Mechanism and simulation of droplet coalescence in molten steel

Bing Ni\textsuperscript{1)}, Tao Zhang\textsuperscript{2)}, Hai-qi Ni\textsuperscript{2)}, and Zhi-guo Luo\textsuperscript{2)}

1) Department of Metallurgical Technology, Central Iron and Steel Research Institute, Beijing 100081, China
2) School of Metallurgy, Northeastern University, Shenyang 110004, China

(Received: 20 February 2017; revised: 29 April 2017; accepted: 4 May 2017)

Abstract: Droplet coalescence in liquid steel was carefully investigated through observations of the distribution pattern of inclusions in solidified steel samples. The process of droplet coalescence was slow, and the critical Weber number ($\textit{We}$) was used to evaluate the coalescence or separation of droplets. The relationship between the collision parameter and the critical $\textit{We}$ indicated whether slow coalescence or bouncing of droplets occurred. The critical $\textit{We}$ was 5.5, which means that the droplets gradually coalesce when $\textit{We} \leq 5.5$, whereas they bounce when $\textit{We} > 5.5$. For the carbonate wire feeding into liquid steel, a mathematical model implementing a combined computational fluid dynamics (CFD)–discrete element method (DEM) approach was developed to simulate the movement and coalescence of variably sized droplets in a bottom-argon-blowing ladle. In the CFD model, the flow field was solved on the premise that the fluid was a continuous medium. Meanwhile, the droplets were dispersed in the DEM model, and the coalescence criterion of the particles was added to simulate the collision-coalescence process of the particles. The numerical simulation results and observations of inclusion coalescence in steel samples are consistent.

Keywords: mechanism; simulation; droplet; collision; coalescence; molten steel

1. Introduction

Particle aggregation is used to remove the inclusions generated during multiphase flow in molten steel [1–3]. During composite deoxidation, small droplets are formed in molten steel and polymerized inclusions along with droplets in excellent condition are washed away [4–5]. In addition, several class-D inclusions containing MnS are removed, facilitating droplet coalescence. Unlike the bubble removal of solid inclusions [6–7], the droplets generated in molten steel combine with the solid and liquid inclusions and float on the slag. Thus, observing the input and output of droplets is difficult. The collision and coalescence of particles including the droplets are used to remove the inclusions in molten steel. Previous studies on sparse two-phase flow, i.e., where the volume fraction of particles in the dilute phase is $\leq 10\%$, have mainly ignored the precondition of particle collision. Nevertheless, recent studies have shown that, even if the volume fraction of particles is only $4 \times 10^{-4}$, particle collision cannot be ignored [8–9]. The conditions in the interior of the liquid steel cannot be observed at high temperatures. Therefore, numerical simulations of the dynamic behavior of particle motion, collision, aggregation, and coalescence in molten steel are critical.

In this study, we investigated the coalescence of droplets in liquid steel by observing the distribution patterns of inclusions in solid steel samples. Generally, the computational fluid dynamics (CFD) methods of numerical simulation of multiple phases include both Eulerian and Lagrangian methods. The former regards both the fluid and the particles as a continuum; the latter regards the fluid as a continuum and the particles as a discrete system. In the traditional sense, the Lagrangian method (including the Euler–Lagrangian method, the direct numerical simulation method, and the volume-of-fluid method) does not take into account the interactions among the particles or the effect of the particle volume fraction on the continuous phase. Because ignoring the collisions among particles is inappropriate, a numerical simulation should be carried out using, for example, the discrete element method (DEM). The DEM includes solving the Newton’s second law under the Lagrangian system, dynamically simulating each particle in the system, and assessing the interaction
of particles under the effect of the fluid field as well as the exchange of mass, momentum, and energy among particles. Therefore, in the present work, a mathematical model based on a CFD + DEM approach was used to simulate the movement and coalescence of droplets of various sizes in a continuously bottom-argon-blown ladle. The simulation results indicate the capture and removal of inclusions. This study provides a theoretical basis for the production of clean steel.

