1-1-2010

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Neslihan Dogan  
*University of Wollongong, ndogan@uow.edu.au*

Geoffrey A. Brooks

Muhammad A. Rhamdhani

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**Recommended Citation**

Dogan, Neslihan; Brooks, Geoffrey A.; and Rhamdhani, Muhammad A.: Kinetics of decarburization reaction in oxygen steelmaking process 2010, 9-11.  

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KINETICS OF DECARBURIZATION REACTION IN OXYGEN STEELMAKING PROCESS

Neslihan Dogan, Geoffrey A. Brooks and Muhammad A. Rhamdhani
Swinburne University of Technology, Hawthorn, VIC 3122 Australia

Key words: global model, decarburization, emulsion, oxygen steelmaking, bloated droplet

The steelmaking process is complex since it involves simultaneous multi-phase (solid-gas-liquid) interactions, chemical reactions, heat and mass transfer and complex flow patterns at high temperatures. The transient nature of the process also adds more complexities and the severe operating conditions inhibit the direct measurement and observation of the process. This difficulty can be addressed by developing models, which make it possible to describe the complicated nature of the process itself and to understand the interconnection of important process variables. A global model of oxygen steelmaking focusing on the overall decarburization of the process and including the new bloated droplet theory has been developed.

Decarburization reaction occurs in different reaction zones using various reaction mechanisms. There are two main reaction zones considered in this study, which are bath and emulsion zone. At the impact zone, as top-blown oxygen reaches to the surface of the liquid bath, it reacts with carbon dissolved in the metal and forms a mixture of CO-CO2 gases as product. Carbon monoxide further oxidized to carbon dioxide. Subsequently, dissolved carbon also reacts with CO2 simultaneously at this region. The sequence of the decarburization reactions as follows;

\[
\begin{align*}
\text{[C]} + \frac{1}{2}\text{O}_2(g) & = \text{CO}(g) \quad \text{(Eq. 1)} \\
\text{[C]} + \text{CO}_2(g) & = 2\text{CO}(g) \quad \text{(Eq. 2)}
\end{align*}
\]

It is suggested that gaseous diffusion controls the decarburization rate down to the critical level of carbon, where carbon diffusion in liquid phase becomes rate-limiting step. However, some investigators suggested that sulphur has a determining effect on the reaction rate and chemical reaction at the interface also controls the reaction rate. The mixed control mechanism involving both mass transfer in the gas phase and dissociative adsorption of CO2 was selected to be the rate determining step.

In the case of emulsion zone, it is proposed that FeO supplies oxygen and liberates CO2. Oxygen then reacts with CO at slag-gas interface and followed by reaction at the metal-gas interface with CO2 diffusion through the gas halo. CO2 provides oxygen to react with carbon in the melt. These reactions involve the sequence as below

\[
\begin{align*}
\text{CO}(g) + \text{(FeO)} & = \text{Fe} + \text{CO}_2(g) \quad \text{slag surface} \quad \text{(Eq. 3)} \\
\text{CO}_2(g) + \text{[C]} & = 2\text{CO}(g) \quad \text{metal surface} \quad \text{(Eq. 4)}
\end{align*}
\]

The overall reaction is

\[
\text{(FeO)} + \text{[C]} = \text{Fe} + \text{CO}(g) \quad \text{(Eq. 5)}
\]
There is no agreement on the description of the mechanism of this reaction and also the rate controlling step of this reaction under various operating conditions. In this study, carbon diffusion in the metal droplet was considered to be rate determining step. The total decarburization rate is obtained by the summation of decarburization rates of droplets with various residence times given in (Eq.6). The procedure to calculate the residence time of droplets was taken from the study of Brooks et al.\textsuperscript{1)} The generated droplets, whose residence time is smaller than given time-step, are returning from the emulsion phase.

\[
M_e \frac{dC}{dt} = \sum_{i=1}^{n} \frac{m_i}{100} \left( C_{i+\Delta t} - C_i \right) 
\]

(Eq. 6)

where \( n \) is number of present droplets in the emulsion, \( m_i \) is weight of a single droplet (kg) and \( C \) is the carbon content of droplet (mass%). In this model, carbon content of the metal droplet is assumed to be the same as bulk carbon content. The values for \( C_i \) are obtained from the mass balance calculation including scrap melting, decarburization reaction in emulsion and at the impact zone.

The global model, which utilizes numerical computational technique, has enabled us to predict the carbon content of bulk metal and metal droplets and the rate of decarburization reaction in the emulsion zone and impact zone throughout the blow for a given operating conditions of dynamics and materials additions for a given input conditions, weights, analysis of scrap and hot metal. The outcome of other refining reactions is entered as known variables from the industrial data. At the end of each time step, the new carbon composition can be evaluated, by means of mass transfer equations. It is considered to utilize the updated values from each sub-routine for the next step. The calculation in this model include the submodels kinetics of scrap melting, kinetics of flux dissolution, droplet generation, droplet residence time, decarburization in the emulsion and at the impact zone and offgas generation and temperature profile of the metal and slag phase. The required process data was obtained from the study of Cicuttì et al.\textsuperscript{2, 3}) Several of the submodels such as flux dissolution and droplet generation that form the global model were validated against industrial data and the results have been published.\textsuperscript{4, 5})

![Figure 1 - The comparison of bulk carbon content in metal bath calculated by the global model with the study of Cicuttì et al.](image-url)
Figure 1 shows the comparison of preliminary results of bulk carbon content of the bath as a function of time obtained from the global model with the study of Cicutti et al. It can be seen that the model can predict the change of carbon content well up to approximately two thirds of the blowing period.

The comparison of decarburization reaction in the process predicted by the global model is illustrated in Figure 2. The majority of decarburization during the main blow takes place in the emulsion zone based on the global model. This result is agreement with previous findings\(^6\), \(^7\) that showed that decarburization within the metal droplets dominates the refining of carbon in oxygen steelmaking process. Further optimisations are being carried out especially for the final stage of the blowing, e.g. including the effect of bath stirring.

![Figure 2 - The comparison of decarburization rates in oxygen steelmaking process calculated by the global model](image)

References: