structural units are considered as liquid constituents in the framework of the modified non-ideal associate species model. This fact indicates that the modified non-ideal associate species model is appropriate for the prediction of the structural features in the liquid phase with a direct link to, for example, the viscosity of the melt published by Wu et al. [Wu2019].

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CaO-ZnO-P₂O₅

The following ternary phases are included in the present database along with the Slag phase: the solid solutions based on Ca₃P₂O₈ (C3P-C2S, HT; C3P-alpha, MT; C3P-beta, LT) and on Zn₃P₂O₈ (Z3P-beta, HT; Z3P- alpha, LT) as well as the intermediate solid solution based on CaZn₂P₂O₈-HT (CZ2P-HT) according to [Kreidler1967, Carbajal2011]. The phase boundaries reported in these two sources have been used to optimize the parameters of the liquid phase as well as the various solid phases. The resulting phase diagrams are shown in Figure 17 and Figure 18. It should be noted in particular that the system has been considered as fully water-free. Thus, the phase Ca₄P₂O₉ appears in the diagrams instead of HAp (HAp=hydroxyapatite Ca₁₀(PO₄)₆(OH)₂), which is observed experimentally due to water impurities.

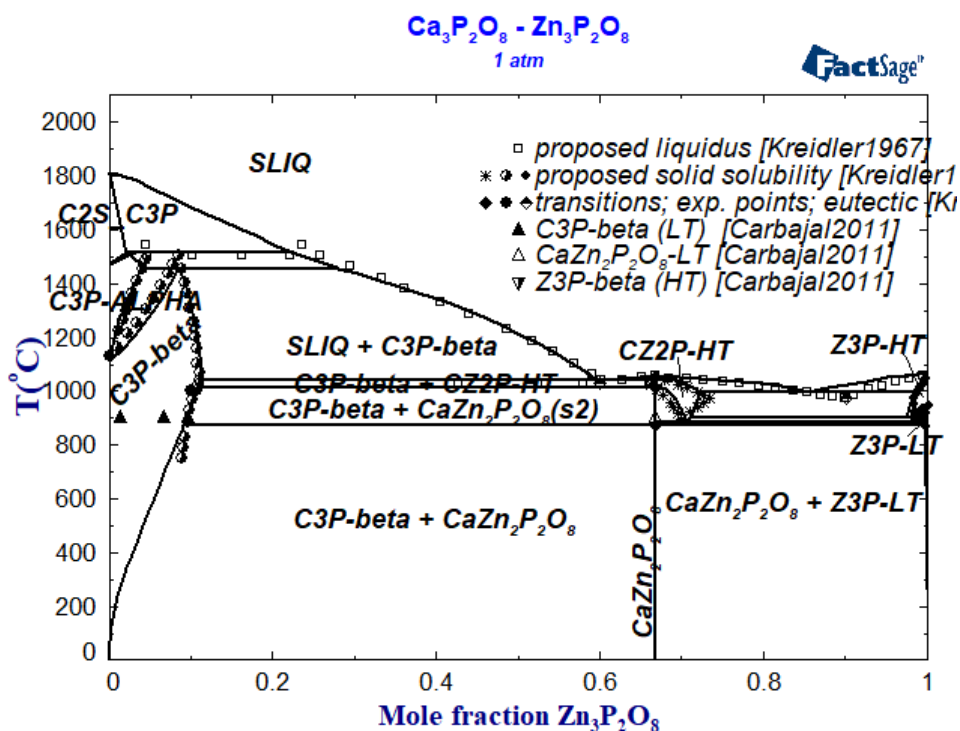


Figure 17: Calculated phase diagram of the system Ca₃P₂O₈-Zn₃P₂O₈ compared with experimental data [Kreidler1967, Carbajal2011].

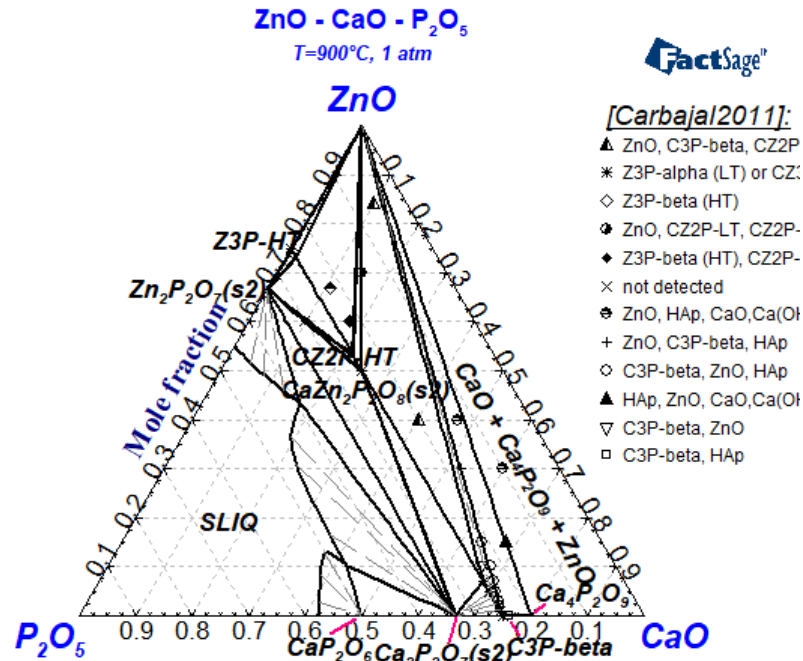


Figure 18: Calculated isothermal section at 900 °C in the ternary system CaO-P₂O₅-ZnO compared with experimental data [Carbajal2011].

References

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Al₂O₃-Li₂O-MgO

MgAl₂O₄ and LiAl₅O₈ (or Li_{0.5}Al_{0.5}Al₂O₄) form a complete spinel solid solution in the Li₂O-MgO-Al₂O₃ system [Menzheres1978, Izquierdo1980]. Spinel is an oxide of the general type A^TB^O₂O₄ which has a very compact oxygen structure, with cations in tetrahedral (T) and octahedral (O) oxygen coordination. Simple examples are MeO·Me₂O₃ which can be described with the formula (Me²⁺)(Me³⁺)₂(O²⁻)₄, where the divalent cations occupy the tetrahedral and the trivalent cations the octahedral sublattice sites. This makes it more obvious that the valence state of the metals plays an important part for the existence of this phase. MgAl₂O₄ has a normal spinel structure where Mg²⁺ is mostly placed on tetrahedral sites and Al³⁺ occupies octahedral sites. In the opposite system, Li_{0.5}Al_{2.5}O₄ has an inverse spinel structure where Al³⁺ combined with Li¹⁺ are located on the octahedral sublattice, and Al³⁺ occupies the tetrahedral sublattice. Using a combined cationic species on the tetrahedral sublattice (Li_{0.5}Al_{0.5}²⁺) deals with the charge compensation between the monovalent and the trivalent ion. The isothermal section for 1400 °C in the Al₂O₃-Li₂O-MgO system is presented in Figure 19 where MgAl₂O₄ and LiAl₅O₈ form a complete solid solution.