2. Droplet coalescence in molten steel

2.1. Experimental procedure

A 60-t ladle furnace was used, and the molten steel was maintained at (1873 ± 10) K. The chemical composition (wt%) of ship plate steel is C 0.15, Si 0.32, Mn 1.45, P 0.021, S 0.018, and Al 0.030. The Si–Mn–Al–Fe alloy with a chemical composition (wt%) of Si 30, Mn 45, Al 10, and Fe 15 was added to the ladle to deoxygenate and produce a white slag, which was sampled every minute. We collected a steel sample 20 min after adjusting the chemical composition. The samples were rapidly cooled to room temperature to preserve their original high-temperature characteristics. The steel samples were cut, ground, and polished, and the inclusions were characterized using a metallographic microscope, a Philips Quanta 400 scanning electron microscope, and an Oxford INCA spectrometer.

2.2. Droplet coalescence

The number and morphology of inclusions are shown in Fig. 1. There are many inclusions at the beginning of deoxidation, and a majority of the inclusions had diameters between 5 and 50 μm. Inclusions greater than 10 μm were nearly nonexistent after 20 min. During deoxidation, early in the refining stage, the initial tiny inclusions rapidly aggregated and formed complex compounds of Si, Al, and Mn oxides and occasionally Ca or Ti oxides, which were homogeneously distributed and apparently liquid at steelmaking temperatures. The inclusions collided, grew, and floated prior to removal. After 20 min, few large oxide inclusions remained in the molten steel. The residual inclusions were mainly Al–Mg–O compounds, occasionally contained Si and Mn oxides, and spherical MnS.

An example of droplet polymerization is shown in Fig. 2. The energy-dispersive X-ray spectra corresponding to the three labeled areas in Fig. 2 are shown in Fig. 3.

The large inclusions in Fig. 1(a) have diameters of 32 and 53 μm and have nearly the same composition, i.e., O, Al, Si, Mn, and some Ti. The composition of the inclusions is plotted on the Al2O3–SiO2–MnO ternary phase diagram in Fig. 4. The projection of the composition of the inclusions in the Al2O3–SiO2–MnO ternary phase diagram and the 1873 and 1473 K isotherms are clearly observed. Because the melting point of these compounds is less than 1473 K, i.e., far below the steelmaking temperature of 1873 K, the inclusions generated by the deoxidation reaction are likely to be in the liquid state. Moreover, the circular outline of the inclusions to be in the liquid state. Moreover, the circular outline of the inclusions
also suggests the presence of liquid droplets. When two droplets are in contact, the liquid between the contact films is discharged. Because of the force acting on the liquid film between the droplets, this film is insufficient to resist the droplets’ relative movement; thus, the droplets coalesce. The state of coalesced droplets is shown in Fig. 1(a). We used these droplets to investigate the coalescence mechanism of liquid inclusions in molten steel.

3. Droplet coalescence and bounce mechanism

3.1. Collision

To determine whether collisions occur among droplets, we compare the distance between the centers of two droplets and their radii. When the distance between the centers of two droplets is less than their radii, collision occurs [10]. The droplet collision is described by the dimensionless Weber number (We), the collision parameter B, the droplet size parameters A and γ, and the Reynolds number (Re) [11]. We is expressed as

\[
We = \frac{D_a u_p}{\rho \sigma}
\]

where \(D_a\) is the average diameter of the droplet, \(u_p\) is the relative velocity of the droplet, \(\rho\) is the density of the liquid, and \(\sigma\) is the liquid surface-tension coefficient.

The collision parameter is

\[
B = \frac{b}{D_0}
\]

where \(b\) is the projection of the line of the two colliding droplet centers in the normal direction of the relative velocity vector. It determines the effect of collision droplets on the spatial orientation. \(D_0\) is the sum of the radii of the two droplets.

The ratio \(\gamma\) is related to the droplet size parameter \(A\) via the following equation:

\[
\gamma = \frac{1}{A} = \frac{D_1}{D_2}
\]

where \(D_1\) and \(D_2\) are the diameters of the large and small droplets, respectively.

