Application of Multiphysics in the Simulation of Metallurgical Processes

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Abstract: In the steelmaking processes, the stirring of the metal bath by argon (or nitrogen) injection is a widely used method to achieve thermal homogeneity. chemical or Computational fluid dynamic can be used as a very powerful tool to gain an insight into the mass transfer and heat transfer in liquid steel. In the present paper, the flow behaviors in two different steelmaking reactors were simulated using COMSOL 3.5. The first model was used to calculate the Argon-stir induced flow in the metal bath inside a 300 ton converter. In the second model, the effect of gas stirring on the mixing time in a 180 ton ladle for chemical homogenization was investigated. In both cases, the effect of argon gas flow rate on flow in the reactors was investigated.

Keywords: steelmaking, stirring, mixing, converter, ladle

1. Introduction

The production of steel involves a number of different processes which utilize stirring of the metal bath by argon gas injection. One of these processes is the basic oxygen steelmaking process (BOS) in which pig iron is decarburized by oxygen blowing. Another process during the secondary steel making is the ladle treatment in which chemical and thermal homogenizations are crucial objectives.

In both of these processes the metal bath is stirred to improve the kinetic conditions in the processes. In the BOS process it is important to have a sufficient rate of stirring so that the metal is as close to chemical homogeneity as possible. A too low carbon concentration close to the slag would result in a slower decarburization rate. The ladle treatment utilizes the stirring to achieve chemical and thermal homogeneity in the steel. However, a too high flow causes increased refractory wear and higher process cost. Hence, it is important to find an optimum stirring rate for process. Computational fluid dynamic (CFD) is a powerful tool to get an insight into the various metallurgical processes. In this paper two different models are looked at. One investigates the flow induced by Argon stirring in 300 ton BOS vessel. The other one calculates the mixing time in a 180 ton vessel in ladle treatment.

2. Governing Equations

All governing equations used for the models were taken from COMSOL Multiphysics 3.5 Chemical Engineering module. In both models the bubbly flow was utilized to model the flow induced by Argon stirring. In the ladle model mass transfer was coupled with bubbly flow to simulate the mixing. In this section the conservation equations are described.

2.1 Conservation of momentum

The governing equations used by the bubbly flow mode in COMSOL 3.5 is a two-phase model, with each phase having a separate velocity field. The momentum equation is expressed as:

$$\phi_{l}\rho_{l}\frac{\partial u_{l}}{\partial t} + \phi_{l}\rho_{l}u_{l} = -\nabla p_{l} + \phi_{l}\rho_{l}g + F$$
$$+\nabla \left[\phi_{l}(\eta_{l} + \eta_{T})\left(\nabla u_{l} + \nabla u_{l}^{T} - \frac{2}{3}(\nabla u_{l})I\right)\right]^{(1)}$$

The continuity equation is expressed as:

$$\frac{\partial}{\partial t} \left(\rho_l \phi_l + \rho_g \phi_g \right) + \nabla \cdot \left(\rho_l \phi_l u_l + \rho_g \phi_g u_g \right) = 0 \quad (2)$$

Where ϕ is the fraction of liquid or gas phase, ρ is the density [kgm⁻³], **u** is the velocity vector [ms⁻¹] and η the viscosity [Pas].

2.2 Conservation of Mass

In the ladle simulation, the mixing of alloying elements is modeled with the Convection and diffusion mode in COMSOL shown in equation (3),

$$\frac{\partial c_i}{\partial t} + \nabla \left(-D_i \nabla c_i \right) = R_i - u \nabla \cdot c_i \quad (3)$$

Where c is element transported, D $[m^2s^{-1}]$ is the diffusion coefficient, R $[molm^{-3}s^{-1}]$ is the rate of generation, **u** is the velocity vector $[ms^{-1}]$. The velocity vector u was coupled with the velocity vector in equation (1) for liquid.

3. Model descriptions

The model of the 300 ton BOS vessel (see Figure 1) consists of one domain with 3 inlets. The vessel has a diameter of 6 m and the metal bath height is 1.5 m. The model only utilized to the bubbly flow mode to calculate the flow profile within the converter vessel. The BOS model has a tetrahedral mesh consisting of roughly 20,000 elements.

The model of the ladle can be seen in figure 2. The model consists of two domains both which makes up the metal volume inside the ladle. The vessel has a height of 3.18m and lower and upper diameter of 2.97m and 3.25m respectively. The small sub domain at $0.5m^3$ acts as the container of alloying element at the beginning of the calculation. The mesh used for calculations is tetrahedral with about 18000 elements.

The following assumptions were made for both of the models:

(1) Only 2 phases are present in the system, liquid metal and gas.

(2) Temperature is assumed to be constant throughout the model. This assumption is justified by fact that the forced convection due to stirring is the dominant factor.

(3) As an consequence of the assumption of constant temperature, the density and viscosity are assumed to be constant. The values of these properties are given in Table 1.

(4) No top phase (slag) is present and the surface is assumed to flat.



Figure 1. The simulating Domain of the BOS vessel.



Figure 2. The Simulating domain of the Ladle vessel.

(5) The stirring rate is assumed to be constant throughout the entire calculation time.

