Mathematical Modeling on the Fluid Flow and Desulfurization During KR Hot Metal Treatment

Chao Fan, Alexis GoSa, Lifeng Zhang, Qingcai Liu and Dayong Chen

Abstract In the current study, the fluid flow and desulfurization in a 160 t KR ladle were simulated using FLUENT combined with user-developed subroutines. The velocity distribution of the hot metal, the motion and distribution of CaO particles, and the desulfurization rate of the hot metal were calculated. With the increase of rotation speed of the impeller, the velocity of CaO particles increased as well, which resulted in the increase of desulfurization efficiency. The desulfurization rate varied at different positions of the ladle, with a higher rate in the higher speed zone and slower in the dead zone. The desulfurization rate increased slightly with growing rotation speed of the impeller. When the particle diameter increased from 1.3 to 2 mm, the desulfurization rate decreased approximately 3 or 4 times.

Keywords Hot-metal pretreatment · KR · Desulfurization · Desulfurizer particle · Fluid flow · Mathematical modeling

Introduction

As demand for high-quality steel increases, high efficiency of hot metal desulfurization has become one of main objectives in the steelmaking process. Sulfur which is harmful in most steel always leads to the crack on the surface of steel when the temperature is very high [1]. Almost all of the sulfur in hot metal can be removed by hot metal pretreatment in the process of steelmaking. Kambara Reactor (KR) desulfurization is widely used as a high efficiency and low cost desulfurization

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method [2, 3]. During KR stirring process, the CaO particles are involved into hot metal by the cross impeller which is rotating at a high speed under the liquid level [4]. The desulfurization reaction between sulfur and CaO particles that occurred in hot metal was investigated by CFD software, because the fluid flow and particles distribution in invisible hot metal internal were invisible only by the experiment. In the current study, the multi-phase flow and the distribution of added CaO particle during KR stirring process were firstly discussed. Then, the characteristics of desulfurization reaction within the metal steel was investigated with the in-house user-developed subroutines. Finally, the effects of rotation speed of the impeller, immersion depth of impeller, and size of CaO particles on the desulfurization reaction were compared.

Models

Calculation Domain and Mesh System

A schematic of calculation domain and meshes of the current model are shown in Fig. 1. In order to simplify the calculation and avoid the convergence problem caused by complex mesh, the bottom of hot metal ladle was regarded as flat which was round in fact. The impeller was cross shape and the diameter of connecting rod was 150 mm. The mesh type was unstructured hexahedral mesh with a total mesh number of about 400,000. The sizes of the 160 t hot metal ladle and the impeller are showed in Table 1 and Table 2, respectively [5].
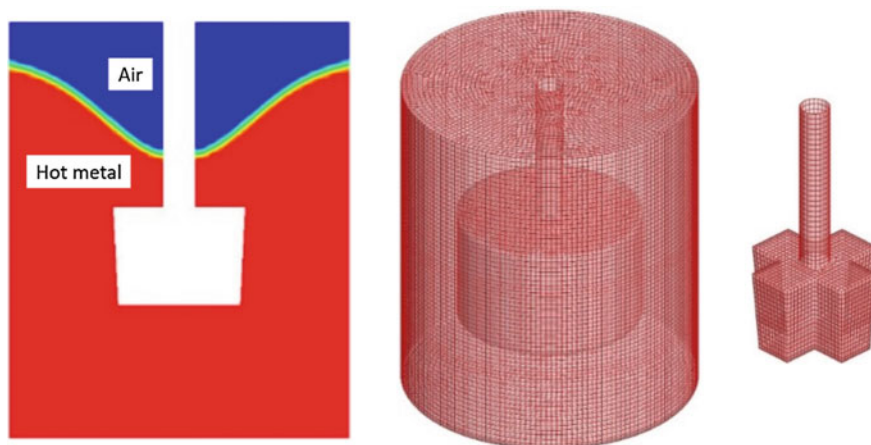
Fig. 1 Schematic of calculation domain and mesh of the current model

Table 1 160 t hot metal ladle size [5]

| Diameter of top (mm)	Diameter of bottom (mm)	Height (mm)	Liquid level (mm)
3200	3200	3600	3000

Table 2 Impeller size [5]

	Diameter (mm)	Width (mm)	Height (mm)
Top	1240	470	850
Bottom	1140	390	

Models Used and Boundary Conditions

The turbulence model used in the calculation was standard $k - \varepsilon$ model. In order to obtain the vortex surface distribution, multiphase flow VOF model was used [6]. The desulfurizer particles were added via a discrete phase model (DPM) [7]. The diameter of all the particles was 1 mm. The diffusion of S in hot metal and the desulfurization of CaO particles were performed by solving UDS equations [8].

