Modeling of Decarburization in Metal Droplet in Basic Oxygen Steelmaking

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Abstract: Basic Oxygen Steelmaking is the process of refining hot metal obtained from blast furnace using oxygen. In the process, supersonic jet of oxygen is blown over the metal bath resulting in formation of droplets. The droplets mix with slag to form an emulsion in which refining reactions take place. Among those reactions, decarburization reaction is the most important one. In present study decarburization reaction in the droplet is simulated. The possibility of formation of carbon monoxide and subsequent effect on the droplet too is evaluated. The carbon and oxygen are allowed to react to form carbon monoxide. The oxygen concentration is fixed at the boundary and all three species are considered to take part in the diffusion reaction. The effect of presence of bubble inside the droplet as well as concentration profile in deformed droplet has been attempted in this paper.

Keywords: Steelmaking, diffusion

1. Introduction

The Basic oxygen steelmaking is the process of refining the hot metal produced from a blast furnace [1]. The objective is to reduce the amount of carbon, silicon and phosphorous to a predefined limit by means of oxidizing them by supplying oxygen at supersonic speed. Due to the impact of oxygen at such high momentum, the metal droplets are ejected and get embedded in slag resulting into the formation of an emulsion as metal and slag are immiscible. The metal droplets undergo refining reactions in emulsion where the oxidizing slag acts as oxygen supplier. The droplets also show complex behavior like bloating and breakage [2]. The origin of these phenomena lies in the change of the composition of species within the droplet due to chemical reactions. Hence, the study of carbon composition field inside the droplet is undertaken in this study.

2. Theory

In steelmaking converter, the generated droplet underdo different reactions. Among them decarburization is one of the most important reaction. A fraction of total decarburization occurs in emulsion where the metal droplets react. The carbon in the droplet reacts with oxygen to form carbon monoxide according to the following reaction (R1) [3].

$$[C]+[O] \rightarrow CO \qquad \ldots (R1)$$

The amount of oxygen is determined by the oxidizing potential of the slag. There remains a supply of oxygen from the boundary towards the center of the droplet. The carbon and carbon monoxide formed also diffuse towards the interface.

3. Use of COMSOL Multiphysics

COMSOL Multiphysics (R) was used as the tool for simulation studies for the ease of coupling different physics together. The chemical reaction engineering module coupled with the transport of dilute species module was used for the study of composition field. Two domains were defined with one representing metal droplet and the other representing slag. The chemical species (carbon) was distributed in the metal domain and allowed to react. The reacting species considered were carbon and oxygen with carbon monoxide being the product. The interface between slag and metal was the boundary and the composition of this layer in equilibrium was taken as the boundary condition for solving the diffusion and transport equation.

4. Governing Equations

Based on reaction R1, the following equations was used which included diffusion of the species:

$$\frac{dc_i}{dt} + \nabla(-D_i \nabla c_i) = R_i \qquad \ldots (E1)$$

where, c_i is the concentration of species i, D_i is the diffusion coefficient of species i and R_i is the

rate constant. Convention term was not used in the equation as no convention was considered in the system under study.

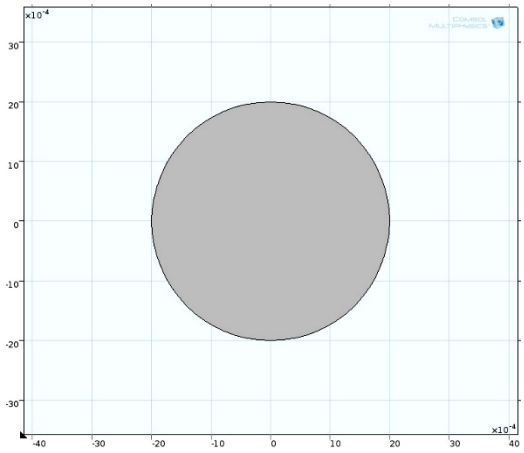

Figure 1: Geometry of the droplet under study

5. Model Development

The dimensions of the system are shown in Figure 1. A batch type constant volume reactor was considered for the system. The reaction 1 was taken as irreversible. The initial condition was carbon: 2 mol/m^3, oxygen: 0.1 mol/m^3 and CO: 0.01 mol/m^3. Only diffusion was considered as transport mechanism. The values of diffusion coefficient are shown in Table 1. For carbon and carbon monoxide, a no flux boundary condition was used i.e. all carbon monoxide generated stayed inside the droplet. For oxygen, a fixed concentration of 0.1 mol/$m^3$was considered at the boundaries. The system was solved using COMSOL Multiphysics®.