The Reynolds number is expressed as

\[
Re = \frac{\rho \frac{u_p}{\mu}}{\mu_i}
\]
where $D$ is the droplet diameter, $u_p$ is the droplet velocity, $\rho_l$ is the density of the liquid, and $\mu_l$ is the dynamic viscosity of the liquid.

The range of the parameters for the droplets in molten steel are as follows: (1) droplet diameters of 5–50 µm, with an average of 30 µm; (2) droplet velocities of 0–0.5 m·s$^{-1}$, with an average of 0.20 m·s$^{-1}$; (3) surface tension of 0.31–0.70 N·m$^{-1}$, with an average of 0.40 N·m$^{-1}$; (4) densities of 2500–3500 kg·m$^{-3}$, with an average of 3000 kg·m$^{-3}$; and (5) kinematic viscosities of $794$–$3968 \times 10^{-6}$ m$^2$·s$^{-1}$, with an average of $2500 \times 10^{-6}$ m$^2$·s$^{-1}$. Consequently, the calculated $We$ and $Re$ are 0.01 and 0.24, respectively. In molten steel, the initial collision angle of the droplets ranges from 0° to 90°, and $0 \leq B < 1$ [12]. In addition, the vast majority of droplets are moving with the steel; therefore, the value of $B$ is very small. We assume $B = 0$ at the center of the collision.

Many researchers have studied the effect of airflow on droplets [13–20]. Pairs of droplets collide with each other in five different ways [17]: by slow merging, bouncing, merging, reflexive separation, and stretching separation. However, the droplets in molten steel differ from the droplets in the gas stream. Their velocity is typically 5 m·s$^{-1}$ or less, and $We$ is very small ($\leq 10$). Therefore, the last three cases are unlikely to occur, whereas the slow coalescence and bouncing of the droplets are more common [21].

### 3.2. Criteria for slow coalescence and bouncing

When two droplets move toward each other, the liquid between them forms a film that resists coalescence of the droplet. However, as the pressure increases, the droplets deform. If the droplets move sufficiently slowly, the liquid film is pushed away and the droplets contact each other and slightly deform as they coalesce [22–23] (Fig. 1(a)).

With increasing $We$, the relative velocity of the droplets increases and the liquid does not have sufficient time to flow out. The pressure at the droplet contact points increases dramatically before the droplets coalesce, and bouncing occurs [24]. Based on our experiments using water, the critical $We$ is 5.5, which is used to evaluate whether coalescence or separation of droplets occurs. For $We \leq 5.5$, a completely inelastic collision occurs and the droplets coalesce slowly; by contrast, for $We > 5.5$, the droplets bounce. According to the similarity principle, the value 5.5 of the critical $We$ is chosen as the criterion for the coalescence and separation of droplets in molten steel. This criterion can be included in the numerical simulations, and the velocity of the coalesced droplets can be calculated on the basis of the rule of momentum conservation.

### 4. Droplet coalescence simulation

#### 4.1. Model assumptions

Because of the difficulty of observing high-temperature molten steel, directly observing the collision-coalescence of small inclusions is not feasible. Therefore, the process is indirectly observed using steel samples. However, numerical simulations are superior because they can visualize the motion and collision of inclusions. Using the established droplet collision model and a combination of CFD and DEM, we add the droplet coalescence and rebound to calculate the droplet movement in the ladle. In a bottom-argon-blowing ladle with a carbonate line feeder, the droplets are released at certain depths in molten steel. The droplets coalesce because of the collision between the continuous and dispersed phases. By tracking each discrete phase, the process of collision and coalescence of droplets is demonstrated.

#### 4.2. Meshing and boundary conditions

The diameter of the upper part of the ladle is 3000 mm, the diameter of the lower part is 2700 mm, and the height of the lower part is 4000 mm. The argon-blowing hole is located at $R/2$ from the center of the ladle bottom. The inlet of the feed line is at the $R/2$ position, 500 mm from the ladle bottom. A hexahedral mesh is adopted to divide the structure. In the literature [25], a similar ladle was simulated using $8 \times 10^5$ grid points. In the present study, we divided the ladle into four groups of $3 \times 10^5$, $6 \times 10^5$, $8 \times 10^5$, and $12 \times 10^5$ grid points. For example, the velocity difference of the fluid is less than 3% at the three points (as shown in Fig. 5) under different grid numbers, which shows that the number of grids has little effect on the calculation results. We selected three points at the central plane (as shown in Fig. 5), and the results are shown in Fig. 6.