In the stirring process of KR desulfurization, CaO particles were added into the hot metal to react with sulfur. The main reaction was shown as Eq. 1.

$$CaO(s) + [S] = CaS(s) + [O] \tag{1}$$
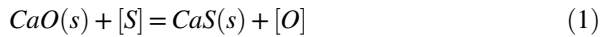
According to chemical reaction kinetics, the desulfurization rate can be expressed as Eq. 2 by assuming that the rate-controlling step is the mass transfer of [S] in hot metal.

$$-\frac{d[S]}{dt} = -k \cdot \frac{A}{V_m} \cdot [S] \tag{2}$$

where, k is mass transfer rate, A (m^2) is the interfacial area that can be expressed as the sum of surface area of all particles, V_m is hot metal volume (m^3), and $[S]$ (ppm) is the sulfur concentration in hot metal. The mass transfer rate, k, was obtained by Eq. 3, which was proposed by Nakanishi et al. [9].

$$k = 0.82 \times D_s^{0.5} \times v_t^{0.5} \times \left(\frac{D_t}{2}\right)^{-0.5} \tag{3}$$

where D_s is the diffusion coefficient of S in hot metal (= 2.58 $\times$ 10^{-9} m^2/s), v_t is the relative velocity of particle compared with hot metal (m/s), and D_t is the diameter of particles (m). Desulfurization behaviors during KR stirring process were estimated by Eqs. (1)–(3).

Table 3 Materials physical properties [11, 12]

|	Hot metal	CaO particle	Air
Density (kg/m^3)	7100	2718	1.225
Viscosity (Pa · s)	0.0065	–	1.789×10^{-5}
Molar mass (g/mol)	56	56	29

The boundary conditions were set as follows:

a. The bottom and side wall of the ladle were non-slip walls;
b. The upper outlet of the ladle was a plane without shear stress;
c. The impeller wall was a rotation wall;
d. The rotation of hot metal and the stirrer were calculated by the multiple reference frame model (MRF) [10].

The properties of materials used in the calculation are shown in Table 3 [11, 12].

Results and Discussion

Flow Field

After the flow was stable, the streamline and the distribution of flow velocity under the condition of the rotation speed was 120 rpm (revolution per minute) are presented in Fig. 2. As the figure shows, the flow of hot metal was divided into two parts of the upper and lower circulation. The flow velocity of hot metal at different
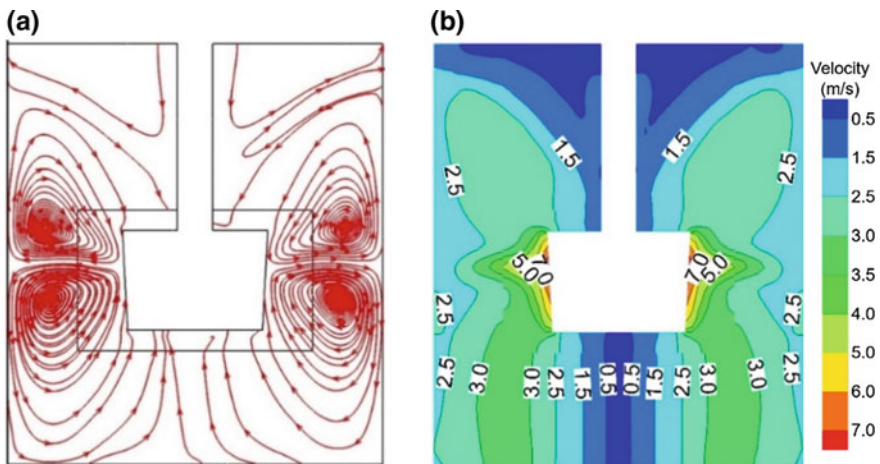

Fig. 2 Predicted velocity field with the rotation speed of 120 rpm

positions is very different. It can be seen that the flow velocity of hot metal is inversely proportional to the distance from the stirring impeller. The flow velocity besides the impeller reaches 7.0 m/s while near the wall it is below 2.5 m/s. The movement of hot metal under the impeller is much worse than other positions. In this paper, the zone in which the flow velocity of hot metal is below 0.5 m/s is defined as dead zone. During the hot metal pretreatment, the dead zone always leads to an increase of sulfur content after the desulfurization is finished.

