19th Australasian Fluid Mechanics Conference
Melbourne, Australia
8-11 December 2014

Preliminary Numerical Simulation of Chemically Reacting Gas and Liquid Phases in Oxygen Steelmaking

K.H.A. Kalyani, J. Naser and G. Brooks

Faculty of Science, Engineering and Technology
Swinburne University of Technology, Hawthorn, VIC3122, Australia

Abstract

A preliminary dynamic model is developed to predict the foaming phenomenon in oxygen steelmaking incorporating Computational Fluid Dynamics, which will be able to simulate the evolution of the physical properties throughout a blow and predict the foaming height with time.

The computational fluid dynamic (CFD) model developed by Sattar et al (Sattar et al., 2013a, Sattar et al., 2013c, Sattar et al., 2013b) was extended to incorporate the chemical reactions on removal of impurity elements. The model includes three phases: gas, liquid and foam. The major removal reactions of carbon (C), silicon (Si), manganese (Mn) and phosphorus (P) were included with the mass transfer within and between gas and liquid phases.

The model incorporated the first order diffusion kinetics with static equilibrium values for carbon and silicon, while for manganese and phosphorus, the first order diffusion kinetics with dynamic equilibrium values were used. The real plant data reported in IMPHOS (Millman et al., 2011) report was used for the simulation validation, after simulating it for 20 minutes of real time.

The results obtained were in reasonable agreement with the real plant data as reported in the IMPHOS (Millman et al., 2011) report. The observed deviations were mainly due to the merging of slag phase with the liquid phase and limited number of reactions used, compared to the actual process.

Introduction

Basic Oxygen Steelmaking has become one of the most commonly used refining methods for producing steel nowadays. In this process an oxygen jet is injected to the molten metal bath causing the oxidising reactions which produce the oxides of the elements (building up the slag), and carbon monoxide gas. The evolution of slag and the high gas flow causes the slag to foam. The extreme foaming called sloping is disastrous and reduces the efficiency of the process. The phenomenon of slag foaming in steelmaking is investigated by researchers with different approaches of modelling the foaming (FRUEHAN, 1991, Sattar et al., 2013b, DOGAN, 2011, Sattar, 2013). Those models are limited in size, temperature variation and chemical composition evolution in comparison with the real process. So still there is the need for a dynamic model, which can simulate the evolution of properties of the liquid and slag in the bath.

Therefore the present research aims at developing a dynamic model to predict the foaming phenomenon incorporating Computational Fluid Dynamics, which will be able to simulate the evolution of the physical properties throughout a blow and predict the foaming height with time. The first step is to incorporate the chemical reactions in the model for predicting the physical properties' evolution and of which the results are presented in this paper.

Introduction to the Model

A 3D CFD model is used in the present study for simulating the operation of a 6 tonne pilot plant BOS (Basic Oxygen Steelmaking) converter including the chemical reactions in the metal bath and the emulsion. The geometrical model developed by Sattar et al (Sattar, 2013) was used together with their CFD model for foaming. The developed model consists of only three phases: gas, liquid and foam, and incorporates only the decarburisation reaction. In the present study all the other major chemical reactions are included in the model through user subroutines written in FORTRAN programming language. The simulation results will demonstrate the removal behaviour of impure elements (Si, C, P and Mn), and the results are validated against the data published by Millman et al (Millman et al., 2011).

Chemical Reactions with First Order Diffusion Kinetics

The following major reactions that occur in the BOF converter are included in the present model. The [] and () indicate the dissolution in iron and slag respectively.

$$[\mathrm{C}] + [\mathrm{O}] = \mathrm{CO}_{\mathrm{g}}$$

$$\mathrm{Fe} + [\mathrm{O}] = (\mathrm{FeO})$$

$$[\mathrm{Si}] + 2[\mathrm{O}] = (\mathrm{SiO_2})$$

$$[\mathrm{Mn}] + [\mathrm{O}] = (\mathrm{MnO})$$

$$2[\mathrm{P}] + 5[\mathrm{O}] = (\mathrm{P_2O_5})$$

$$[\mathrm{C}] + (\mathrm{FeO}) = \mathrm{Fe} + \mathrm{CO}_{(\mathrm{g})}$$

$$[\mathrm{Si}] + 2(\mathrm{FeO}) = 2\mathrm{Fe} + (\mathrm{SiO_2})$$

$$[\mathrm{Mn}] + (\mathrm{FeO}) = \mathrm{Fe} + (\mathrm{MnO})$$

$$[\mathrm{C}] + (\mathrm{MnO}) = [\mathrm{Mn}] + \mathrm{CO}_{(\mathrm{g})}$$

$$[\mathrm{Si}] + 2(\mathrm{MnO}) = 2[\mathrm{Mn}] + (\mathrm{SiO_2})$$

$$5[\mathrm{Si}] + 2(\mathrm{P_2O_5}) = 4[\mathrm{P}] + 5(\mathrm{SiO_2})$$

$$5[\mathrm{C}] + (\mathrm{P_2O_5}) = 2[\mathrm{P}] + 5\mathrm{CO}_{(\mathrm{g})}$$