![Fig. 5. Location of the three points which were selected to measure the fluid velocity.](image)
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4.3. Flow model and convergence criterion

4.3.1. Fluid-phase models

Mass and momentum conservation for an incompressible fluid are given by

$$\frac{\partial}{\partial t} \left( \alpha_i \rho_i \right) + \nabla \cdot \left( \alpha_i \rho_i \mathbf{u}_i \right) = 0$$

$$\frac{\partial}{\partial t} \left( \alpha_i \mathbf{u}_i \right) + \nabla \cdot \left( \alpha_i \mathbf{u}_i \mathbf{u}_i \right) = -\nabla P + \nabla \cdot \left[ \alpha_i \left( \mu_i + \mu_t \right) \nabla \mathbf{u}_i + \mathbf{F}_i \right]$$

where \( \alpha_i \) is the continue-phase volume fraction, \( \rho_i \) is the liquid-phase density, \( \mathbf{u}_i \) is the fluid-phase average velocity, \( P \) is the pressure, \( \mathbf{F}_i \) is interaction momentum per unit mass transferred from the discrete phases, \( \mu_i \) is the liquid viscosity, and \( \mu_t \) is the turbulent viscosity. Parameter \( F_i \) in Eq. (6) is the source term for momentum exchange with the bubbles, representing the drag force, the lift force, and the virtual mass force. The liquid flow field is calculated using the standard \( k-\epsilon \) equation model [26].

4.3.2. Droplet transport model

The transient transport of droplets is simulated based on the flow fields in the liquid pool. The droplets are treated as discrete phases, and their motion can be simulated by integrating the following transport equation for each droplet, which considers contributions from six different forces:

$$m_b \frac{d \mathbf{u}_p}{dt} = F_D + F_{\text{press}} + F_b + F_{\text{vm}} + F_\gamma + F_L$$

The terms on the right-hand side of Eq. (7) from left to right are the drag force, pressure gradient force, buoyancy force, virtual mass force, gravitational force, and the lift force, respectively. All of the forces in Eq. (7) are expressed as follows; details are presented elsewhere [26].

$$F_D = C_D \frac{1}{2} \rho_\text{l} \left| \mathbf{u}_l - \mathbf{u}_p \right| \left( \left| \mathbf{u}_l - \mathbf{u}_p \right| \right) \pi D^2$$

$$F_{\text{press}} = \frac{1}{6} \pi D^3 \rho \frac{d \mathbf{u}_p}{dt}$$

$$F_b = -\frac{1}{6} \pi D^3 \rho \cdot \mathbf{g}$$

$$F_{\text{vm}} = \frac{1}{6} \pi D^3 C_{\text{vm}} \rho \left( \mathbf{u}_l - \mathbf{u}_p \right)$$

$$F_\gamma = \frac{1}{6} \pi D^3 \rho \cdot \mathbf{g}$$

$$F_L = -\frac{1}{6} \pi D^3 C_L \mathbf{u}_l \cdot \left( \mathbf{u}_l - \mathbf{u}_p \right) \left( \nabla \times \mathbf{u}_l \right)$$

4.3.3. Trajectories of the particles

The trajectories of the bubbles are obtained by integrating Eq. (14):

$$x_p = \int \mathbf{u}_p dt$$

where \( x_p \) is the displacement of droplets.