Distribution of CaO Particles

Figure 3 shows the distribution of 20000 particles at different calculation times after adding into the hot metal, when the rotation speed of the impeller was 100 rpm. It can be seen that under the stirring effect from the impeller, the added particles moved with the hot metal, and at 60 s, the distribution of CaO particles was dispersed well within the hot metal. As the main desulfurizer, the movement and
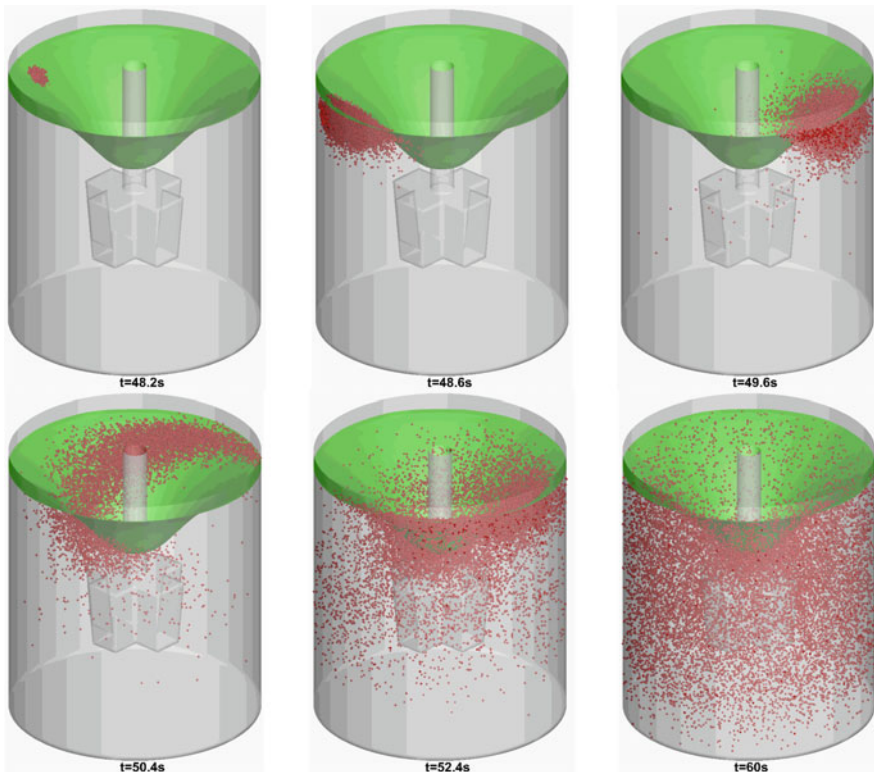

Fig. 3 Predicted particle distribution at different moments

distribution of the CaO particles in the hot metal have significant effect on the desulfurization rate. It is obvious that the CaO particles were moving with hot metal, so the movement situation of CaO particles can be optimized by the optimization of velocity field.
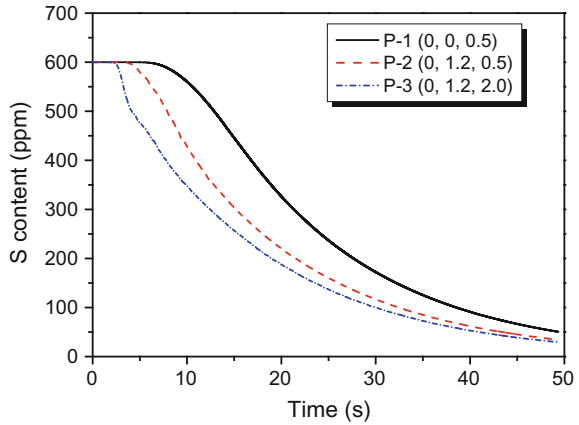
Desulfurization Process