$$5[\mathrm{Mn}] + (\mathrm{P_2O_5}) = 2[\mathrm{P}] + 5(\mathrm{MnO})$$

$$5[\mathrm{Fe}] + (\mathrm{P_2O_5}) = 2[\mathrm{P}] + 5(\mathrm{FeO})$$

In these reactions the reaction rates are governed by the diffusion of the elements to the slag metal interface. Hence the first order diffusion kinetics was used for calculating the rates of the reactions in the present model.

By rearranging the equation; Fick's first law of diffusion the following equation was obtained to address the reaction rate of each element in each cell of the model.

$$\frac{dC}{dt} = K(m_{f_{b,i}} - m_{f_{eq,i}})\alpha_l \rho_l v_c \quad (1)$$

Where,

C: Mass fraction of the element in the cell

K: Constant (k × A)

$m_{f_{b,i}}$: Bulk mass fraction of the element in the cell.

$m_{f_{eq,i}}$: Equilibrium mass fraction of the element.

α_l: Liquid volume fraction.

ρ_l: Density of liquid.

v_c: Volume of the cell.

The equation (1) was used in the subroutine for reaction kinetics of the elements and the value of the constant K was calculated for each element with the published data by Millman et al (Millman et al., 2011). The values of K used for carbon, silicon, manganese and phosphorus were the average for the 20 heats for each element.

Model Geometry and Features

The geometry of the model used in the present study was designed according to the MEFOS 6 tonne pilot plant BOS converter. A schematic diagram of the model is given in figure 1. The simulation was carried out in a 3D thin slice of the model. The surface mesh of the model was developed in CAD software Rhinoceros 3.0 and imported in CFD simulation software AVL FIRE 2009.2 to generate volume mesh of the model.

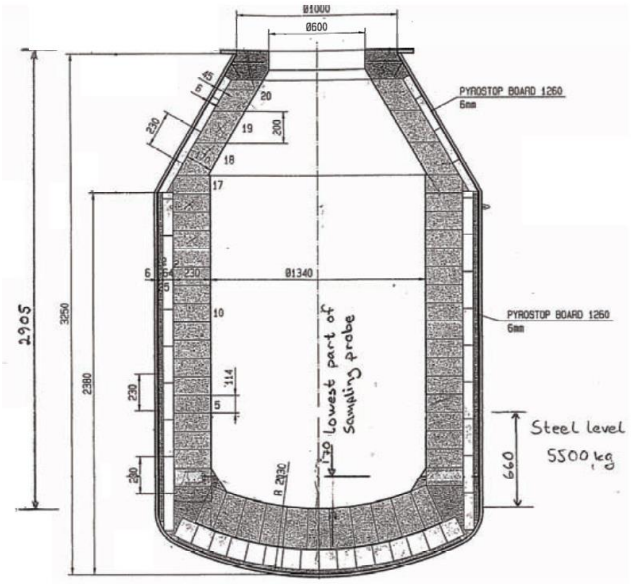

Figure 1. Schematic diagram of the 6 tonne BOS converter (Millman et al., 2011).

In the present study the model was simulated based on finite volume method and the simulation of multiphase flow was conducted according to the Euler-Euler approach. All the phases interact with each other in terms of mass, momentum and energy. The followings were the other conditions used in the simulation and with these conditions the model was simulated iteratively.

- The fluid is incompressible.
- Unsteady state multiphase solution was used for momentum and continuity.
- A standard k-ε model was used for turbulence.
- First order upwind differencing scheme was used for momentum and turbulence.
- Second order central differencing scheme was used for continuity equation.

Boundary Conditions and Initial Conditions

The inlet of the model was at the extended lance tip, which was placed in the middle of the converter. It supplied a supersonic oxygen stream into the converter, but the lance tip was extended and expanded until it becomes subsonic and subsonic inlet velocities were used in the simulation. Oxygen was supplied at a similar temperature to the liquid bath. Normal velocity boundary conditions were applied in the inlet for all the phases.

