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Estimation of softening behavior of BF burden materials using computational phase diagrams for multicomponent systems

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Introduction

One of the first and the most obvious uses of phase diagrams has been to estimate the softening and melting behavior of different materials. Current computational thermodynamics (CTD) software together with thermodynamic databases make it possible to study the behavior of different materials in various conditions with phase diagrams created for multicomponent systems. The purpose of this study was to determine what are the possibilities to estimate the effect of compositional changes on the softening behavior of blast furnace (BF) iron burden materials using multicomponent phase diagrams computed with a commercial CTD software (FactSage v. 6.4 & v. 7.0) and its databases. Furthermore, a correlation between the computed phase diagrams and gas permeability of the material bed was estimated.

Studied materials

The sample materials investigated in this study were acid and olivine fluxed pellets. Average chemical compositions (excluding sulphur and small amounts of alkali oxides) of these materials are presented in Table 1.

Table 1. Chemical compositions (in wt-%), basicities and the amounts of slag forming components (in wt-%) in acid and olivine pellets considered in this study.

	Fe_{tot}	FeO	CaO	SiO_2	MgO	Al_2O_3	CaO/SiO_2	Slag forming components
Acid pellet	65.8	0.6	0.41	4.82	0.15	0.33	0.09	5.71
Olivine pellet	66.6	0.4	0.42	1.98	1.48	0.37	0.21	4.25

Experiments

The softening behavior of acid and olivine pellets was studied experimentally using two different setups. In the first setup, the materials were first pre-reduced using a blast furnace simulator (BFS; cf. [1] for more detailed description) after which the softening behavior was studied using a cohesive zone simulator (CZS; cf. [2] for more detailed description). In the second setup, an Advanced reduction under load -test (ARUL; cf. [3] for more detailed description) was used to study the softening behavior and gas permeability in simulated BF conditions by measuring pressure drops through the material bed.

Samples from both experimental setups were prepared for microstructural analysis, which provided information about the phase composition of the studied materials, which in turn was needed when defining the systems for computations. Additionally, temperatures in which the pressure drop though the sample material in the ARUL test reached the values of 20 mbar, 50 mbar and 70 mbar (TDP20, TDP50 and TDP70, respectively) were defined based on the second setup experiments. The TDP20 value has been chosen to indicate the onset of softening and the TDP70 value is the temperature in which gases cannot penetrate through the material layer and the test ends. Final reduction degrees in the ARUL test were 48.7% for acid pellets and 68.7% for olivine fluxed pellets.

Computations

The results of the experiments were compared with the phase diagrams computed with the FactSage software (versions 6.4 and 7.0) and its oxide database (FToxid). Phase diagrams for four and five component systems describing the studied materials were computed in order to verify the need to take the sufficient amount of components into account (cf. Figure 1). The phase compositions of the studied systems were computed as a function of temperature and the amounts of the molten phase were compared with the experimentally defined TDP values describing the gas permeability through the sample materials (cf. Figure 2). Finally, phase diagrams for the single pellet composition were computed as a function of temperature and partial pressure of oxygen in order to get a more comprehensive picture on the softening and melting behavior in the BF conditions (cf. Figure 3).

Departing from the compositions presented in Table 1, iron was defined as divalent oxide (FeO) in the systems described in Figures 1 and 2, because the softening of the raw materials in the blast furnace takes place in the conditions in which trivalent iron is already reduced to divalent form. In the system described in Figure 3 iron was defined as trivalent, because the reduction is taken into account with varying partial pressure of oxygen. Total compositions in all the computations were scaled to 100%.