The variation of sulfur content in the hot metal after the injection of CaO particles is shown in Fig. 4, in which the rotation speed of impeller was 100 rpm and the initial sulfur content was 600 ppm. As the figure shows, with the addition of CaO particles, the desulfurization reaction occurred in the hot metal. Figure 5 shows the
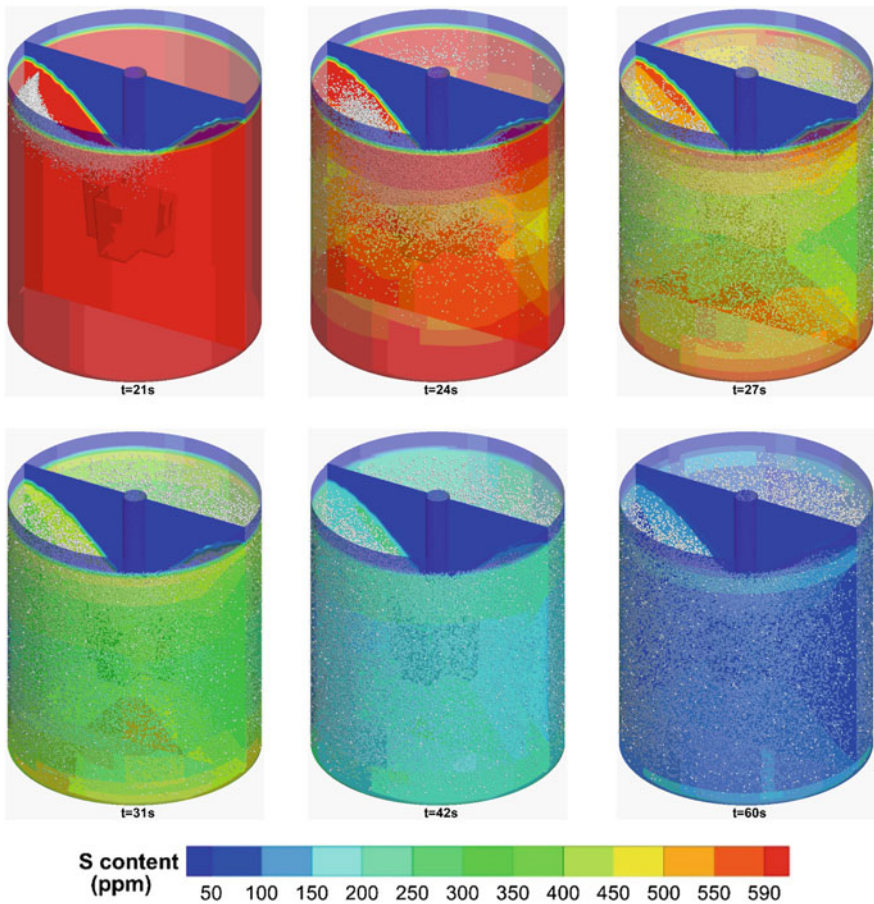
Fig. 4 Predicted sulfur content at different moments

**Fig. 5** Predicted change curve of sulfur content at different positions

change of sulfur content monitored in three positions. Obviously, the desulfurization rate at P-3 was much higher than P-1. The reason for this phenomenon is that P-1 is in the dead zone where the flow is the worst in the ladle. On the contrary, P-3 is besides the impeller where the stirring is much stronger than other positions in the ladle. In combination with Eq. (3), it can be seen that the rate of desulfurization was increased due to the high stirring strength near the impeller and the faster rate of hot metal regeneration.

## Effect of Parameters on Desulfurization

In this paper, the desulfurization rate under different conditions were simulated, respectively. Figure 6 shows the desulfurization results with different rotation speeds (under the immersion depth of 1.85 m). From the result, it indicated that the