5. Simulation results and discussion

5.1. Droplet motion behavior in the flow field

After the molten steel flow field is stabilized by the bottom-blowing argon, the cored wire is melted 0.5 m from the bottom and the droplets are released at \( R/2 \). Thus, the droplets move with the flow field, as shown in Fig. 7(a). After the droplets flow into the region of argon blowing, some of them directly rise to the surface, whereas the majority moves to the deep parts of the ladle as the flow field moves.
downward as shown in Fig. 7(b). When the droplets move to half the depth of the ladle, their production stops and some of them directly move downward to the lower part of the ladle sidewall and are removed; the rest of the droplets move with the molten steel deep into the ladle as shown in Fig. 7(c). After entering the bottom of the vortex, the droplets begin to disperse. They do not move as much as they did before; however, the relative motion of particles becomes more significant. Thus, turbulence transport begins to dominate particle collisions [27]. Some droplets move to the ladle bottom wall and are removed, whereas most of the droplets continue to float as shown in Fig. 7(d). In secondary flotation, the dispersion of the dispersed phase flow is very large, showing an S-type flotation route. Consequently, droplets are conducive to adsorption with more droplets or inclusions colliding, which improves the droplet removal efficiency.

Droplet coalescence is divided into two cases. Initially, droplet collisions occur among droplets of the same size; this process increases the diameter of the droplets. The probability of collision with small droplets then increases. The following simulations describe the droplet coalescence.

5.2. Coalescence of same-sized droplets

The coalescence behavior of the droplets is shown in Fig. 8. Figs. 8(a) and 8(b) show how small droplets with the same diameter coalesce. Figs. 8(c) and 8(d) show the collision and coalescence.

The volume of each of the droplets 1 and 2 before coalescence is $1.80 \times 10^{-4}$ mm$^3$, and the $We$ is 0.02. The two small droplets collide as they move and reach the coalescence critical level and produce droplet 3 with a volume of $3.60 \times 10^{-4}$ mm$^3$. The volume of droplet 3 is equal to the sum of the volumes of droplets 1 and 2, which suggests that they follow the law of mass conservation.

5.3. Coalescence of different-sized droplets

Droplets of different sizes are produced because of the interactions among droplets; thus, large and small droplets collide and coalesce. Fig. 9 shows the coalescence of droplets with different diameters.
Fig. 8. Collision and coalescence of same-size droplets in liquid steel: (a) before coalescence, low magnification; (b) after coalescence, low magnification; (c) before coalescence, high magnification; (d) after coalescence, high magnification.

Fig. 9. Collision and coalescence of droplets with different diameters in liquid steel: (a) before coalescence, low magnification; (b) after coalescence, low magnification; (c) before coalescence, high magnification; (d) after coalescence, high magnification.
The volume of droplet 1 before coalescence is 1.13 × 10^{-4} \text{mm}^3, and its \textit{We} is 0.02; the volume of droplet 2 is 5.23 × 10^{-4} \text{mm}^3, and its \textit{We} is 0.04. The two small and large droplets collide with each other to form the larger droplet 3 with a volume of 6.36 × 10^{-4} \text{mm}^3, which is equivalent to the sum of the volumes of the two droplets before the collision.

As the wire is fed into the ladle, the liquid droplets collide with each other because of the fluid flow. The simulated collisions resemble those observed in coagulated samples; with time, the collision removal efficiency of the droplets increases. In this study, 2000 particles were selected to simulate the collisions. Because the actual amount of inclusions in molten steel is 10^{10}–10^{15}, the computing power presently limits further study.

6. Conclusions

The distribution of inclusions in solidified steel samples was analyzed, and the basic physics of droplet collision was discussed. A model for droplet collision and bouncing was proposed, and the droplet coalescence with wire feeding in the ladle was investigated.

(1) Droplet coalescence is slow in molten steel. The critical \textit{We} of 5.5 was used to evaluate the coalescence or separation of droplets; for \textit{We} ≤ 5.5, the droplets coalesced slowly, whereas they bounced for \textit{We} > 5.5.

(2) A model coupling the CFD and DEM methods was constructed to simulate the movement and coalescence of droplets of various sizes in a bottom-blowing argon ladle. The simulated collision with carbon dioxide feeding into the ladle agreed with observations in the steel samples. The proposed mathematical model can describe the behavior of droplets in steel in the second refining in a ladle.

Acknowledgements

This work was financially supported by the National Natural Science Foundation of China (No. 51374081).

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