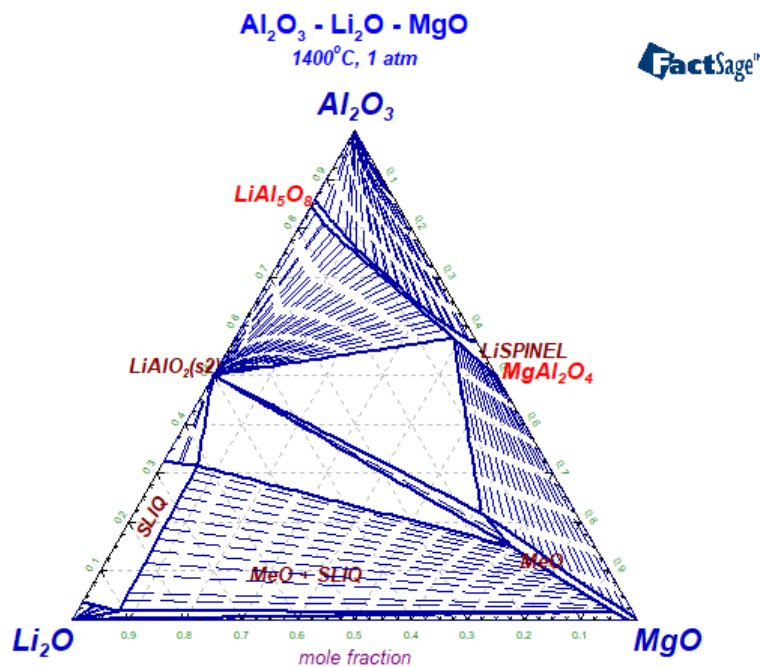


Figure 19: Isothermal section at 1400 °C in the Al₂O₃-Li₂O-MgO system.

References

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Viscosity modelling

Model parameters for the viscosity of oxide melts have been assessed, where available, by using the experimental data for pure oxides and selected binary and ternary systems. Great care has been taken in order to cover the well-known experimental facts by the modelling. These are: the lubricant effect, the weak lubricant effect, and the charge compensation effect. The following series of diagrams (Figure 20) shows the successful use of the model for all these characteristic features.

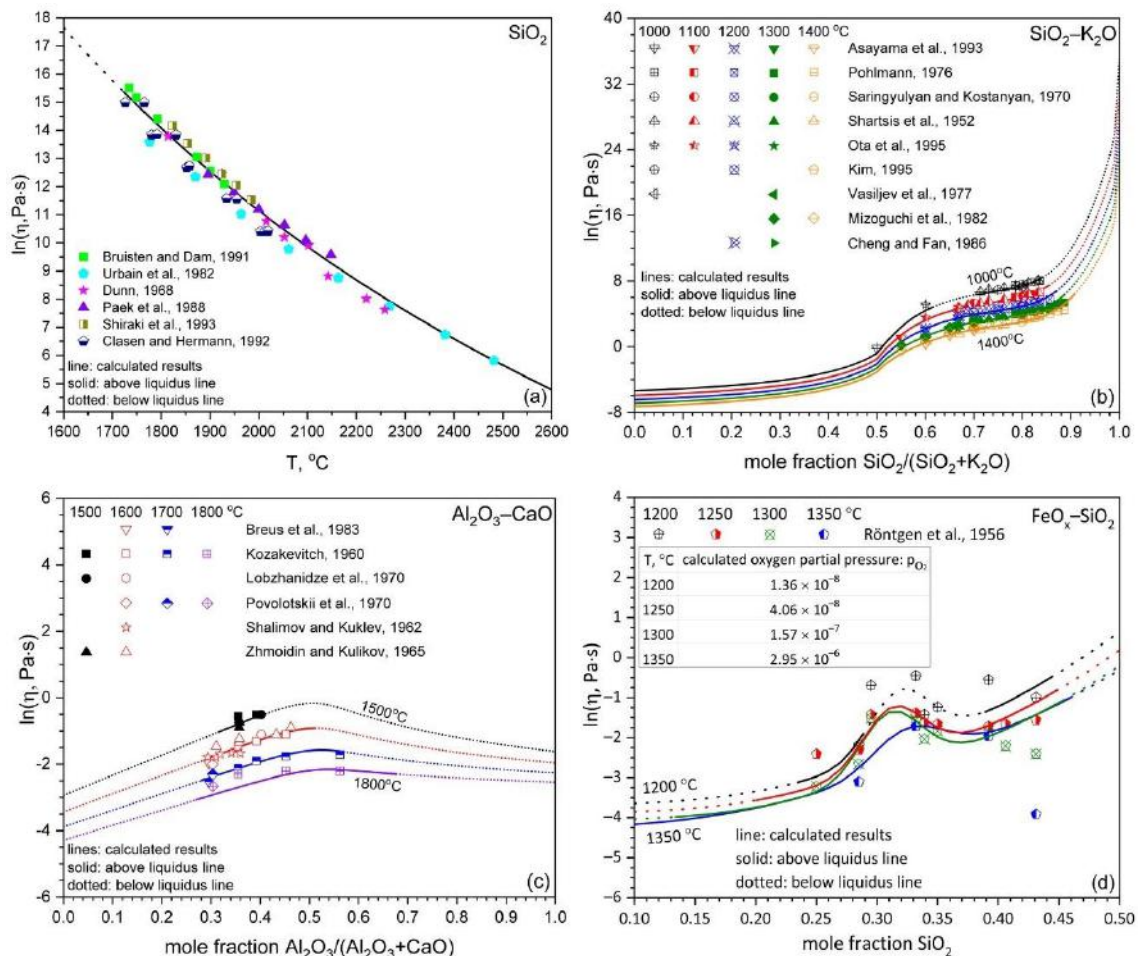


Figure 20: Comparison between experimental data and calculated data for the selected oxide melts SiO_2 (a), $\text{SiO}_2\text{-K}_2\text{O}$ (b), $\text{Al}_2\text{O}_3\text{-CaO}$ (c), and $\text{FeO}_x\text{-SiO}_2$ (d) [Wu2015,Part1] [Wu2018] (Reprint with permission by Elsevier).

For molten silica, the viscosity of more than 5 MPa·s ($\ln(\eta, \text{Pa}\cdot\text{s}) \approx 15.5$) approaching the melting temperature is well reproduced by the present model, as shown in Figure 20(a). It is seen from Figure 20(b) that the viscosity decreases drastically when a small amount of a network modifier, here K_2O , is added into the pure silica melt, where the network modifier plays the role of a lubricant allowing silica clusters to glide more easily alongside each other ("*lubricant effect*"). Another clearly

noticeable but less strong decrease of the viscosity occurs around the SiO_2 content of 0.55 mole fraction (“*weak lubricant effect*”) due to possible ring structures. The present model can very well describe both these effects.

The present model also reproduces the viscosity maximum due to the “*charge compensation*” of Al_2O_3 with CaO , as shown in Figure 20(c). The influence of the oxygen partial pressure on the viscosity behavior of systems containing multivalent iron oxide has also been considered. It is seen from Figure 20 (d) that a local viscosity maximum around the fayalite composition occurring in the binary system FeO - SiO_2 is described by the present model, where the position of the local viscosity maximum and its order of magnitude vary with temperature and oxygen partial pressure.