Table 1: Diffusivity Coefficients (D_i) of species

Species	D_i **(in m^2 s^{-1})**
Carbon	2 x 10 $^{-9}$ [4]
Oxygen	2 x 10^{-7} [5]
Carbon Monoxide	9.8 x 10 $^{-9}$ [6]

6. Results:

The results are shown in Figure 2 - 7. Figure 2 - 4 correspond to time of 2.2 seconds from the start and figures 5 - 7 correspond to time 9.2 seconds from the start.

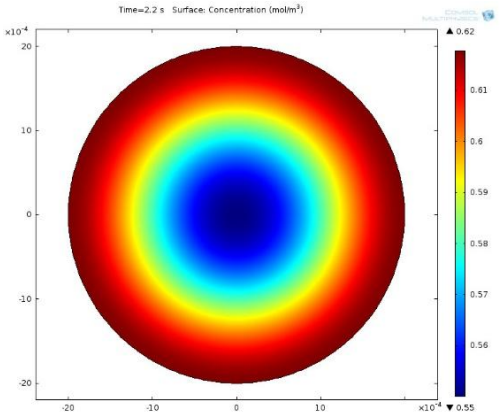

Figure 2: Concentration profile of CO in the droplet at 2.2 seconds

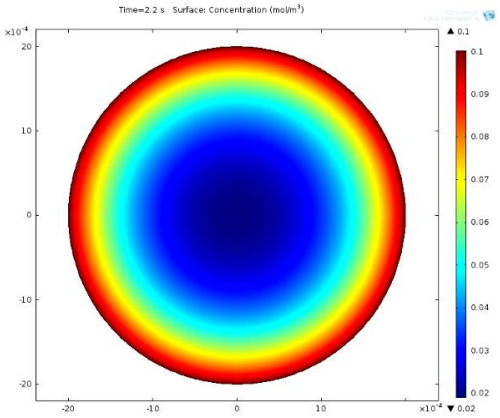

Figure 3: Concentration profile of O in the droplet at 2.2 seconds

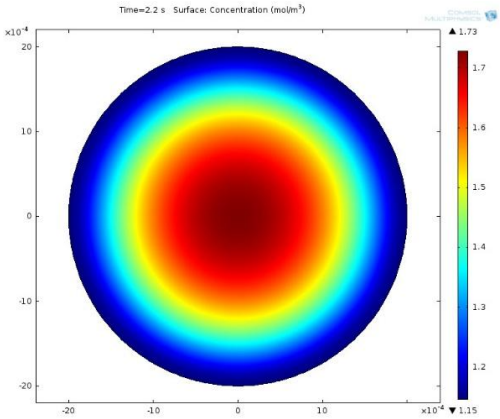

Figure 4: Concentration profile of C in the droplet at 2.2 seconds

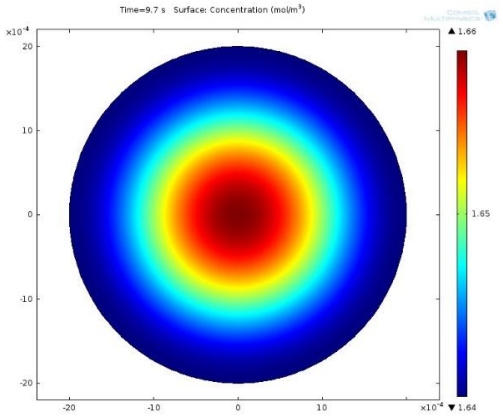

Figure 5: Concentration profile of CO in the droplet at 9.2 seconds

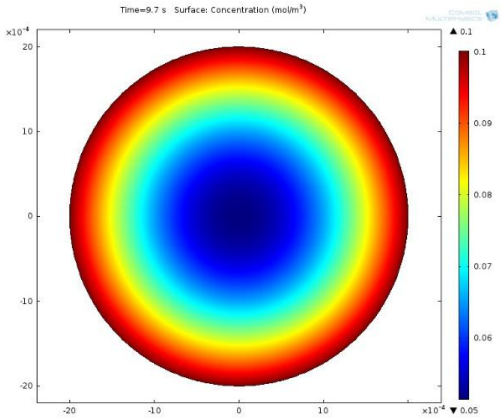

Figure 6: Concentration profile of O in the droplet at 9.2 seconds

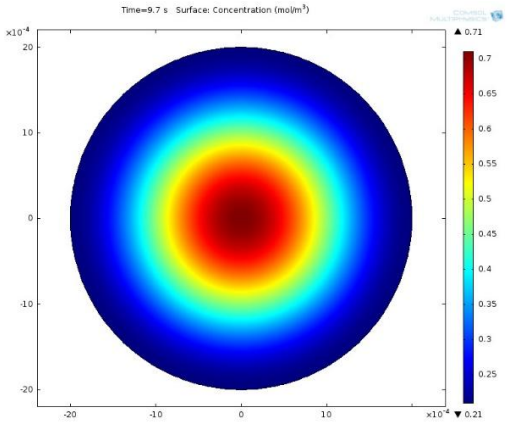

Figure 7: Concentration profile of C in the droplet at 9.2 seconds

7. Discussion

As seed from figures 2-7, the concentration profiles have been satisfactorily simulated. In the initial states, the concentration of carbon monoxide is higher near the edges than in the bulk as the oxygen is supplied at the interface. Thus in the initial stages of the reaction, the possibility of nucleation and growth of carbon monoxide bubble is higher near the surface. Near the surface, the bubble can escape the droplet and get transferred to slag or even escapes to atmosphere. This has been reported in literature that a gas halo has been observed around the droplet in the slag undergoing reactions. Another possibility is the nucleation of CO bubble inside the droplet and the droplet does not escape. The possibility of this case increases with time as seen from the figures 5-7. The concentration of the CO has increased and nucleation inside the droplet too has started. The droplet generated inside can be stabilized by the hydrostatic