(6) The K- \mathcal{E} model is employed to calculate turbulent flow.

The following assumptions are made only for Ladle model:

(7) All alloying elements are assumed to exist in the small sub domain from start of calculation.

(8) The mass transfer is solved in transient mode using a pre-solved flow profile in the vessel.

(9) No mass of alloying element is being added or lost through chemical reaction, R=0.

3.1 Boundary Conditions

The following boundary conditions are adopted in the simulation.

(A) The vessel walls are set to the logarithmic wall function.

(B) The walls are insulating for the gas phase.

(C) The gas inlets are set to a gas flux $[kgm^{-2}s^{-1}]$ to get right flow rate $[Nm^{3}h^{-1}]$.

(**D**) The steel surface boundary is set to outlet for the gas phase.



Figure 3. The flow profile through center inlet at (A) $400 \text{Nm}^3 \text{h}^{-1}$, (B) $600 \text{Nm}^3 \text{h}^{-1}$ and (C) $800 \text{Nm}^3 \text{h}^{-1}$.



Figure 4. Plot showing the Z velocities on a line through the center porous plug at a height of 0.6m.

3.2 Computing

For all calculations, the Paradiso solver is used. The fluid flows for both vessels are solved in transient mode with a solution time of 300 second. The solution at 300s is used as initial condition for a stationary solution in case of the converter model. In the case of the ladle model, the flow is calculated first. Once the flow is obtained, it is used for the calculation of mass transfer inside the ladle.

4. Results

4.1 Converter model

The flow profile within the vessel is calculated for 3 different total flow rates between

400 and $800Nm^3h^{-1}$ through three porous plugs. In Figure 3 the flow profile in slice through the central plug can be seen. All three cases display very similar flow profiles with higher velocities at higher flow rates. The Z velocities along the line at a height of 0.6m in the plane seen in figure 3 are presented in Figure 4 for different gas flow rates. The figure shows that higher flow rate does give higher velocities although the difference is not profound.

4.2 Ladle model

The mixing time is calculated for a number of different flow rates ranging from $5Nm^3h^{-1}$ to $40Nm^3h^{-1}$. In each case the mixing time is investigated at different positions within the model domain.

The mixing time, $\tau_{95,99}$, is the time required to reach a degree of mixing of 99% and 95% respectively.

$$\tau_{95,99} = \frac{|c|}{c_{\infty}} \quad (4)$$

The apparent mixing time varies depending on the position, as seen in figure 5. The mixing time is decided by the longest mixing time among the analyzed points within the domain. The obtained mixing time for six different flow rates can be seen in Figure 6. The calculation shows a significant decrease in mixing time at higher stirring rates.



Figure 5. A plot showing the apparent mixing time at 3 different positions within the ladle.



Figure 6. The mixing time in the ladle for 6 different stirring rates.

The gap between τ_{95} and τ_{99} is seen to decrease with increased stirring intensity. The velocity field in a slice through the porous plug can be seen in figure 7. A noticeable increase in the velocity along the walls can be seen with higher stirring rate.

5. Discussion

The CFD calculations, figure 6 ,show a mixing between 2 to 3 minutes for stirring rates above $15Nm^3h^{-1}$. For lower stirring rates the mixing show a significant increase. Industrial experiments^[11] carried in a 185 ton ladle reveal a mixing time, τ_{95} , of 200 to 240 seconds for a stirring rate of $6Nm^3h^{-1}$ on single porous plug, depending on the location. In the same experiments with a single porous plug at $12Nm^3h^{-1}$, a mixing time about 140 seconds is observed. This is in good agreement with the CFD calculation put forward in this paper.

A mixing time of 2 to 3 minutes is a short time compared to the full operational time for a ladle treatment. In cases where it is not important to achieve chemical homogeneity quickly it might be preferable to keep stirring rate down. In fact higher velocities associated with higher flow rate (see figure 7) cause refractory wear which would act as a inclusion source to the melt^[2].

In the converter process the surface of the metal bath will see a decrease in reacting elements as a result of the decarburization as well as dephosphorization. It is thus important to achieve good mixing of metal bath, so the stirring will bring fresh steel from lower bath up to the surface. The calculations show similar flow profiles for the used stirring rates and higher velocities with flow intensities. However the difference, as seen in Figure 4, is not profound. A doubling of the gas flow rate from $400 \text{Nm}^3\text{h}^{-1}$ to $800 \text{Nm}^3\text{h}^{-1}$ would only bring about a 20% increase in Z-velocity in the plume.

5. Conclusions

Two simplified models of steel making processes were successfully developed using COMSOL 3.5. The gas stirred induced flow and associated mixing times were predicted in the models. The mixing time in the ladle model was found to be in agreement with industrial trials for similar vessel size and stirring.



Figure 7. Showing the velocity field in a slice through the porous plug at (A) $20Nm^3h^{-1}$, (B) $40Nm^3h^{-1}$.

6 References

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7. Appendix

 Table 1: Physical properties used in the model calculation

Fluid	Density ρ [kgm ⁻³]	Viscosity η [PaS]
Steel	7000	7*10 ⁻³