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Simulation of molten steel refining in a gas-stirred ladle using a coupled CFD and thermodynamic model

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Abstract

In secondary steelmaking, the gas-stirred ladle refining process is enhanced by applying a vacuum. A three phase (steel/gas/slag) mathematical model based on the fundamental transport equations has been reported in the literature. This model was used to study the steelmaking refining process. In this approach, the gas-stirred ladle system fluid flow prediction from Computational Fluid Dynamics (CFD) analysis was linked with thermodynamic analysis, with some thermal simplification. The model predicts the changes in the mass concentration of the elements of concern (Al, O, and S) during the refining process.

In the present work we aim to enhance the modeling in the literature. Here we use Fluent as the CFD package to predict the flow pattern of the three phase (steel/gas/slag) system. The thermodynamic package is MTDATA from the National Physical Laboratory (NPL), which has the capability to make thermodynamic predictions for multi-component systems containing up to 30 elements. Therefore, it is possible to solve for the properties of the slag as a function of composition and temperature. The two packages are being linked in a Visual Basic environment. The mass concentration of the different elements at the steel/slag interface is being updated at a pre-defined Δt time step.

Comparison of the model calculated results with data from the literature show the potential of this model. Real plant data will be used to validate this multi phase simulation model.

Introduction

Extensive efforts have been made to investigate and improve the secondary steelmaking process since it was first envisioned by Sir Henry Bessemer almost hundred and fifty years ago. In secondary steelmaking ladle metallurgical processes, the driving force of chemical reactions can be verified using thermodynamics and an estimation of the rate of the industrial process can be obtained based on, for example, laboratory experiments, plant data, and industrial experience. The driving forces in the metallurgical processes include the heat and mass transfer on the micro scale at the metal/slag interface, the heat and mass transfer at the metal and/or the slag phase, and the chemical reactions them selves. Today, the mass and heat transport in the metal and slag phases can be predicted by solving the fundamental transport equations using Computational Fluid Dynamics (CFD) as a tool. In addition, developed at the National Physical Laboratory (NPL), the MTDATA thermodynamics package is capable of predicting the different phases formed at the metal/slag interface at a chemical equilibrium.

Mazumdar and Guthrie [1] published comprehensive review in the mid-nineties; this illustrated the great potential of mathematical modeling in metallurgical process enhancement. They also noted that most of the published computational studies assume isothermal conditions. Furthermore, the prediction of heat and mass transfer using the ***k-ε*** turbulent model in the computational procedure was in good agreement with the experimental measurements.

It is widely accepted now that the fully developed region of the two-phase system within the control volume is independent of the gas injection device and pressure inlet conditions [1]. The influence of the gas injection device used (nozzle/porous plug) and the gas input kinetic energy is limited to the local area near the inlet [1, 2]. The injected gas velocity is drastically reduced within a short distance from the inlet due to the gas kinetic energy losses [2], as illustrated in figure (1). Furthermore, due to the huge difference in heat capacity between the injected gas and the molten steel, most of the heat exchange between the two phases occurs within a small region around the gas inlet nozzle. Also, Jonsson and Jönsson [3] reported a high temperature rise of the injected gas within the nozzle body before it came into contact with the liquid path.

In the industrial ladle vessel, the refractory lining usually includes an insulation layer to reduce the heat losses to the surroundings. However, due to the high working temperature of the molten steel (~1600 ^{o}C), and the large size of the industrial ladle vessel, the heat losses cannot be eliminated. Therefore, during the ladle holding time, whilst waiting for processing, temperature variation within the molten steel occurs due to the heat losses from the ladle sidewalls, the ladle bottom and the top slag layer. This variation in temperature results in natural convection heat transfer within the liquid phase and in turn this leads to turbulent flow. Xia and Ahokainen [4] conclude that, at an early stage of the ladle holding time, a single flow recirculation is formed where the molten steel flows upward at the ladle central region and downward along the wall side. This single recirculation loop provides the highest flow velocity due to natural convection. However, for a holding time of more than 40 seconds more vortices are formed, leading to reduced flow velocity. The flow pattern gradually becomes unstable. Austin el, at. [5] report that the flow velocity magnitude of the standing ladle decreases with the holding time, and the formed recirculation regions shrink. Furthermore, the maximum velocity magnitude reported by Xia and Ahokainen due to the natural convection phenomena is roughly less than 20% of the maximum velocity magnitude due to gas stirring reported by Jonsson and Jönsson [3].