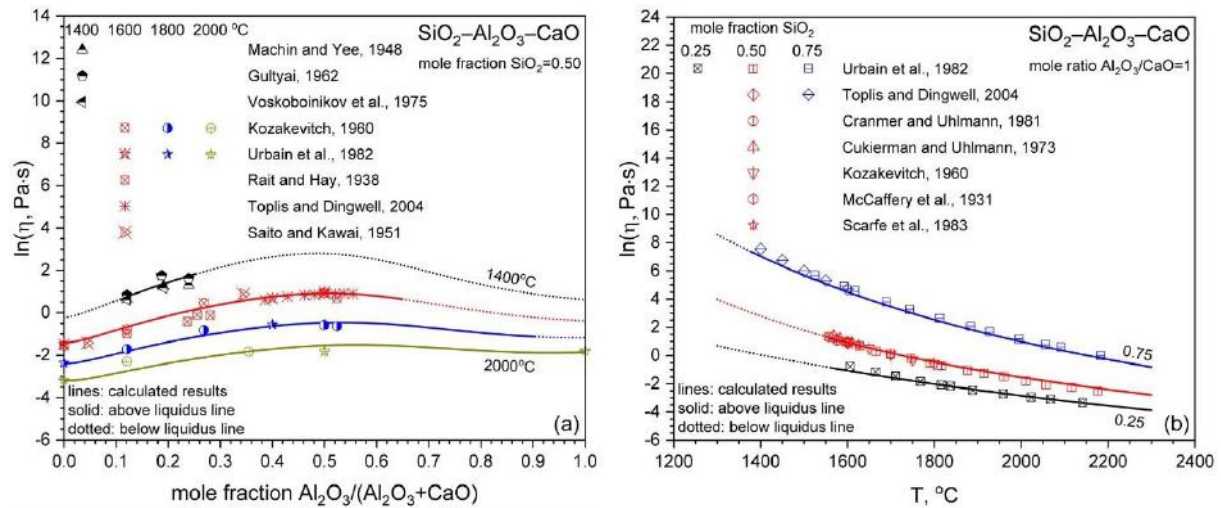


Figure 21: Comparison between experimental data and calculated data for the system SiO_2 - Al_2O_3 - CaO [Wu2015,Part2] (Reprinted with permission by Elsevier).

The extension of the model from low-order systems to high-order systems has been evaluated, as reported in detail elsewhere [Wu2015,Part2] [Wu2019] [Hack2019]. Figure 21 shows an example regarding the viscosity behavior induced by the charge compensation effect in the ternary system SiO_2 - Al_2O_3 - CaO . As shown in Figure 21(a), the viscosity maximum is well described by the present model around the fully charge-compensated composition, which is CaAl_2O_4 . The present model reproduces the order of magnitude of the viscosity maximum with increasing SiO_2 content. At the fully charge-compensated composition, the trend of the viscosity with temperature, as shown in Figure 21(b), has also been well predicted. This indicates a good quality regarding the assessment of model parameters.

It is worth noting that the values of the model parameters are not just fitting parameters determined by minimization of the difference between experimental data and model calculations. They have a clear-cut physical meaning, i.e. for each structural unit they represent the activation energy for viscous flow which increases as the ability of network formation rises. In addition, viscosities extrapolated to regions where no experimental data are available in literature have also been checked for reasonable behavior.

References

- [Wu2015,Part1] Guixuan Wu, Elena Yazhenskikh, Klaus Hack, Erwin Wosch, Michael Müller, Viscosity Model for Oxide Melts Relevant to Fuel Slags. Part 1: Pure Oxides and Binary Systems in the System $\text{SiO}_2\text{--Al}_2\text{O}_3\text{--CaO--MgO--Na}_2\text{O--K}_2\text{O}$, Fuel Processing Technology 137 (2015) 93–103.
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- [Wu2015,Part2] Guixuan Wu, Elena Yazhenskikh, Klaus Hack, Michael Müller, Viscosity Model for Oxide Melts Relevant to Fuel Slags. Part 2: The System $\text{SiO}_2\text{--Al}_2\text{O}_3\text{--CaO--MgO--Na}_2\text{O--K}_2\text{O}$, Fuel Processing Technology 138 (2015) 520–533.
- [Wu2019] Guixuan Wu, Sören Seebold, Elena Yazhenskikh, Joanne Tanner, Klaus Hack, Michael Müller, Slag mobility in entrained flow gasifiers optimized using a new reliable viscosity model of iron oxide containing multicomponent melts, Applied Energy 236 (2019) 837–849.
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Density modelling

The model parameters have been assessed using the existing experimental data for pure oxides as well as binary and ternary subsystems. Due to a limited availability of experimental density data for pure oxides, the calculated densities by Ghiorso and Kress [Ghiorso2004] are used to derive the model parameters regarding the partial molar volume and partial molar thermal expansion.

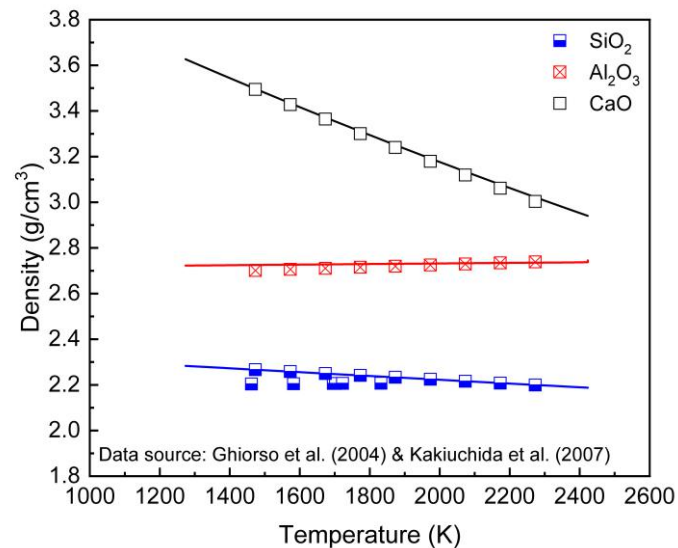


Figure 22: Comparison between the existing data [Ghiorso2004] [Kakiuchida2007] and model predictions for SiO₂, Al₂O₃ and CaO.

As shown in Figure 23, for SiO₂ and CaO the density usually decreases as temperature increases. However, the figure also shows that the density of Al₂O₃ increases slightly with increasing temperature. This unusual effect may be caused by the structural evolution of OAl₃ triclusters. As temperature increases, the stability of these triclusters decreases and the oxygen coordination number increases, which leads to a decrease in the molar volume of Al₂O₃. This structural variation with respect to the temperature requires a negative partial molar thermal expansivity of Al₂O₃.