Static pressure boundary conditions were applied in the outlet, which was the top surface of the model. This outlet does not include the area of the lance. A non-slip wall boundary condition was applied to the wall of the model. The wall was assigned the same fixed temperature as the liquid.

In the present model, the converter was initially charged with approximately 5.5tonnes of molten pig iron at 1648^0C in to the converter and oxygen was injected on to it. The liquid height was around 660mm from the bottom of the converter. The simulation was run in an Intel(R) Xenon(R) CPU E5-1620 0 machine, where the RAM and the speed of the processor were 16GB and 3.60GHz respectively. And transient results were obtained by a time step of 0.1seconds for 20minutes in real time.

Results and Discussion

Oxygen gas was injected at $25ms^{-1}$ in to the converter. This oxygen oxidised the elements in the bath and produced the oxides. This caused the volume fractions of the gas, liquid and foam phases to change. The volume fractions of each phase at four intermediate occasions are given in figure 2. It is evident from the figures that;

- The gas injected reacts and lifts the liquid around the nozzle and the excess gas escapes along the outer periphery of the nozzle. Oxygen is spent for oxidising the elements and carbon monoxide is generated by the reactions involving carbon.
- The liquid volume fraction stays unchanged. The increase of liquid due to the formation of oxides has balanced by the reduction of liquid due to the formation of foam.
- The foam formation is high at the middle part of the blow reaching its maximum height around 6 minutes into the blow, which is also observed by the Millman et al (Millman et al., 2011). The height of the foam increases towards the middle of the blow and reduces in a small amount towards the end of the blow.

Composition Change of the Impure Elements (C, Si, Mn and P)

In steelmaking the required steel composition is achieved through oxidising the impure elements from the liquid bath. Carbon and silicon in the bath oxidise in the first part of the blow and their removal kinetics is hardly dependant on the chemical composition of the bath. Phosphorus and manganese oxidise and de-oxidise throughout the blow, due to the dependence of their removal kinetics on the chemical composition of the bath.

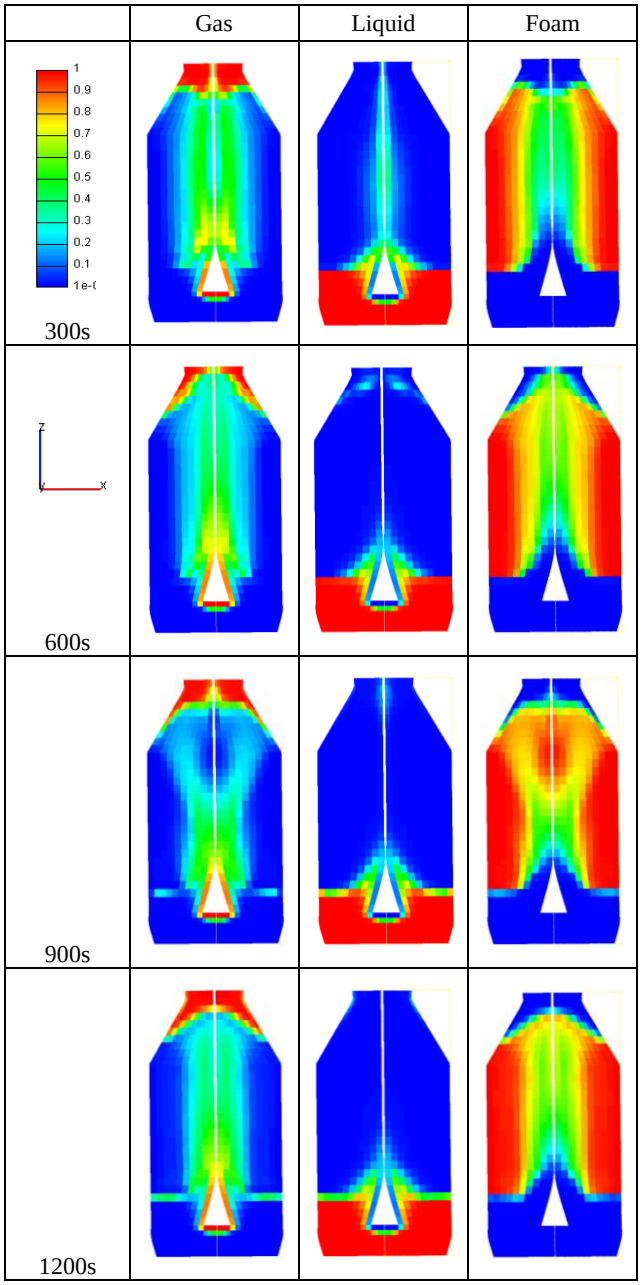

Figure 2. Volume fraction of each phase at selected time steps.