The presence of the upper buoyant phase is responsible for significant energy dissipation and slowing of the lower liquid phase, as illustrated in figure (2) [1]. Han el. at, [6] investigate the ladle flow characteristics using a water model with a top layer of oil. The mixing time decreased with the increase of gas flow rate. The presence of the top oil layer inhibited mixing, as illustrated in figure (3). Furthermore, mixing time increased with the increase of the thickness of the top oil layer as shown in figure (4). However, recently a three phase model of a gas stirred bath including the top slag layer, has been developed by Jonsson and Jönsson [3]. The agreement with measured values of the radial steel surface velocity was five times better than an earlier comparison with a two-phase simulation where the influence of the slag layer was neglected. Furthermore, the Weber number is a good indicator of the entrapment between slag and steel at the interface. The model was capable of predicting the slag and molten steel fractions in the mixture at the interface.

Jonsson et al. [7] established a new approach to steel refining simulation. The multi-phase steel/slag/gas model was linked with a thermodynamic database to simulate the desulphurization process. However, some simplifications have been made. Only the effect of aluminium, oxygen and sulphur dissolved elements were accounted for in the desulphurization based on the assumption that the concentrations of other elements do not change significantly during the process. The oxygen activity was determined only by the aluminium and alumina activity in the

melt and slag respectively, which were used to determine the sulphur partition ratio between the melt and the slag at constant slag sulphur capacity. The sulphur was assumed to be completely dissolved in the slag.

In this present work, a three phase (steel/gas/slag) mathematical model was developed using Fluent commercial CFD package. MTDATA was used to predict the species exchange at the metal/slag interface.

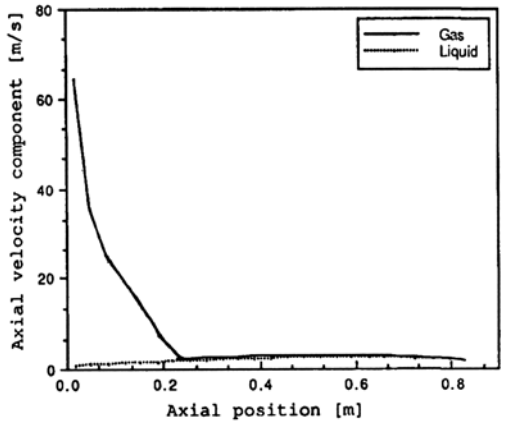

Figure-1. Gas and liquid phase axial velocities along the centre line [2]

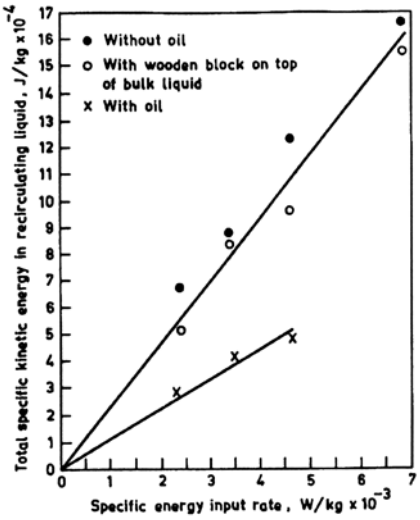

Figure-2. Total specific kinetic energy in recirculation vs. energy input rate for various slag conditions[1].

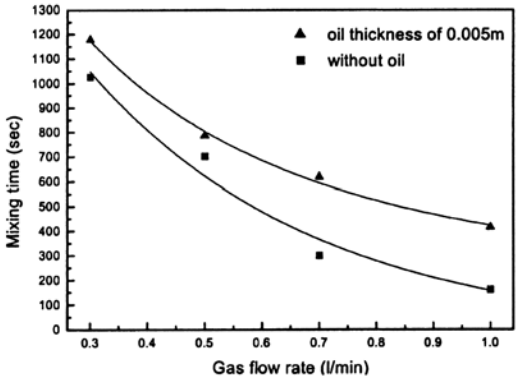

Figure-3. Gas flow rate influence on required mixing time [6].