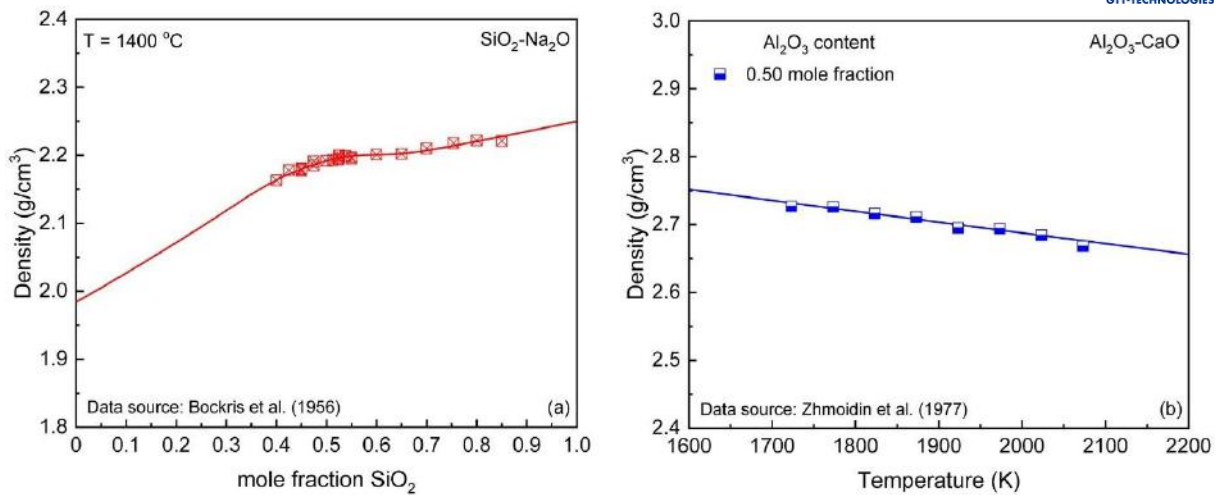


Figure 23: Comparison between the existing data [Bockris1956] [Zhmoldin1977] and model predictions for the binary systems SiO₂-Na₂O (a) and Al₂O₃-CaO (b).

The experimental data of the binary system SiO₂-Na₂O are well reproduced by the present model, as shown in Figure 23(a), where a small hump in density occurs probably due to the formation of a ring structure. Figure 23(b) shows that the model predictions are in good agreement with the experimental data of the binary system Al₂O₃-CaO. It is seen that the density decreases with increasing temperature, where Al₂O₃ plays a different structural role compared to that in a pure Al₂O₃ melt, because Al₂O₃ is almost fully compensated by CaO, and the quasi-tetrahedron CaAl₂O₄, rather than the OAl₃ tricluster, is dominant.

When the model is extended to the ternary system SiO₂-Al₂O₃-CaO, the model predictions are consistent with the experimental density data, as shown in Figure 24. This indicates that the structural dependence of density has been well described by the present model regarding the Al₂O₃-induced charge compensation effect.

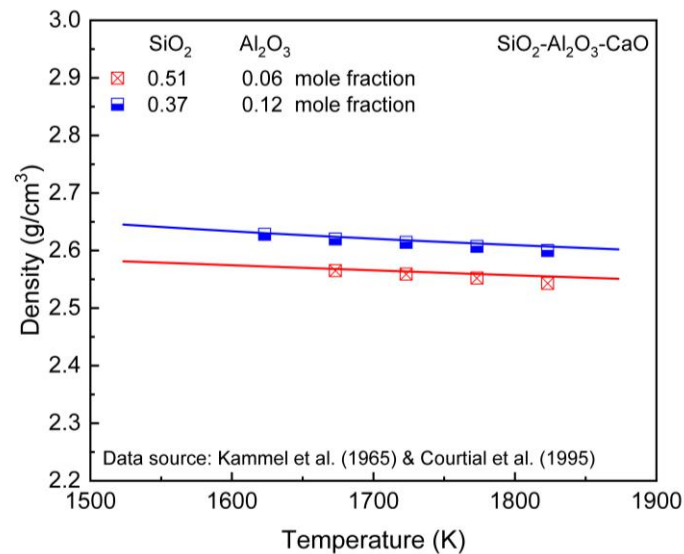


Figure 24: Comparison between the existing data [Kammel1965] [Courtial1995] and model predictions for the ternary system SiO₂-Al₂O₃-CaO.

References

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Database compatibility

GTOx version 18 can be used alone or together with many other databases available in FactSage:

- SGPS (complex gas phases or first-order approximation for any other substance)
- FactPS (complex gas phases or first-order approximation for any other substance) (slightly lower compatibility than with SGPS)
- aiMP / aiOQ (zeroth-order approximation for any other substances, lower compatibility but much larger material system covered)
- FSstel (steels, several superalloys)
- SpMCBN (non-oxide ceramics and refractory alloys)
- FTlite (light metals)
- FScopp (copper alloys)
- FSlead (lead alloys)
- SGTE solutions (general metal alloys, but data coverage for specific alloys is lower compared to the specialized databases indicated above)

Note: For any combinations that include FSstel, SpMCBN, FTlite, FScopp, FSlead, or SGTE Solutions, our recommendation is to utilize the liquid phase of that database and remove all pure metal endmembers from the SLIQ phase in GTOx using the " * - custom select end-members " option. Metallic solid solutions should be taken only from the respective alternative databases, not from GTOx. Please be aware that oxygen solubilities in liquid metal and solubilities of metallic components in the liquid Slag phase cannot be calculated with this approach.

We will be happy to assist you in the selection of databases, please [contact us](#) if you have any questions!

Phases

Unified Liquid phase (SLiq)

In contrast to all previous versions of the GTOx database the present version contains thermodynamic data for only one liquid phase. The reason for that is given by the fact that in real world systems there are many cases in which it is possible to change composition continuously from a liquid metal state to a molten oxide (Fe-O or Cu-O) or from a molten oxide to a matte (molten sulfide) (Cu-O-S). Even the transition from a molten silicate to a sulphatic melt can be found in reality (Mg₂SiO₄-MgSO₄). It was thus decided to integrate the separated liquids Slag, Sulphate and Metal, which have been so far part of the GTOx database, into one liquid. This is called “**SLiq**” indicating by the name that there is a **Single Liquid** covering all possible liquid states with one dataset. It is obvious that for proper use of the SLiq phase the I- or even the J-option must be used in order to include the possible miscibility gaps into the calculations. For a detailed discussion of the new approach see the chapter “[What's new in version 18](#)” below. The SLiq phase contains data for the following components:

Oxides	Al₂O₃-CaO-CO₂-Cr₂O₃-CuO-Cu₂O-FeO-Fe₂O₃-Li₂O-MgO-MnO-Mn₂O₃-K₂O-Na₂O-NiO-P₂O₅-SO₃-SiO₂-SrO-TiO₂-Ti₂O₃-V₂O₃-V₂O₅-ZnO
Metals	Al, Ca, Cr, Cu, Fe, Li, Mg, Mn, K, Na, Ni, Si, Sr, Ti, V, Zn + C, P, S, O
Phosphates	of the metals Ca, Cu, Fe, Mg, Mn, Sr, Zn
Sulfides	of the metals Al, Ca, Cr, Cu, Fe, Li, Mg, Mn, K, Na, Ni, Si, Sr, Ti, Zn
Sulfates	of the metals Ca, K, Mg, Na, Ni and Pyrosulfates of the metals K, Na
Carbonates	of the metals Ca, K, Mg, Na
Chlorides	of the metals Ca, K, Mg, Na
Fluorides	of the metals Al, Ca, Mg

With the new set of constituents it is possible to calculate even binary metal-oxygen or metal-sulphur systems. All phase diagrams are available in a separate PDF document which is provided by GTT on request.

