Modeling of Decarburization in Metal Droplet in Basic Oxygen Steelmaking

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Introduction: Decarburization is one of the important reactions occurring in basic steelmaking converter. Recent studies have highlighted the role of the droplets in metal slag emulsion in refining reactions. The present work is aimed at simulating the concentration profiles of carbon, oxygen and carbon monoxide in metal droplet undergoing reactions in emulsion.

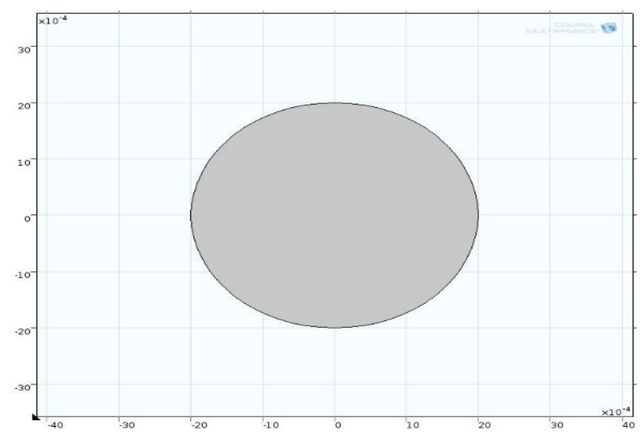

Figure 1. Geometry of the droplet under study

Computational Methods: In COMSOL, 'Reaction Engineering' and Transport of Dilute Species' interfaces' were used. The governing equations were:

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

$$[C] + [O] \rightarrow CO$$

A Batch, constant volume, reactor was considered for the system. The reaction 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, no flux condition was used, i.e. all the carbon monoxide generated remained inside the droplet. For oxygen, a fixed boundary value concentration of 0.1 mol/m^3 was considered.

Results: Results of simulation are shown in Figures 2-4. The concentration profiles of carbon monoxide is plotted against various conditions of the droplet. In figure 3, the droplet already has a bubble and in figure 4, the droplet is deformed.

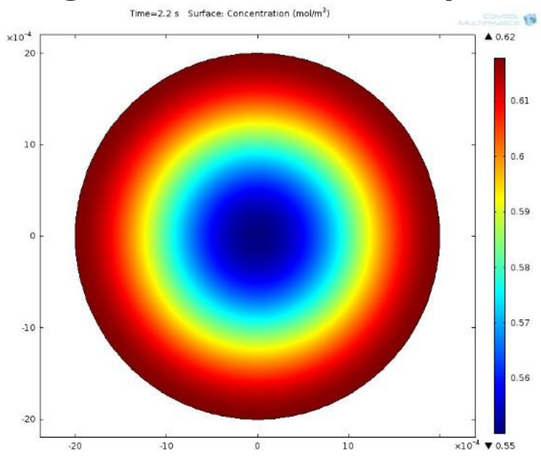

Figure 2. Concentration profile of CO in the droplet at 2.2 seconds

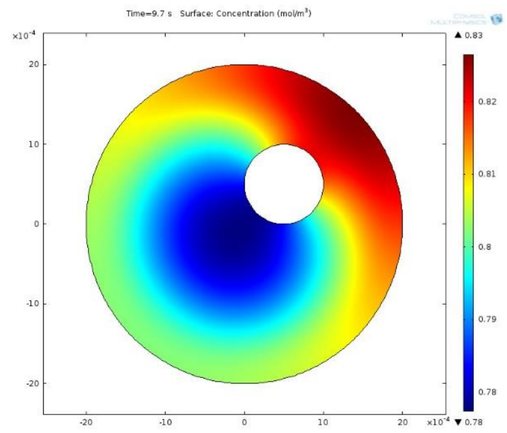

Figure 3 Concentration profile of CO in the bubble filled droplet at 9.2 sec

Species	Diffusion Co-efficient (in m^2 s^{-1})
Carbon	2 x 10 $^{-9}$
Oxygen	2 x 10^{-7}
Carbon Monoxide	9.8 x 10 $^{-9}$

Table 1: Diffusion Coefficients of species

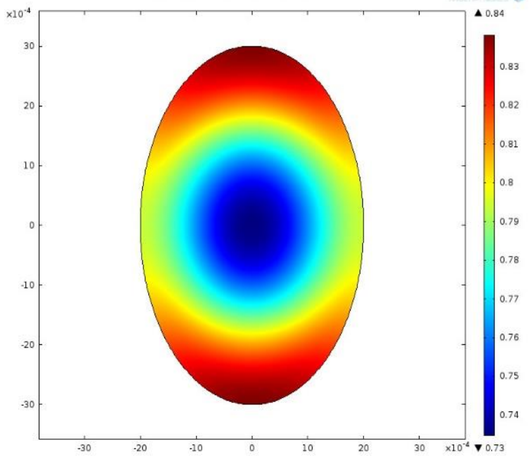

Figure 4. Concentration profile of CO in the deformed droplet at 3.6 sec

Conclusions: The framework has been developed to study the composition field of the metal droplet in the metal-slag emulsion. The results will enable studies of other composition dependent phenomena like surface tension which result in breakage of a droplet.

References:

1. A. Ghosh and A. Chatterjee, Iron making and steelmaking. New Delhi: Prentice-Hall of India, (2008)
2. H. Sun, 'Reaction Rates and Swelling Phenomenon of Fe-C Droplets in FeO bearing Slag', ISIJ Int., vol. 46, no. 11, pp. 1560-1569, (2006)