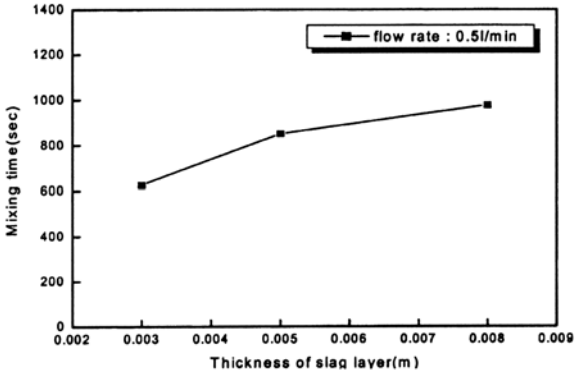

Figure-4 Slag layer thickness influence on mixing time at constant gas flow rate [6].

Mathematical Modeling

Mathematical Formulation

A 2D mathematical model of a gas-stirred ladle accounting for the steel, argon and slag phases was created as illustrated in figure(5). The Eulerian multiphase model approach was used to solve separate transport equations for each of the dissolved elements of interest such as aluminum, oxygen and sulphur.

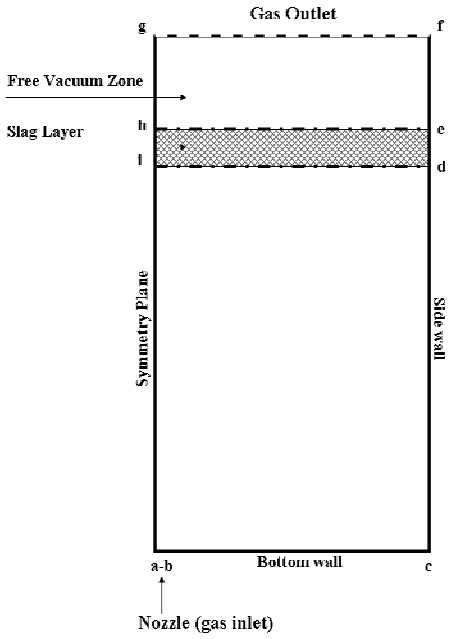

Figure-5. Schematic diagram of the two dimensional control volume domain of the gas stirred ladle system

The simulation was based on the following assumptions:

a. The ladle vessel is axially symmetric;
b. The argon gas bubbles are injected through a jet nozzle located in the center of the ladle bottom. The gas flow rate used is 80 *l*/min;
c. The transient solution approach was used to run the simulation;
d. A free vacuum zone occupied by gas on the top of the slag layer was assumed [2]. A constant gas temperature at the outlet surface was assumed. This temperature value was taken from steelmaking plant ;
e. A non-slip boundary condition was assumed at the ladle side wall and the bottom. An enhanced wall treatment provided by Fluent was used to define the velocity profile, turbulent kinetic energy, energy dissipation rate, and turbulent viscosity in the region near the wall. This method combines a two-layer model with enhanced wall functions. The two-layer model is an integral part of the Fluent enhanced wall treatment approach and is used to specify both ε and the turbulent viscosity in the near-wall cells. The enhanced wall function is an amalgamation of the turbulent and laminar wall flows to obtain a reasonable representation of velocity profiles and resolve the different conditions near the wall region (i.e., laminar sub-layer, buffer region, and fully-turbulent region). The heat loss flux from the molten steel to the refractory lining was assumed to be 24.6 KW/m^2 [7];
f. A homogeneous molten slag composition and temperature were assumed as an initial condition, with slag layer thickness of 9 cm prior to calculation;
g. A homogeneous molten steel composition and temperature were assumed as an initial condition prior to calculation;

Based on the above assumptions, the following transport equations were solved to conduct the simulation.

a. Mass conservation equation for each single phase and dissolved elements of interest.

b. Momentum conservation equation.
c. Energy conservation equation.

The turbulent flow was solved using a modified ***k-ε*** model.

Boundary conditions

A diagram of the two-dimensional domain mesh is illustrated in figure (5). The area (*h-e-d-i*) is occupied by slag phase of thickness 9 cm at the start of calculation. The free vacuum zone (*h-g-f-e*) on the top of the slag layer is occupied by gas under vacuum. The surface (*a-g*) stands for the system symmetrical plane. A homogenous temperature of value 1600 ^{o}C was assumed at the start of calculation. The applied boundary conditions are described below.