In the present study the removal behaviour of each element was monitored and compared against the published data for heat 1843 by Millman et al (Millman et al., 2011).

The figures 3-6 show the results obtained for the removal behaviour of carbon, silicon, manganese and phosphorus after the simulation. Simulation results show that the decarburisation reaction rate was high at the first several minutes and gradually reduced achieving the same composition as the actual process at the end of the blow (Figure 3). The rate of the silicon oxidation used in the simulation was low compared with that of the actual process, but followed a similar pattern and achieved the equilibrium at the end of the blow (Figure 4). Phosphorus removal rate used in the simulation shows a good agreement with the observed data by Millman et al (Figure 5), while manganese does not show any agreement with that observed (Figure 6).

Figure 7 shows the approximate refining behaviour of the iron in the bath during the blow.

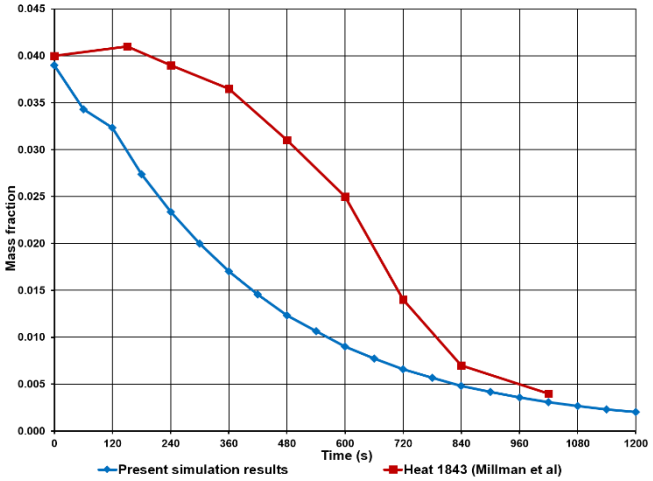

Figure 3. Carbon removal behaviour during the blow.

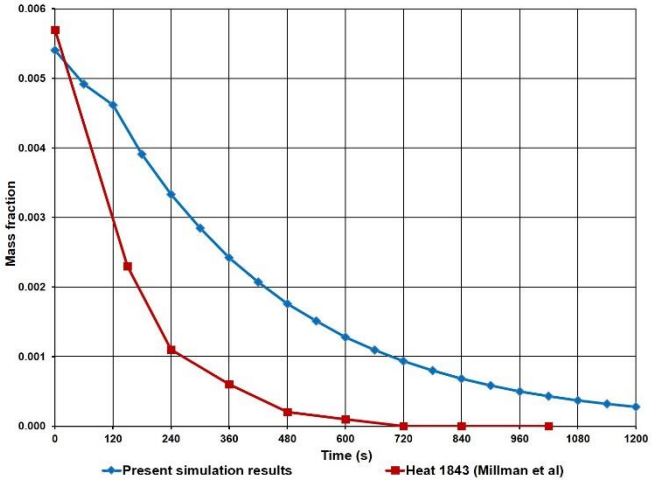

Figure 4. Silicon removal behaviour during the blow.

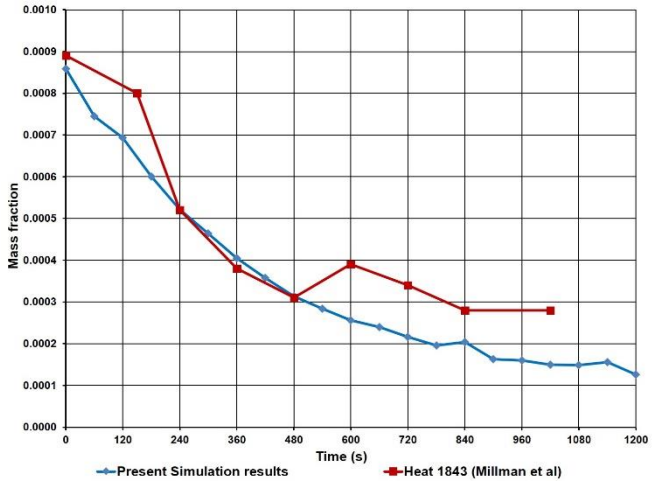

Figure 5. Phosphorus removal behaviour during the blow.