pressure of the droplet and do not escape- thus causing the droplet to bloat. Since, the nucleation and growth of the droplet is a continuous process, the droplet will not maintain its shape throughout the reaction. In figure 8, a bubble was introduced into the droplet to simulate the distribution of CO gas around it. The simulation showed that there is higher chance of the new bubble to be generated in the smaller gap from interface and the existing bubble. It was assumed that the bubble does not take part in the reaction in this case. Thus, a new bubble may be formed and similarly many other bubbles too also can form. The surface tension of the droplet too is a function of the concentration [7] and at certain places, the surface tension may drop and combined with the pressure exerted by the bubbles, the droplet may break into smaller droplets. This has been observed in the steelmaking process but the source of this phenomenon is still a topic of debate [2].

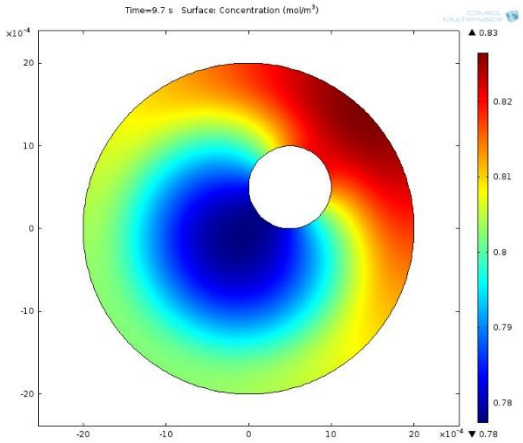

Figure 8: Concentration profile of CO in the bubble filled droplet at 9.2 sec

Apart from having a bubble, the change in interfacial surface tension can cause flattening of droplet thus changing the shape of the droplet from regular spherical [8]. A study of similar case is shown in figure 9.

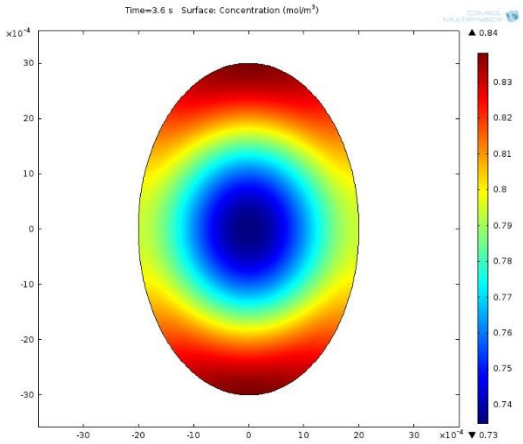

Figure 9: Concentration profile of CO in the deformed droplet at 3.6 sec

8. Conclusions

The framework has been developed to study the composition field of the species in the metal droplet in the metal-slag emulsion. The obtained composition fields can be further used to develop surface tension field according to available relations [7]. Based on the surface tension profiles, and presence of droplets, the breakage of droplet can be predicted which will help in evaluating the instantaneous interfacial area of the droplet while undergoing reactions.

9. References

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