Solid solution phases

The GTOx database contains **166 solid solution phases**. The complete list including a short description for each phase can be provided upon request.

Solid stoichiometric compounds

The GTOx database includes **901 stoichiometric compounds**. The complete list can be provided upon request.

References

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- [Wu2018] Wu G., Seebold S., Yazhenskikh E., Hack K., Müller M. Viscosity model for oxide melts relevant to fuel slags. Part 3: The iron oxide containing low order systems in the system $\text{SiO}_2\text{--Al}_2\text{O}_3\text{--CaO--MgO--Na}_2\text{O--K}_2\text{O--FeO--Fe}_2\text{O}_3$, Fuel Processing Technology 171 (2018), 339–349.
- [Jantzen2017] T. Jantzen, K. Hack, E. Yazhenskikh, M. Müller, Evaluation of thermodynamic data and phase equilibria in the system Ca–Cr–Cu–Fe–Mg–Mn–S part I: Binary and quasi-binary subsystems, Calphad 56 (2017) 270-285.
- [Jantzen2017-2] T. Jantzen, K. Hack, E. Yazhenskikh, M. Müller, Evaluation of thermodynamic data and phase equilibria in the system Ca–Cr–Cu–Fe–Mg–Mn–S Part II: Ternary and quasi-ternary subsystems, Calphad 56 (2017) 286-302.

What is new in version 18?

The current update is important for two major reasons:

- Unification of the data for the liquid phase
- Addition of new and reassessed subsystems

Unification of the data for the liquid phase

The following diagrams illustrate the need for a unified thermodynamic treatment of the liquid state. Figure 25 (below) shows that the miscibility gap in the Fe-O system closes at higher temperatures and this requires a single liquid to be described.

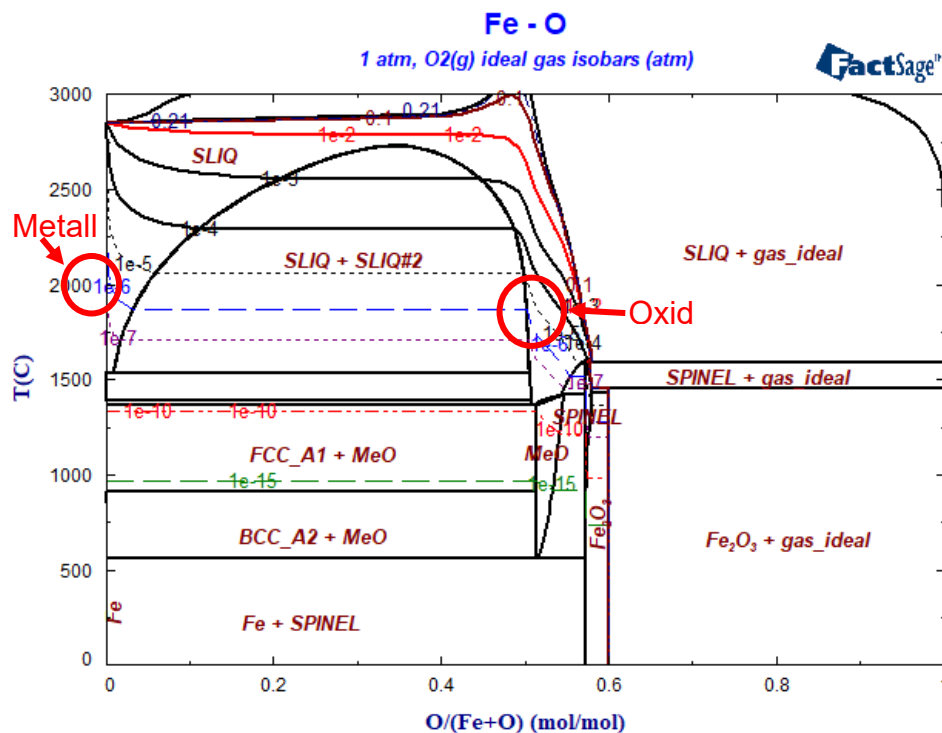


Figure 25: The Fe-O-Phase diagram.

Figure 26 shows by way of the isothermal section of the Fe-O-S system that there is need for a unified description of a liquid state which covers metallic, oxidic as well as sulphidic compositions. There is a miscibility gap on the Fe-O edge which penetrates into the ternary while on the Fe-S edge a metallic liquid begins in the Fe-rich corner and protrudes into the Fe-S binary. On the other hand it is possible to combine molten "FeS" with molten "FeO" without any demixing.

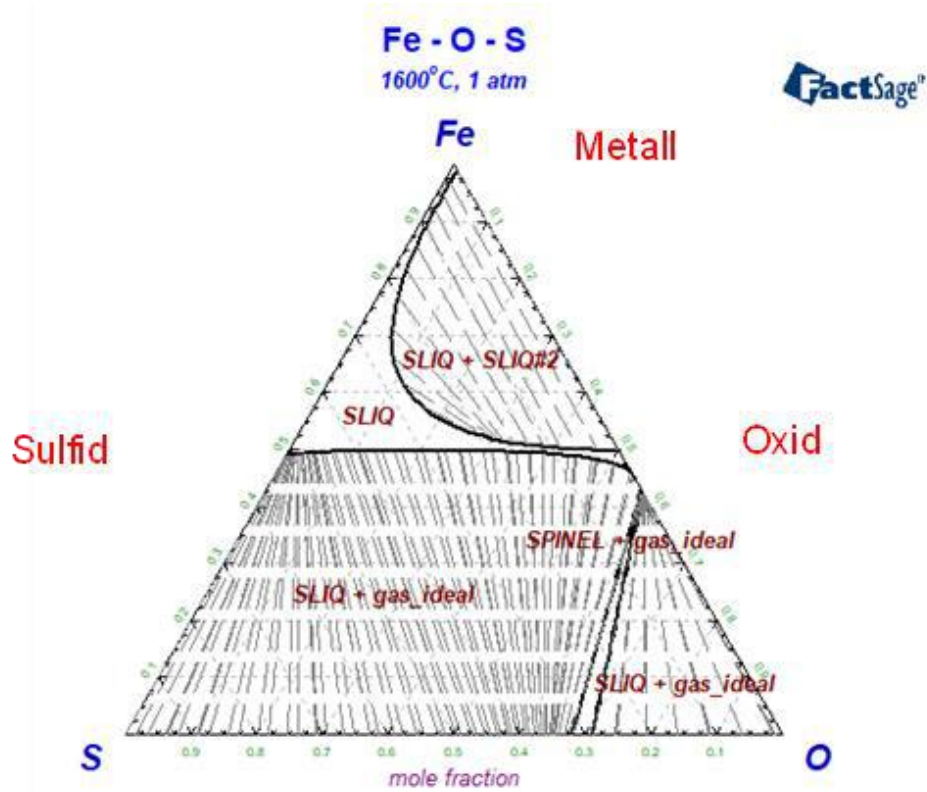


Figure 26: The isothermal section through the system Fe-O-S at $T=1600^{\circ}\text{C}$.

