



The development of simple correlation for carbon particles dissolving into liquid metal by using numerical models

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ABSTRACT

In this study, a single carbon particle dissolving into liquid metal has been numerically investigated by using a quasi-steady flow model and a transient-dissolution model. The dissolution rate is assumed to be controlled by carbon-mass transfer in liquid metal. It is found that the particle Reynolds number has significant effects on the dissolution rate and distribution on particle surface. If the Reynolds number is low, the highest dissolution rate is at the front stagnation point and monotonically decreases to the rear stagnation point. On the other hand, if the Reynolds number is high, the lowest dissolution rate is close to the flow separation point on particle surface, and the highest and the local highest dissolution rates are respectively at front and rear stagnation points because of the wake formed behind the particle. Furthermore, the shape evolution of dissolving particle at low and high Reynolds numbers are also simulated by using a transient-dissolution model. It is found that the particle body evolves into a self-similar shape during dissolution process. Due to the different dissolution rates and distributions on particle surface, the dissolution time and the shape variation during dissolution process are drastically different. It is found that the particle Reynolds number (the flow agitation) significantly affects particle dissolution. In addition, to simulate a large amount of carbon particles dissolving into liquid metal during steelmaking process, a simple correlation of particle dissolution rates is preliminarily established by using the quasi-steady flow model and further modified according to the numerical results obtained by using the transient-dissolution model.

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1. Introduction

In recent years, environmental issues have raised serious concerns and many researchers have put lots of effort into developing energy-saving technologies and green-power systems. It is known that steelmaking is one of the largest energy-consuming processes in manufacturing industries. In order to demonstrate the amount of fossil fuels consumed in the production of steel or iron, the concept of carbon footprint is used in steelmaking industry. In addition to the consideration of cost, low energy-consuming steel/iron (environmentally friendly) products will be more competitive in the future. Therefore, it is imperative to improve energy efficiencies and reduce the emission of pollutants in steelmaking industries.

As societies become increasingly industrialized, the amount of scrap steel/iron becomes noticeable in many developed and developing countries. So, using scrap to replace the virgin iron ore will

play an important role in steelmaking industries in the future. In current steelmaking processes, scrap is usually recycled by using Electric-Arc Furnace (EAF) and Basic Oxygen Furnace (BOF). In EAF process, scrap is the primary raw material (>80%) and is melted by using the electric power. On the other hand, scrap is added as a supplement (< 20%) in BOF process. The melting heat is provided by oxidation of carbon, silicon, etc. contained in liquid metal as oxygen is blown into the converter furnace. Comparing scrap recycling in these two processes, the energy cost and process time in EAF are much higher and longer than those in BOF. In addition, the amount of impurities in the liquid metal from EAF process greatly depends on the source of scrap if no additional process is included. Nevertheless, in BOF process, the impurities can be controlled and/or reduced during scrap-melting process to obtain the required quality. Therefore, it is beneficial to increase the usage of scrap in BOF process with the process period meeting the requirement of production line. For this purpose, additional carbonaceous energy sources are suggested to be added into the liquid metal for melting more scrap efficiently [1,2]. In addition to the addition of

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Nomenclature

Symbols

a	radius of carbon atom (m)	T	temperature (°C)
B	inverse of permeability (m^{-2})	T_0	reference temperature (°C)
C_1	permeability (m^2)	x	distance in the axial coordinate (m)
C_2	inertial resistance factor (m^{-1})	y	distance in the radial coordinate (m)
D	diffusivity of carbon atom in liquid metal ($m^2 \cdot s^{-1}$)	Y	mass fraction
d	particle diameter (m)	δ	distance vertical to the particle surface (m)
K	dissolution rate constant	μ	dynamic viscosity ($kg \cdot m^{-1} \cdot s^{-1}$)
k_c	mass diffusion constant ($m \cdot s^{-1}$)	ν	kinematic viscosity ($m^2 \cdot s^{-1}$)
\dot{m}	total mass dissolution rate ($kg \cdot s^{-1}$)	γ	porosity
\dot{m}''	mass dissolution rate per unit area ($kg \cdot m^{-2} \cdot s^{-1}$)	κ	Boltzmann's constant ($J \cdot K^{-1}$)
n	exponent factor	ρ	density of liquid metal ($kg \cdot m^{-3}$)
P	pressure ($N \cdot m^{-2}$)	ρ_0	reference density of liquid metal at T_0 ($kg \cdot m^{-3}$)
r	Radius of the carbonaceous particle (m)	ρ_c	density of graphite ($kg \cdot m^{-3}$)
\dot{r}	The reduction rate of particle radius ($m \cdot s^{-1}$)	$\bar{\tau}$	stress-strain tensor ($N \cdot m^{-2}$)
R	Gas constant ($J \cdot g \cdot mol^{-1} \cdot K^{-1}$)	Λ	control volume surface (m^2)
Re	The Reynolds number	\forall	control volume (m^3)
S	Source term ($kg \cdot m^{-3} \cdot s^{-1}$)		
Sc	The Schmidt number		
Sh	Sherwood number	<i>Subscript symbols</i>	
t	Time (s)	c	carbon
t_d	Dissolution time (s)	p	correlation system
u	Velocity in the axial coordinate ($m \cdot s^{-1}$)	o	initial condition
U	Inlet (relative) flow velocity ($m \cdot s^{-1}$)	sat	saturated condition
v	Velocity in the radial coordinate ($m \cdot s^{-1}$)	t	terminal condition
\vec{v}	Velocity vector ($m \cdot s^{-1}$)	∞	ambient condition