Gas Inlet Nozzle: Argon gas is injected into the domain volume by a nozzle located at the bottom of the ladle (*a-b*) with a volume flow rate of 80*l*/min. The turbulent kinetic energy and kinetic energy dissipation is calculated using the gas inlet velocity and the estimated turbulent intensity at the inlet. The turbulent intensity is estimated from equation (4) suggested by Fluent CFD package.

$$I = 0.16 \cdot (\mathrm{Re})^{-.125} \tag{4}$$

where *I* is turbulent intensity and (Re) is Reynolds number.

Ladle side and bottom walls: A non slip condition was assumed with the applied Fluent enhanced wall treatment. A constant rate of heat loss was assumed.

Pressure Outlet: A pressure outlet condition with a vacuum pressure was applied at the gas exhaust surface (*g-f*).

Thermodynamics

Desulphurization

In the present work, the authors study the desulphurization of fully aluminum-killed steel during ladle degassing. The slag system (CaO-Al_2O_3-SiO_2-MgO) is used in such a refining process. The slag content is assumed to be 55 wt% CaO, 33 wt% Al_2O_3, 7.5 wt% SiO_2, and 7.5 wt% MgO.

Richardson and Fincham [8] and Richardson [9] have shown that the sulphur is held in the slag totally in the form of sulphide at oxygen partial pressures less than 10^{-5}-10^{-6} atm. Desulphurization is controlled by the equilibrium:

$$\frac{1}{2}S_2(gas) + O^{-2}(slag) = \frac{1}{2}O_2(gas) + S^{-2}(slag) \tag{5}$$

Richardson and Fincham [8] and Richardson [9] formulate the slag sulphide capacity as a function of gas partial pressures in the molten slag and sulphur concentration present in the slag as:

$$C_s = (wt\%S) \times \left(\frac{p_{o_2}}{p_{s_2}}\right)^{1/2} = K.\left(\frac{a_{o^{2-}}}{\gamma_{s^{2-}}}\right) \tag{6}$$

where K is the equilibrium constant for the reaction. Richardson and Fincham suggested this should be defined as follows:

$$K = \left(\frac{a_{s^{2-}}}{a_{o^{2-}}}\right) \times \left(\frac{p_{o_2}}{p_{s_2}}\right)^{1/2} = \frac{(x_{s^{2-}}.\gamma_{s^{2-}})}{a_{o^{2-}}} \times \left(\frac{p_{o_2}}{p_{s_2}}\right)^{1/2} \quad (7)$$

where a_i and γ_i are the thermodynamic activity of the dissolved element (i) and the activity coefficient of the element (i) respectively.

Basis for the Use of the Thermodynamic Prediction Package (MTDATA)

In the steelmaking industry, the oxygen partial pressure within the steel/slag system is within the range of 10^{-8}-$10^{-9.2}$ atm. Therefore, the sulphur tends to be present as sulphide rather than sulphate. In addition, the aluminum present in the fully killed steel means that a reasonable assumption is that the desulphurization process is limited to the three main control elements (Al, O, and, S) [7]. However, the influence of the presence of CaO on sulphur removal during the fully-killed steel refining process, is illustrated in the overall desulphurization reaction expressed as [10]:

$$(CaO)_{slag} + [S]_{steel} + 2/3[Al]_{steel} \rightarrow (CaS)_{slag} + 1/3(Al_2O_3)_{slag} \quad (8)$$

Figure (6) illustrates the influence of SiO_2 slag content on desulphurization. In addition, the notable influence of the initial content of FeO in the slag has been published in the literature[11].

Therefore, the thermodynamic prediction of desulphurization process expected to be enhanced by using the MTDATA package, due to its capability for thermodynamic predictions for multi-component systems containing up to 30 elements. MTDATA is equipped with three different databases named NPLOX2, TCFE, and SUB_SGTE. The database [NPLOX2] contains the data for the oxide system CaO-Al2O3-MgO-SiO2-Fe-O, [TCFE] is the multi-component alloy database specific to steels containing the data about O/S solubility in steel, and finally, [SUB_SGTE] is the gas phase data source.