Figure 27 depicts the continuous transition from a sulphate to a sulfide melt for the system $\text{K}_2\text{S}-\text{K}_2\text{SO}_4$.

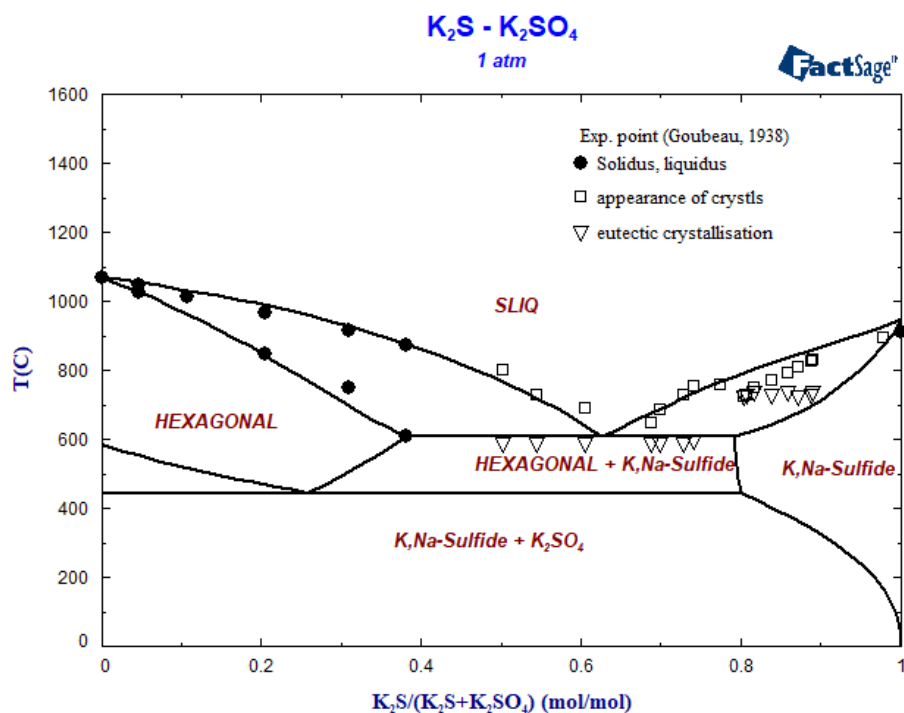


Figure 27: Phase diagram for the system $\text{K}_2\text{S}-\text{K}_2\text{SO}_4$.

In addition to the three phase diagrams shown above, which have all been calculated with the new dataset “SLiQ” for the unified liquid phase, below are given some further highlights of the successful unification of the data for the generalized liquid phase.

Figure 28 shows the Fe-rich corner of the Fe-Cr-O system at $T=1600^\circ\text{C}$. It is worth noticing that the melt from which the different Cr_2O_3 -based solids precipitate is molten iron with small amounts of dissolved oxygen as well as chromium. Molten “slag” is not involved.

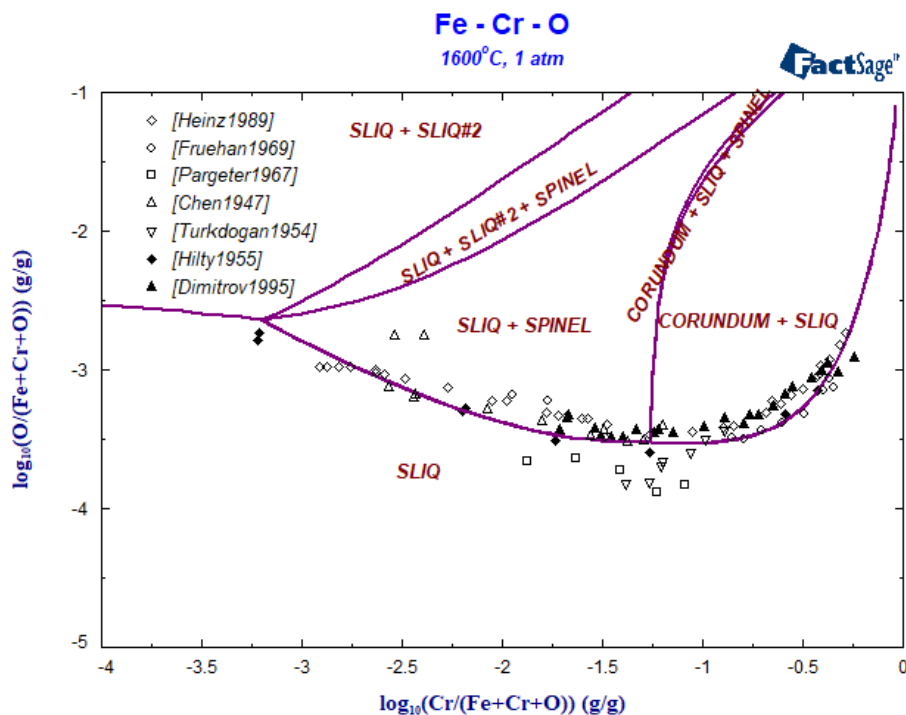


Figure 28: The precipitation range for Fe-rich melts in the Fe-Cr-O system.

Similarly, Figures 29 and 30 show the Fe-rich corners of the Fe-Ti-O and Fe-V-O system in which also different precipitate phases contribute to the respective solubility limits. The agreement with the experimental information is very good. In all cases a new associate of the type Fe_2MeO_4 ($\text{Me}=\text{Al}, \text{Cr}, \text{Ti}, \text{V}\dots$) had to be introduced in order to handle the localized interactions between Fe, the respective metal and oxygen in the very Fe-rich composition range. One particular feature common to all three diagrams (Figure 28 to 30) is especially worth noting: For very low contents of the metal component, all three systems exhibit a miscibility gap (SLIQ + SLIQ#2) which is fully consistent with the behavior of the Fe-O binary subsystem: At 1600°C liquid metal is in equilibrium with the liquid oxide phase. The respective metal component is dissolved in both liquids.