melting heat, the melting temperature is lowered in carburization process [3].

The dissolution process of carbon solids in liquid metal is usually divided into two consecutive steps [3,4]. The first step is the dissociation of carbon atoms liberated from solid structure into the interstitial positions of iron atoms. The second step is the diffusion and/or the convection of carbon atoms from the interface to the bulk liquid metal. Traditionally, the rate of carbon dissolution was considered to be limited by the carbon-mass transfer in liquid metal [5,6]. Later, the importance of the dissociation reaction at interface was also proposed for the less ordered atomic structure of carbonaceous materials [7–11]. Sun [3] developed a kinetic model for the dissolution rates, including the above two limiting mechanisms, to discuss the interdependency between rate influencing factors, e.g. temperature, carbon structure, interfacial active elements, liquid agitation, solid particle size, side reactions, etc. With the experiments carried out in his study, although there was no evidence to rule out the possibility of mixed limiting mechanism, he found that the mass transfer is the major limiting step. Therefore, the limiting mechanism of mass transfer is applied to investigate the carbon dissolution process in this study.

In carburization process, the alloy elements, such as S, Si, P, etc., can influence the dissolution rates in physical and/or chemical ways. It was found experimentally that adding small amount of sulphur in liquid metal can significantly reduce the carbon dissolution rate [7,8,12,13]. In addition, the carbonaceous sources may also affect the dissolution rate significantly. For example, the inorganic mineral substances in coke may form a blocking layer, reducing particle wettability, and therefore, decrease the dissolution rate [7,8,14–21]. Moreover, the volatiles in coal may further complicate the carbon dissolution phenomena [22]. In this study, the emphasis is placed on the mass-transfer-controlled dissolution rate, so the effects of alloy elements, mineral substances and volatiles in carbonaceous materials are currently not considered.

To maximize the contact area, the carbonaceous materials are preferred to be injected into liquid metal as small particles. The

carrier gas can also agitate liquid metal to enhance the dissolution rate. Several laboratory-scale experiments have been done in previous studies [13,23,24]. However, the understanding of the dissolution process and time for a single carbon particle in liquid metal is still limited. Since the fundamental understanding of the dissolution process from experimental measurements is very difficult, numerical models are suggested to help with the further investigation. In this study, in addition to the study of the dynamic dissolution process for a single carbon particle, a simple dissolution formula is also developed by using numerical models for further modeling and practical application.

2. Numerical model

The compositions of carbonaceous materials (coal, coke, etc.) are complicated and those compositions can affect carbon dissolution rates in different ways. Therefore, to simplify the dissolution phenomena, graphite (almost 100% carbon) is chosen and the effects of alloy elements in liquid metal are not considered. In the model simulation, the carbon particle is fixed in a forced flow with uniform inlet velocity, which represents the relative velocity between liquid metal and carbon particle. In addition, the carbon particle is assumed to be spherical, so two-dimensional axisymmetric models are developed in this study: transient-dissolution model and quasi-steady flow model. The model configuration is shown in Fig. 1. The transient-dissolution model, applying the modeling technique of porous medium, is used to simulate the dynamic dissolution process of a carbon particle in liquid metal. The porosities in the region occupied by carbon particle are initially 0, so the flow of liquid metal cannot pass through it. On the other hand, the porosities in the region of liquid metal are 1. As the particle dissolves into liquid metal, the porosities in the region of carbon particle will gradually become 1. For the quasi-steady flow model, it is assumed that the reduction rate of carbon particle is negligible on the flow time scale, and the flow pattern around it is at the quasi-steady state in dissolution process. There-

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