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Thermodynamic Evaluation of the Slag System CaO-MgO-SiO₂-Al₂O₃

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Topics



- Introduction
- Materials and Methods
- Results and Discussion
- Conclusions



Introduction

- Knowledge of the fundamentals of steel production is very important for companies to keep their position – as the market becomes increasingly competitive.
- Consequently, there is no quality steels production without the knowledge of the slag behavior.
- Knowledge of the physico-chemical properties of the slag, such as viscosity, interfacial tension, density, basicity, thermal conductivity, among others, is essential.
- These properties, in turn, are influenced by the chemical composition and temperature of the system.



- The oxide system CaO-MgO-SiO₂-Al₂O₃ (denoted as C-M-S-A) plays an important role in a large number of industrial processes, especially in the steel industry.
- In modern secondary steelmaking, ladle treatment has become increasingly important in the production of clean steels.
- In the case of basic ladle slag, C-M-S-A slags close to CaO/MgO saturation with moderate AI_2O_3 and SiO_2 contents are used.

Introduction



- Figure 1 shows the pseudo-ternary CaO-MgO-SiO₂ diagram with a fixed 20 wt.% Al₂O₃ content from SLAG ATLAS.
- A series of dotted lines in the liquid surfaces of this diagram denote a quantity of data uncertainties.



Figure 1. C-M-S-A at 20 wt.% Al₂O₃.



(1) To perform a thermodynamic study of the phases at equilibrium at a high basicity value (binary basicity, B_2 , equal to 2) in C-M-S-A slags.

(2) To evaluate the slag viscosity values (checking results obtained *via* thermodynamic software with data coming from the literature) as a function of the slag composition and temperature, establishing therefore a critical analysis.

Materials and Methods



- The focused oxide systems is a pseudo-ternary system CaO-MgO-SiO₂ with fixed levels of Al₂O₃
- The thermodynamic approach was executed with the help of the computational thermodynamic software FactSage 6.3 (Equilibrium module) using FToxid subsystems.
- The thermodynamic simulations were performed under the following conditions:
- ✓ wt.% CaO / wt.% SiO₂ mass ratio (binary basicity, B_2) kept constant (generally $B_2 = 2$) for any MgO content;
- ✓ fixed amount of 20 wt.% AI_2O_3 for all simulations;
- ✓ constant total mass of 100 g;
- ✓ temperatures of 1,500°C; 1,550°C; 1,600°C.

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Figure 2. Schematic diagram of the quaternary system C-M-S-A indicating the *plane* at 20 wt.% Al₂O₃ (light gray) and the area used to plot the phase equilibrium diagrams (dark gray) which illustrate this work (*not to scale*).





Figure 3. CaO-MgO-SiO₂ pseudo-ternary phase diagram depicting the CaOrich corner (C-M-S-A system at 20 wt.% AI_2O_3) at the temperature of 1,500°C.





Figure 4. CaO-MgO-SiO₂ pseudo-ternary phase diagram depicting the CaOrich corner (C-M-S-A system at 20 wt.% AI_2O_3) at the temperature of 1,550°C.





Figure 5. CaO-MgO-SiO₂ pseudo-ternary phase diagram depicting the CaOrich corner (C-M-S-A system at 20 wt.% AI_2O_3) at the temperature of 1,600°C.

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Phase Amount for Binary Basicity B₂ Equal to 2



Figure 6. Mass of phases in the equilibrium state for wt.%CaO/wt.%SiO₂ = 2, $AI_2O_3 = 20$ wt.% and variable amount of MgO (0 to 35 wt.%); T = 1,500°C; FactSage.

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Figure 7. Mass of phases in the equilibrium state for wt.%CaO/wt.%SiO₂ = 2, $AI_2O_3 = 20$ wt.% and variable amount of MgO (0 to 35 wt.%); T = 1,550°C; FactSage.





Figure 8. Mass of phases in the equilibrium state for wt.%CaO/wt.%SiO₂ = 2, $AI_2O_3 = 20$ wt.% and variable amount of MgO (0 to 35 wt.%); T = 1,600°C; FactSage.

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C-M-S-A system at 20 wt.% AI_2O_3 Isothermal section at T = 1,600°C





Table 1. Comparison of MgO wt.% values between Slag Atlas data (C-M-S-Asystem at 20 wt.% Al_2O_3) and simulation results (FactSage) towt.%CaO/wt.%SiO_2 = 2.

	Slag Atlas CMSA phase diagram (20 wt.% Al ₂ O ₃)			FactSage			
	1500 °C	1550 °C	1600 °C	1500 °C	1550 °C	1600 °C	
100% Liquid	*	9.5	8.0	8.6	7.3	5.9	
Periclase saturation	*	11.9	12.7	8.8	9.5	10.3	
∆ wt.% MgO	-	2.4	4.7	0.2	2.2	4.4	

* B_2 isobasicity line equal to 2 does not cross the *Liquid* slag phase field.



Pure Liquid Slag Viscosity

The viscosity of the pure Liquid slag was calculated *via* FactSage (using *melts* database).

Table 2. Viscosity (Poise) values comparison between Slag Atlas data and
simulation results (FactSage),

(C-M-S-A system at 10 wt.% MgO and 20 wt.% AI_2O_3 , variable 35-50 wt.% SiO_2).

		wt.%			
	35	40	45	50	T [ºC]
Slag Atlas	4	7	11	22	1500
	3.1	4.9	8.9	19.0	1500
FactSage	2.4	3.6	6.4	13.2	1550
	1.8	2.8	4.7	9.3	1600



Solid-Liquid Slag Viscosity

- Most slag models are conceived for fully molten slags since their theoretical basis is not applicable to solid–liquid mixtures.
- The presence of solid phases in the slag will affect viscosity in two ways.

First, the components which form the solids are no longer part of the liquid phase. This changes the liquid phase composition and hence its viscosity.

Second, the interaction of solid particles with each other and the liquid phase will affect the bulk slag viscosity. This effect will vary with the size, shape, orientation and mass fraction of the particles.

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 Pretorius e Carlisle provided the concept of *effective* viscosity, which was defined to relate viscosity to the amount of second phase particles. It is based of Roscoe-Einstein model, as follows:

$$\eta_e = \eta \left(1 - 1.35\Theta \right)^{-5/2}$$

were:

- $\eta_{\scriptscriptstyle e}~$ effective viscosity of the Slag
- η viscosity of the molten (Liquid) Slag
- (h) fraction of precipitated solid phases





Figure 9. Solid fraction for slags in Figures 6 to 8 at 1,500°C, 1,550°C and 1,600°C





Figure 10. Effective viscosity determined for the Liquid Slag: 10.3 wt.% MgO; 20 wt.% Al₂O₃; 46.5 wt.% CaO e 23.3 wt.% SiO₂ at 1,600°C.



- Comparing the line for the 1600°C isotherm in Figure 1 (C-M-S-A system at 20 wt.% Al₂O₃) with that of corresponding phase diagram from FactSage, it can be said that there is an acceptable similarity between them.
- However, it can be noted also that MgO content for some Periclase saturation points determined with the help of FactSage software, in comparison with Slag Atlas data, are somewhat smaller.
- The Slag Atlas does not give viscosity values for slags of binary basicity equal to 2; nevertheless, for some compositions at 1,500°C, it shows some consistencies with FactSage calculated values for the C-M-S-A system.

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THANK YOU!!

QUESTIONS?

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