Fig. 6 Predicted change curve of average desulfurization rate with different rotational speed. The immersion depth is 1.85 m
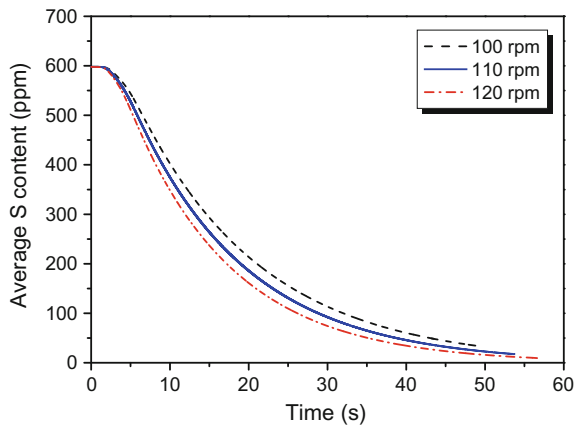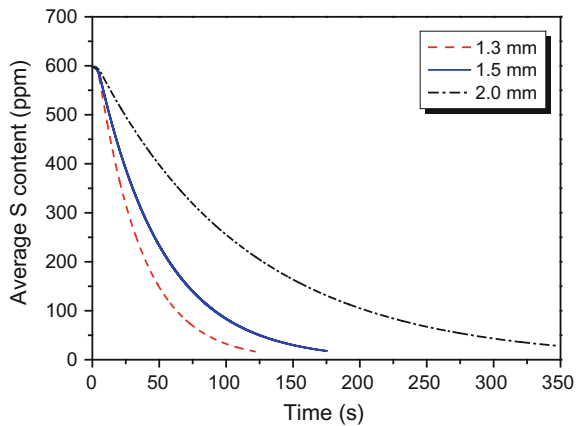
Fig. 7 Predicted change curve of average desulfurization rate with different immersion depths. The rotation speed is 100 rpm
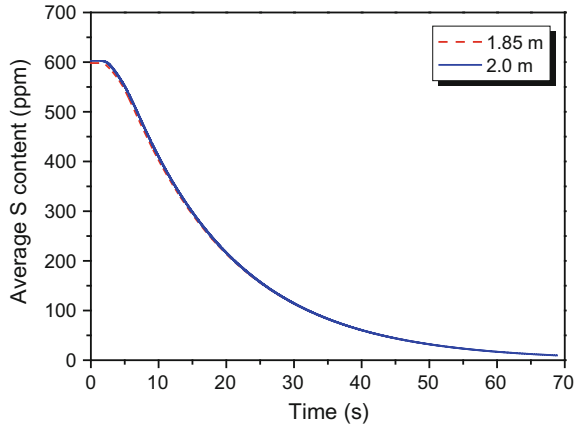
Fig. 8 Predicted change curve of average desulfurization rate with different particle sizes. The rotation speed is 100 rpm. The immersion depth is 1.85 m

desulfurization rate was slightly increased by the increase of rotation speed. That is because the desulfurization rate is not directly effected by the rotation speed, but by the relative velocity of particles compared with hot metal. The increasing rotation speed has a little effect on the relative velocity.

The results of desulfurization rate with different immersion depths and particle sizes are shown in Fig. 7 and Fig. 8, respectively. As Fig. 7 shows, the increasing of immersion depth has no effect on the desulfurization rate. This is because with the increasing of immersion depth, the desulfurization rate of the lower part of the ladle was accelerated, but at the same time the desulfurization rate of the upper part of the ladle was decreased, resulting in no change in the overall desulfurization rate. Figure 8 shows the relationship between the desulfurization rate and particle size. Here, three different diameters of CaO particles were calculated as a contrast. As the

result shows, the desulfurization rate was greatly effected by the particle size. When the particle diameter increased from 1.3 to 2.0 mm, the overall desulfurization efficiency reduced by 3 times mainly due to the surface area reduction of particles.

Conclusions

The KR desulfurization process in hot metal under different conditions were investigated by CFD. The conclusions are summarized as follows.

(1) During KR stirring desulfurization process in the ladle, the flow of hot metal was greatly effected by the rotation speed.
(2) The movement and dispersion of CaO particles were simulated by DPM model. After the desulfurizer was added into the ladle, it can be well dispersed in the hot metal. The desulfurization reaction between the CaO particles and the S in hot metal was also evident.
(3) Desulfurization behavior was simulated using the reaction model. The results obtained show that the increasing of rotation speed and immersion depth have a little effect on the desulfurization rate. It is a significant method to improve the desulfurization rate by controlling the CaO particle size.
(4) The simulation of the KR desulfurization process seems to be feasible and parameter studies give plausible results. Nevertheless, some important phenomena like aggregation of the desulfurizer have not be considered so far. Therefore, it should be careful to analyze simulation results. Further investigations should incorporate these effects in order to achieve more realistic predictions.

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