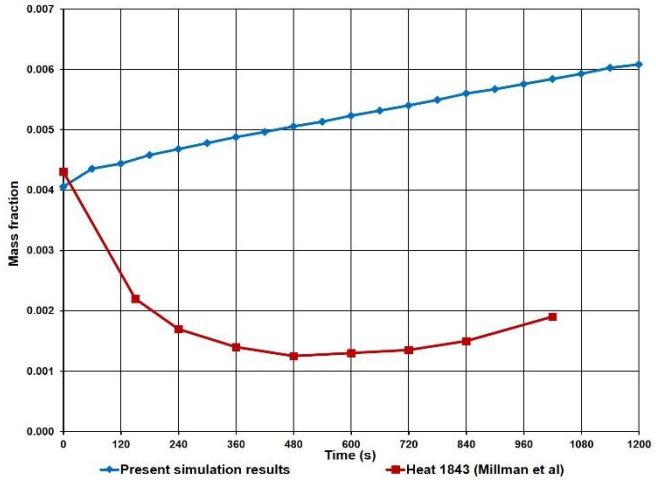

Figure 6. Manganese removal behaviour during the blow.

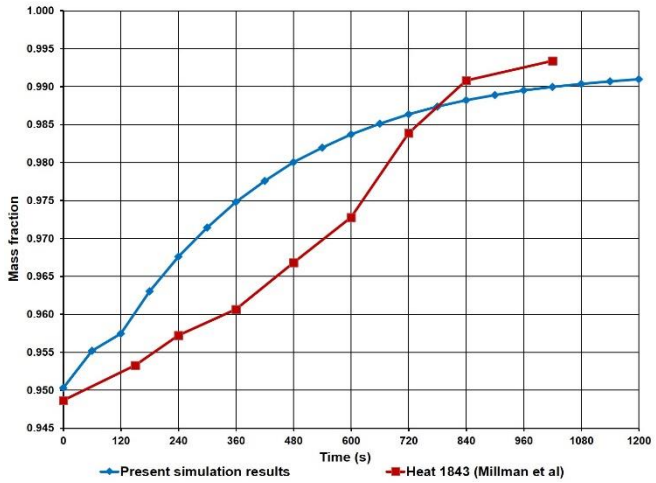

Figure 7. Iron refining behaviour during the blow.

The reaction rates of the refining reactions in the steelmaking process are highly dependent on the chemical composition of the metal bath. The evolution of the chemical composition is a combined result of oxidising reactions of impure elements in the bath and the dissolution of added fluxes and scrap to the bath during the process. Although the former effect is addressed in this study the latter effect is not included. Therefore incorporation of the flux and scrap is to be included in the present model.

Conclusions

According to the obtained results, the removal behaviour of carbon and silicon follows a similar trend to that of actual process, but the rate of reaction of carbon is over-predicted while that of the silicon is under-predicted. For phosphorus, the predicted removal behaviour agrees well with the observed data, but manganese removal behaviour does not show any compliance. This is a preliminary investigation and the authors are looking into the care of anomalous behaviour of manganese removal.

Future Work

In the present study the model only has three phases; gas, liquid and foam, but in real steelmaking process the oxides form a separate phase called slag. And the slag forms the foam. Therefore a separate phase for slag will be introduced into the model simultaneously with the chemical reactions. Then the physical properties of the slag will be calculated with the evolution of the slag and thereby calculate the formation and drainage of foam from slag. Therefore incorporation of the separate slag phase and physical properties will reduce the deviations in the results of the simulation. Also the evolution of slag depends on the dissolution of added flux and scrap. So the dissolution of scrap and fluxes will be included in the model.

References

[1]. Dogan, N., *Mathematical Modelling of Oxygen Steelmaking.* Doctor of Philosophy, Swinburne University of Technology, 2011.

[2]. Fruehan, R. J. & Jiang, R., Slag foaming in bath smelting. *Metallurgical transactions B*, 22B**,** 1991, 481-489.

[3]. Millman, M. S., Kapilashrami, A., Bramming, M. & Malmberg, D., *Imphos: improving phosphorus refining*, 2011.

[4]. Sattar, M. A., *Numerical simulation of foaming in metal processing with population balance modelling.* Doctor of Philosophy, Swinburne University of Technology, 2013.

[5]. Sattar, M. A., Naser, J. & Brooks, G., Numerical simulation of creaming and foam formation in aerated liquid with population balance modeling. *Chemical Engineering Science,* 94**,** 2013a, 69-78.

[6]. Sattar, M. A., Naser, J. & Brooks, G., Numerical Simulation of Slag Foaming in High Temperature Molten Metal with Population Balance Modeling. *Procedia Engineering,* 56**,** 2013b, 421-428.

[7]. Sattar, M. A., Naser, J. & Brooks, G., Numerical simulation of two-phase flow with bubble break-up and coalescence coupled with population balance modeling. *Chemical Engineering and Processing: Process Intensification*, 2013c