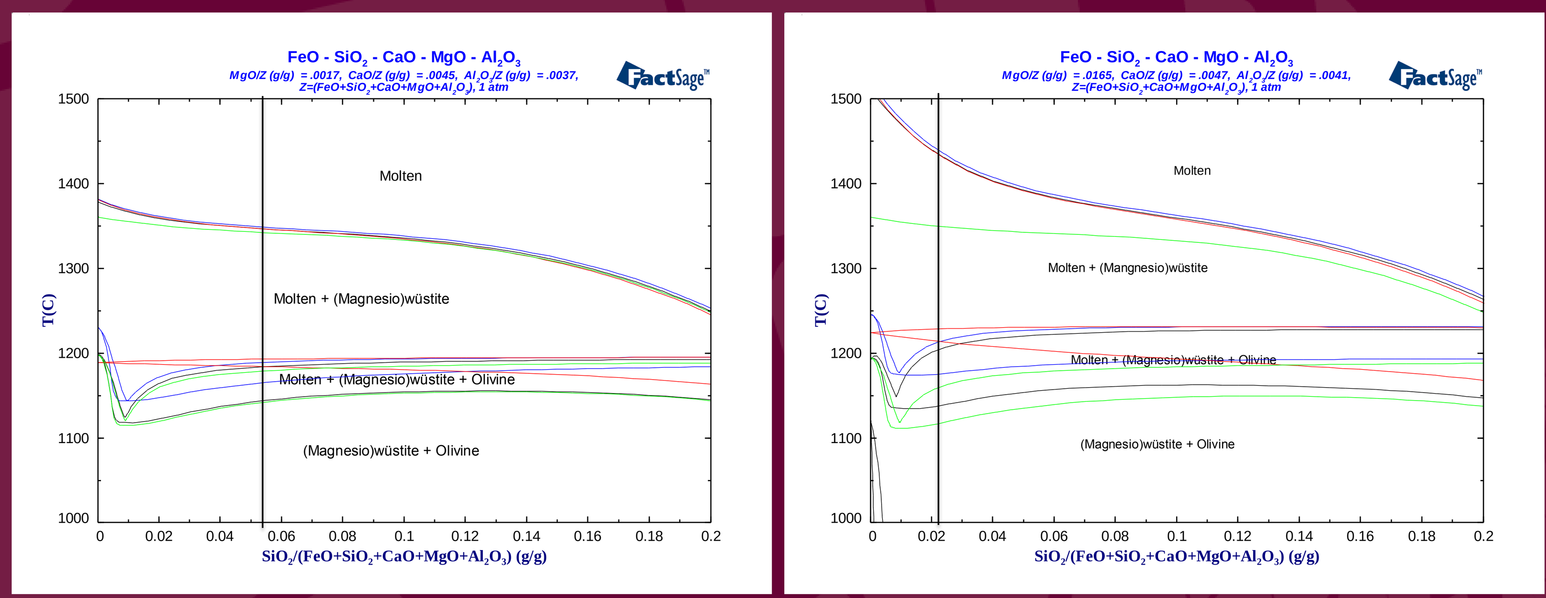

Figure 1. Phase diagrams for FeO-SiO_2-CaO-MgO-Al_2O_3-system illustrating the melting behavior of acid (left) and olivine (right) pellets: Black lines = All five components included in the system. Blue lines = Al_2O_3 excluded. Red lines = CaO excluded. Green lines = MgO excluded.

As shown in Figure 1, it is necessary to consider at least five major components in order to describe the behavior of the pellets. Due to its small amount MgO could be excluded if only acid pellets were studied, but it is necessary to take it into account while studying olivine fluxed pellets in which its amount is larger. Since the exclusion of CaO would change the type of the diagram completely, it would be least problematic to exclude Al_2O_3 if it were necessary to simplify the system. However, this would also cause significant deviance especially in the solidus temperatures.

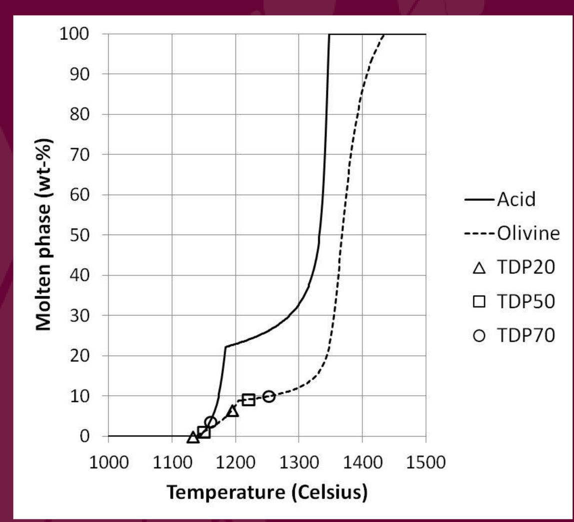

Figure 2. Comparison between computational molten phase fractions and experimental TDP values.

