The behaviour of Al$_2$O$_3$ precipitation at the steel-slag interface

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Abstract. The paper focuses on the numerical investigation of the Al$_2$O$_3$ precipitation behaviour at the steel-slag phases interface. Several assumptions were made to simplify the process in order to prepare its description. A mathematical model of the steel-slag-precipitation system was introduced. The model base on the equation of motion, and takes into account forces balance of buoyancy force, added mass force, drag force and rebound force. Mentioned forces act in the same direction which is perpendicular with the steel-slag interface surface, but is positive or negative. The precipitation initial velocity can be calculated on the base of steel and inclusion density, liquid steel viscosity and particle radius. The numerical model based on the firstly prepared mathematical model was presented. Results of the computations show what is the precipitation radius size influence on particle movement and its assimilation to the slag.

1 Introduction
Stirring of liquid steel with neutral gas or its convection movement caused by the gravity force causes the movement of the metal as well as non-metallic precipitants. At the same time precipitants are effusing to the slag, where they can be assimilated or pushed away. Stirring force is crucial for the intensity of mentioned processes [1, 2].

The chemical composition of slag depends on the type of steel to be cast. However in the case of certain steels a considerable change of content of particular components can be expected, depending on the advancement of the casting process. The composition may change as a result of flowing off, interaction with solidification front, adsorption of inclusions and reactions on the metal/slag interface [3-8]. Adsorption and dissolution of Al$_2$O$_3$ particles by liquid slag solution can be a problem while casting, e.g. TRIP steel, mainly as far as the proper selection of the mould flux is concerned [9, 10]. Experiments performed by [9] revealed that casting steel with Al as an alloy additive resulted in a considerable change of chemical composition of slag during casting after 10-15 minutes from its beginning. A high value of Al$_2$O$_3$ absorption index was observed, and consequently lower SiO$_2$ content in slag, being a result of the reaction:

$$3(\text{SiO}_2) + 4[\text{Al}] = 3[\text{Si}] + 2(\text{Al}_2\text{O}_3)$$

Apart from this reaction the evolution of slag composition was caused by the adsorption of flowing off Al$_2$O$_3$ inclusions.

The calculation of the process of flowing off Al$_2$O$_3$ and interaction of an Al$_2$O$_3$ particle on the liquid steel/liquid slag/particle interface was performed with the use of a computer program.
2 Mathematical model

Mathematical model of precipitation behavior at the steel slag interface basis on several assumptions:

• precipitations have a shape of sphere;
• precipitations do not change shape or volume;
• the liquid is Newtonian;
• the computational domain is isothermal;
• slag has characteristic of liquid;
• front between slag and steel is flat;
• interfacial tension between any phases is constant during computations;
• the forces which causes precipitations movement is driven by following forces [1,12,13]:
  • buoyancy force
    \[ F_w = \frac{4}{3} \pi R^3 \Delta_b \rho_s - \rho_w \]  
  (2)
  • added Newton mass
    \[ F_m = \frac{2}{3} \pi R^3 \rho_s \Delta_b \frac{d^2Z}{dt^2} \]  
  (3)
  • drag force
    \[ F_{vis} = 6 \pi R \eta_s B \frac{dZ}{dt} \]  
  (4)
  • repulsive force
    \[ F_{rep} = 2 \pi R \sigma_{MS} \left( \frac{Z}{R} - 1 - \cos \theta \right) \]  
  (5)

where: \( R \) denotes the radius of the precipitation [m]; \( \Delta_b \) is a coefficient which depends on the position of the precipitation in liquid and slag, and is given by formula:

\[ \Delta_b = \frac{1}{4} \left( \frac{\rho_m}{\rho_s} - 1 \right) \left( \frac{Z}{R} \right)^3 - \frac{1}{3} \left( \frac{\rho_m}{\rho_s} - 1 \right) \left( \frac{Z}{R} \right)^2 + \frac{\rho_m}{\rho_s} \]  
(6)

\( \rho_s, \rho_m, \rho_w \) denotes density of slag, steel and precipitation respectively [kg m\(^{-3}\)]; \( Z \) is location of the particle in the slag, so it’s equal 0 at the moment when particle is touching the slag, but is still all in liquid [m]; \( g \) is gravity acceleration [m s\(^{-2}\)]; \( \eta_s, \eta_m, \eta_w \) is dynamic viscosity of slag, steel and precipitation respectively [Pa s]; coefficient \( B \) denotes impact of location of the particle in the slag on drag force, and is given by formula:

\[ B = \left( \frac{\eta_m}{\eta_s} - 1 \right) \left( \frac{Z}{R} \right)^2 - 2 \left( \frac{\eta_m}{\eta_s} - 1 \right) \left( \frac{Z}{R} \right) + \frac{\eta_m}{\eta_s} \]  
(7)

\( \cos \theta = \frac{\sigma_{WM} - \sigma_{WS}}{\sigma_{MS}} \) is cosine of wetting angle, which can be calculated basing on the knowledge about the values of interfacial tensions between: \( \sigma_{WM} \) - particle and steel, \( \sigma_{WS} \) - particle and slag, \( \sigma_{MS} \) - steel and slag [N m\(^{-1}\)].