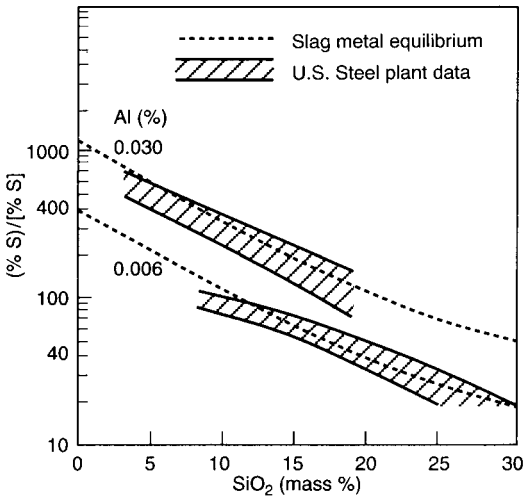

Figure-6 **Slag/metal sulphur distribution ratio after desulphurisation with lime-saturated CaO-MgO-Al_2O_3-SiO_2 slags at 1600 +/- 15 °C [10].**

Solution Method Strategy

A pre-defined CFD file was built and solved until the injected gas penetrates the top slag layer and a slag free hole created (this is called the 'open-eye'). This is taken as the start point for the coupling analysis (i.e. the iterative linking of the CFD program with the thermodynamic prediction package MTDATA). Also, a pre-defined thermodynamics file was created. The multiphase thermal system components are defined as (CaO-SiO_2-MgO-Al-Fe-O-S). Alumina from the slag was broken down into pure aluminium and oxygen. This allows easier tracing of the aluminium element at the interface between the steel and the slag.

A data exchange control macro was created using the Visual Basic 6.0 environment. Figure (7) illustrates the coupling flow chart. First, Fluent is executed to run the pre-defined file for a defined Δt time step. Then the volume fractions of the different phases in the mixture, temperature, and pressure values for each single cell are stored in a defined text file. Next, the macrocode reads the CFD results text file, and in each cell with steel/slag mixture, the moles weights of the multiphase thermodynamic system components are calculated from the steel/slag volume fractions. MTDATA is only executed for each single cell that contains steel/slag mixture (as opposed to the cells which contain steel or slag alone). The thermodynamic results are stored in a text file. This first step is repeated until the end of the refining process. However, starting from the second step, at the beginning of the Fluent session, the species mass concentration at the steel/slag interface is updated by reading the MTDATA results text file from the previous time step, using the customised species mass transfer Fluent user define function.

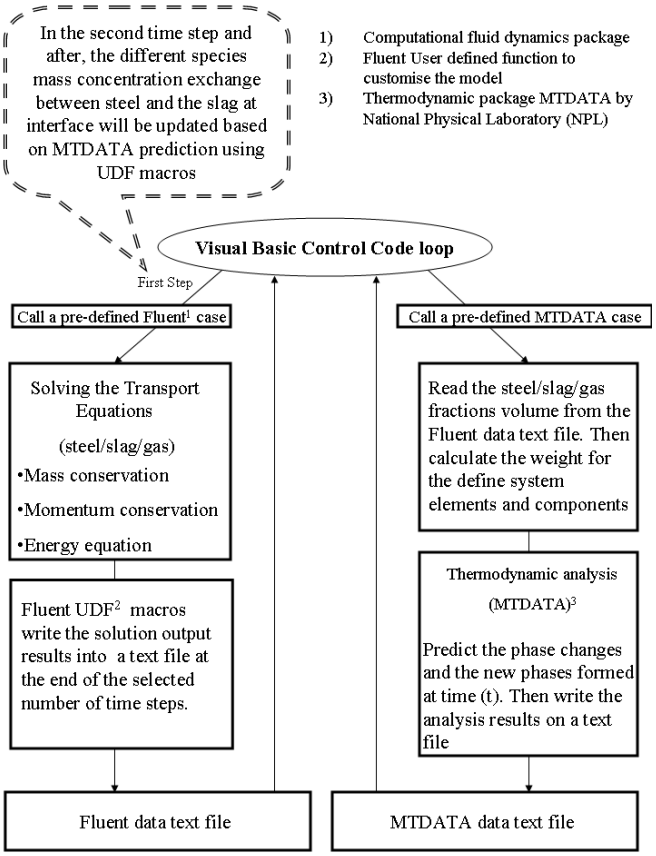

Figure-7. Flow chart diagram of the coupling strategy method used to link Fluent CFD analysis with MTDATA thermodynamics package.

Concluding Remarks

The validity of the model is being tested by comparison with experimental results. The present model predict molten steel near-surface horizontal velocities in good agreement with Hsiao et al. [12] who reported experimental results for a 60 ton gas stirred ladle. Further results will be presented in due course.

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