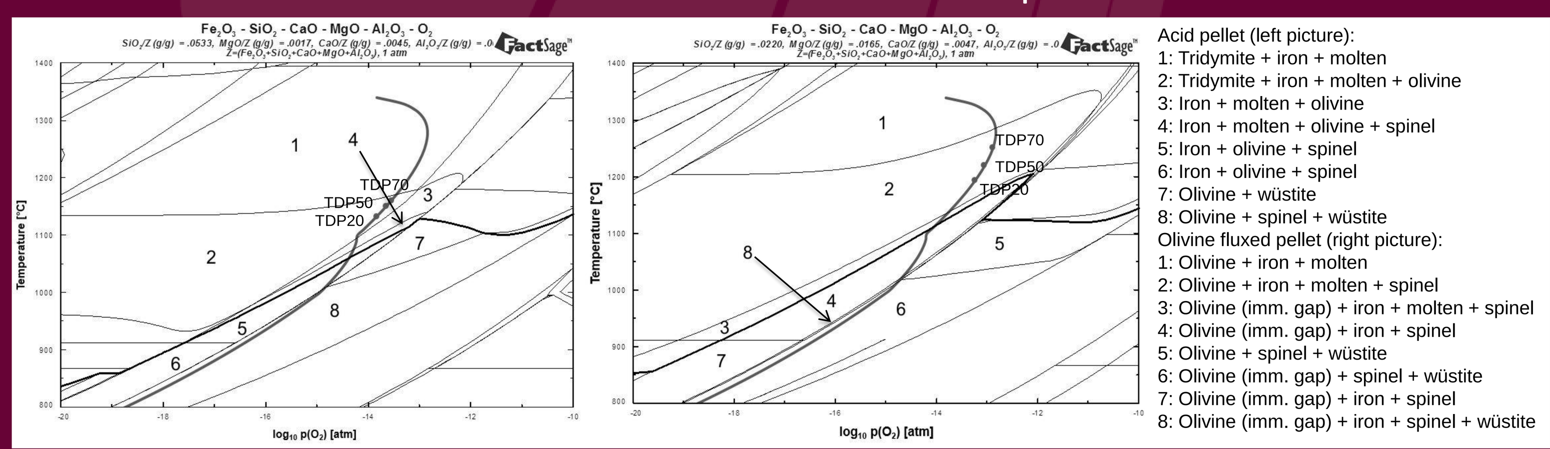

Figure 3. Fe_2O_3-SiO_2-CaO-MgO-O_2 phase diagrams for the acid pellet and the olivine fluxed pellet. The bold grey-coloured curve illustrates the reduction conditions, the dots are the TDP20, TDP50 and TDP70 values and the bold black-coloured curve highlights the solidus of the system.

According to the results, the estimation of the softening behavior of the BF iron burden materials is possible using computational phase diagrams computed for Ca-Fe-Mg-Si-Al-O-systems. However, since the conditions inside the BF vary considerably as a function of location, it was noticed that the diagrams computed to illustrate the behavior of oxide systems in inert atmosphere (cf. Figures 1 and 2) did not correspond with the experimental results as accurately as the diagrams in which partial pressure of oxygen was used as a variable in addition to temperature (cf. Figure 3). For practical purposes, it is important to know that the effect of the pellet composition can be studied computationally with sufficient accuracy. Diagrams similar to figures 1-3 describing the pellet systems with different compositions have been used when optimizing the pellet compositions with an overall goal to improve the BF efficiency and productivity.

References

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