At the beginning of the computations the center of the precipitation is in \( R \) distance from slag, at this moment start of the frame of reference is in the particle center and its location is set to be \( Z = 0 \). Computations runs until \( Z = R \).

Analyzing process of particle flow in liquid metal at the beginning the particle which density is less than the steel density is accelerating until buoyancy and drag forces are equal. Equilibrium of those forces allows one to calculate speed of the particle:

\[ v_{eq} = \frac{2}{9} R^2 \left( \rho_m - \rho_w \right) \frac{\theta}{\eta_m} \]  
(8)

This speed is chosen to be initial in the model as most of the particles reach this speed as their distance from slag is significant.
Finally the process is governed by ordinary differential equation, which takes into account balance of forces (2) – (5), and initial condition for $Z$ and speed eq.(8):

$$\left\{ \begin{aligned}
(4/3 \pi R^3 \rho_w + 2/3 \pi R^3 \rho_3 \Delta_b) \frac{d^2Z}{dt^2} + 6 \pi R \eta_S B \frac{dZ}{dt} &+ 2 \pi R \sigma_{MS} \frac{Z}{R} - (1 + \cos \theta) \\
\frac{4}{3} \pi R^3 (\Delta_b \rho_S - \rho_w) g
\end{aligned} \right. \quad \frac{dZ}{dt} (t = 0) = \frac{2}{9} R^2 (\rho_M - \rho_w) \frac{\eta_M}{\eta_S}$$

$$Z(t = 0) = 0$$

(9)

Discretization of the equation (9) was performed with the use of Runge-Kutta fourth rank scheme.

3 \hspace{1cm} \textbf{Results of the simulation}

To analyze the movement of the $\text{Al}_2\text{O}_3$ particle based on the mathematical model introduced above the Dev-Cpp environment was used to prepare computer software. The computer program works in console window and as a result prepare the file, where the time, actual speed and position of the particle is stored. An exemplary calculation window has been presented in Fig. 1.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{simulation_window.png}
\caption{Window of the simulation software with some messages about uniqueness conditions of the model}
\end{figure}

The following assumptions were made in the calculations [1]: $\rho_M$ – density of steel 7000 kg $\text{m}^{-3}$, $\rho_I$ – density of inclusions $\text{Al}_2\text{O}_3$ 3990 kg $\text{m}^{-3}$, $\rho_S$ – density of slag 2750 kg $\text{m}^{-3}$, $\eta_M$ – viscosity of steel 0.006 Pa·s, $\eta_S$ – viscosity of slag 0.006 Pa·s, $\sigma_{MS}$ – tension on steel/slag interface 1.389 N/m, $\sigma_{IS}$ – tension on inclusion/slag interface 1.504 N/m, $\sigma_{IM}$ – tension on inclusion/steel interface 0.379 N/m.

The results of calculations performed for variant 1: $\text{Al}_2\text{O}_3$ particle radius: $r=0.0001; 0.0003$ and $0.0005$ m, and variant 2: particles with radius $r=0.00001; 0.00003; 0.00005$ m have been presented in figures 2 and 3, respectively.
A system of forces associated with the speed of free flow-off regulated by the Stokes law and force of entrainment resulting from the steel speed, act on the particle. Particles of very small radius reach low speed $U$ values and so their removal and absorption by slag is hindered. The operation of capillary and gravity forces counteract buoyancy defined with Stokes equation. The change of placement of particle $H(m)$ with respect to particle radius has been presented in figures 4 and 5.
Figure 4. Change of placement $H(m)$ of $\text{Al}_2\text{O}_3$ particle with respect to surface for particle radius $1\cdot10^{-4}, 3\cdot10^{-4}; 5\cdot10^{-4}$ m

Figure 5. Change of placement $H(m)$ of $\text{Al}_2\text{O}_3$ particle with respect to surface for particle radius $1\cdot10^{-6}, 3\cdot10^{-6}; 5\cdot10^{-6}$ m

A particle which reaches the liquid steel/slag interface may pass through this boundary and be dissolved in slag or pushed off. It was assumed in the calculations that for $H(m)=0$ the particle is in the initial position, for $H(m)$ the particle is in slag.

4 Conclusions

The removal of non-metallic inclusions to slag is most importantly determined by the system of forces acting on a particle, and so physicochemical parameters, hydrodynamic conditions of the analyzed system and radius of the particle. These parameters determine the position of the particle in reference to the interface. $\text{Al}_2\text{O}_3$ particles have higher density than slag, therefore they stay close to the interface. Moreover the presented results refer to the behavior of a single particle, which is a
considerable simplification. This type of simulation should be performed for a population of
inclusions, taking into account agglomeration. The performed calculations are a starting point for
proper experimental works, first with a water model of two immiscible fluids, then observations with a
high-temperature microscope.

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