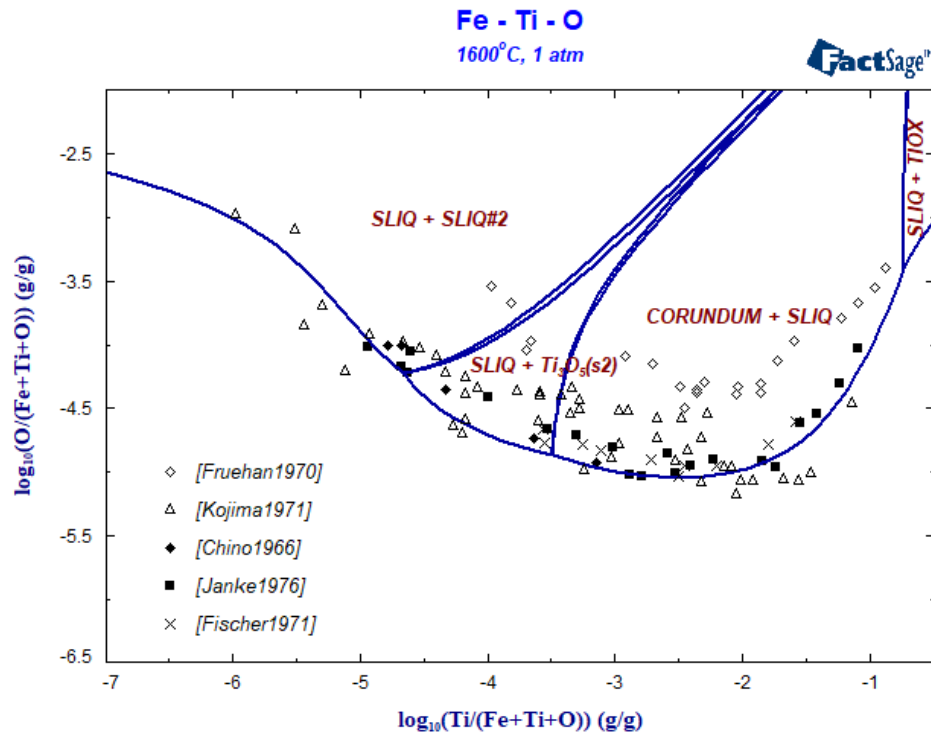


Figure 29: The precipitation range for Fe-rich melts in the Fe-Ti-O system.

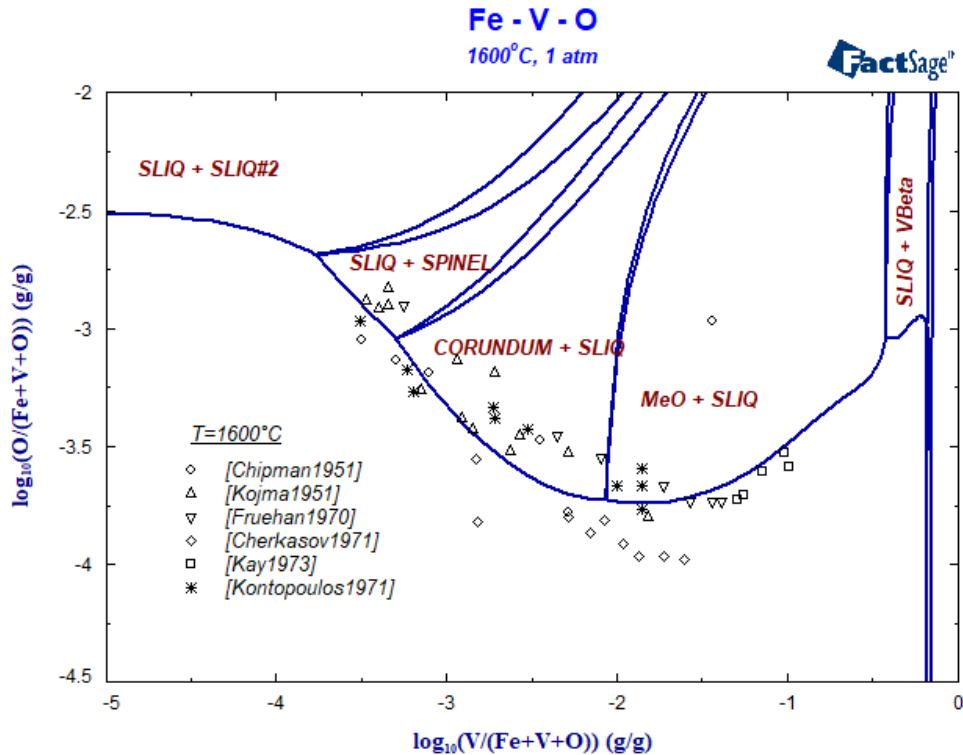


Figure 30: The precipitation range for Fe-rich melts in the Fe-V-O system.

An extreme case with threefold demixing is given in Figure 31. The system is $\text{FeO-SiO}_2\text{-P}_2\text{O}_5$ in contact with Fe. Because of the temperature (1600 °C) iron is liquid.

Thus, a metallic melt (with solubility for Ca, Si, O and P) will be in contact with the solid and/or liquid phases in the oxide subsystem (FeO-CaO-SiO₂). Since at certain compositions in the oxide subsystem there is demixing in the liquid slag in total three liquid phases can be in equilibrium.

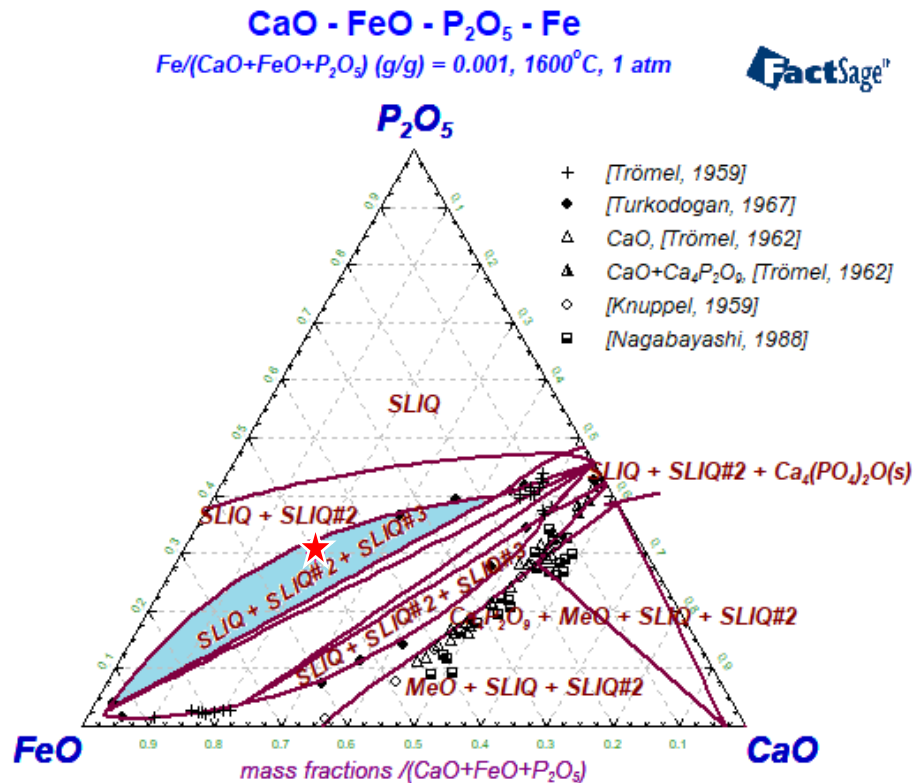


Figure 31: Threefold demixing in the system CaO-FeO-SiO₂-Fe at 1600°C.

The following Figure 32 shows in tabular form the compositions of the three different liquids for the overall composition as marked with ★ in the liquid three phase region (Fig.31). One P₂O₅-rich and one FeO-rich oxide melt as well as an Fe-based liquid can easily be identified.

Sliq #1	Sliq #2	Sliq #3
<pre> 0.78008 gram SLIQ#1 (0.78008 gram, 3.0984E-03 mol) (1600 C, 1 atm, a=1.0000) (8.7041E-05 wt.% Ca2O2 + 3.4575E-03 wt.% Fe + 0.30603 wt.% Fe2O3 + 18.133 wt.% Fe2O2 + 0.25220 wt.% CaFe2O4 + 2.7571E-08 wt.% P2O5 + 3.5664E-02 wt.% FePO4 + 9.3192E-02 wt.% CaP2O6 + 12.825 wt.% Ca2P2O7 + 34.033 wt.% Ca3P2O8 + 5.9708 wt.% Fe2P2O7 + 3.5518E-02 wt.% FeP2O6 + 23.962 wt.% Fe3P2O8 + 4.3485 wt.% Fe3O4 + 5.7441E-10 wt.% Ca + 2.1634E-03 wt.% P + 1.8206E-06 wt.% O </pre>	<pre> + 0.20700 gram SLIQ#2 (0.20700 gram, 1.2514E-03 mol) (1600 C, 1 atm, a=1.0000) (3.0790E-03 wt.% Ca2O2 + 4.1813E-02 wt.% Fe + 1.1734 wt.% Fe2O3 + 72.508 wt.% Fe2O2 + 0.56525 wt.% CaFe2O4 + 2.5841E-09 wt.% P2O5 + 4.8883E-02 wt.% FePO4 + 3.2306E-02 wt.% CaP2O6 + 5.1808 wt.% Ca3P2O8 + 2.4704 wt.% Ca3P2O7 + 5.5180 wt.% Fe2P2O7 + 3.2848E-02 wt.% FeP2O6 + 8.4032 wt.% Fe3P2O8 + 4.0203 wt.% Fe3O4 + 5.3253E-10 wt.% Ca + 2.0331E-03 wt.% P + 1.7182E-06 wt.% O </pre>	<pre> + 1.2520E-02 gram SLIQ#3 (1.2520E-02 gram, 2.3416E-04 mol) (1600 C, 1 atm, a=1.0000) (3.8781E-09 wt.% Ca2O2 + 97.362 wt.% Fe + 1.0290E-05 wt.% Fe2O3 + 0.76730 wt.% Fe2O2 + 3.1242E-05 wt.% CaFe2O4 + 1.7171E-12 wt.% P2O5 + 4.7822E-06 wt.% FePO4 + 7.7293E-06 wt.% CaP2O6 + 1.2554E-03 wt.% Ca2P2O7 + 3.9317E-03 wt.% Ca3P2O8 + 3.6918E-04 wt.% Fe2P2O7 + 2.2734E-06 wt.% FeP2O6 + 1.6590E-03 wt.% Fe3P2O8 + 2.6785E-04 wt.% Fe3O4 + 5.1990E-13 wt.% Ca + 1.7492 wt.% P + 0.11389 wt.% O </pre>
P ₂ O ₅ -rich melt	FeO-rich melt	Fe-rich melt

Figure 32: Tabular output of the composition of the three melt calculated for the overall composition marked with ★ in Fig. 31.

A list of all new and reassessed systems is provided below

Binary systems

new		reassessed	
Al-S	K ₂ CO ₃ -K ₂ SO ₄	Cu-O	Cu ₂ O-Fe ₃ O ₄
Li-S	K ₂ CO ₃ -MgCO ₃	Ca-S	CuO-Mn ₂ O ₃
S-Si	MgCO ₃ -Na ₂ CO ₃	Mg-S	CuO-NiO
S-Sr	CaCO ₃ -MgCO ₃	Mg-O	Cu ₂ O-NiO
S-Ti	CaCl ₂ -Ca ₃ P ₂ O ₈	Ni-O	CuO-P ₂ O ₅
S-V	CaCO ₃ -CaCl ₂	Zn-O	CuO-SrO
K-O	CaO-CaCl ₂	CuO-SiO ₂	Cu ₂ O-SrO
Na-O	MgO-MgCl ₂	Cu ₂ O-SiO ₂	CuO-TiO ₂
Si-O	CaCl ₂ -KCl	CaO-Cu ₂ O	CuO-V ₂ O ₅
Na-S	CaCl ₂ -NaCl	CaO-CuO	CuO-ZnO
K-S	KCl-NaCl	Cu ₂ O-Cr ₂ O ₃	Cu ₂ O-ZnO
P ₂ O ₅ -V ₂ O ₅	K ₂ CO ₃ -Na ₂ CO ₃	CuO-Fe ₂ O ₃	

Ternary systems

new		reassessed
Al-Fe-O	Li ₂ O-P ₂ O ₅ -TiO ₂	CaO-Na ₂ O-SiO ₂
Ca-Fe-O	Li ₂ O-P ₂ O ₅ -ZnO	
Cr-Fe-O	Al ₂ O ₃ -K ₂ O-P ₂ O ₅	
Fe-Mg-O	Al ₂ O ₃ -P ₂ O ₅ -SrO	
Fe-Mn-O	CaO-P ₂ O ₅ -SrO	
Fe-Si-O	FeO-MgO-P ₂ O ₅	
Fe-Ti-O	FeO-P ₂ O ₅ -SrO	
Fe-V-O	K ₂ O-P ₂ O ₅ -TiO ₂	
FeO-Li ₂ O-P ₂ O ₅	K ₂ O-P ₂ O ₅ -V ₂ O ₅	
Fe ₂ O ₃ -Li ₂ O-P ₂ O ₅	MgO-P ₂ O ₅ -SrO	
K ₂ O-Li ₂ O-P ₂ O ₅	P ₂ O ₅ -SrO-ZnO	
Li ₂ O-FeO-SiO ₂	P ₂ O ₅ -V ₂ O ₅ -ZnO	
Li ₂ O-Fe ₂ O ₃ -SiO ₂	Al ₂ O ₃ -Na ₂ O-P ₂ O ₅	
Li ₂ O-MgO-P ₂ O ₅	Na ₂ O-SiO ₂ -TiO ₂	
Li ₂ O-MnO-P ₂ O ₅	K ₂ CO ₃ -MgCO ₃ -Na ₂ CO ₃	
Li ₂ O-NiO-P ₂ O ₅	CaO-CaCO ₃ -CaCl ₂	
Li ₂ O-P ₂ O ₅ -SiO ₂	Al ₂ O ₃ -CaO-CaSO ₄	

Quaternary systems

new	reassessed
Al ₂ O ₃ -CaO-Fe ₂ O ₃ -SiO ₂	
Al ₂ O ₃ -CaO-K ₂ O-SiO ₂	
Al ₂ O ₃ -CaO-Na ₂ O-SiO ₂	

Quinary systems

new	reassessed
Al ₂ O ₃ -CaO-K ₂ O-Na ₂ O-SiO ₂	

Contact

In case of questions or to provide feedback, please open a new ticket in our support center: <https://support.gtt-technologies.de/> or contact us via

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