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Numerical investigation of desulfurization behavior in electroslag remelting process

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ABSTRACT

A transient three-dimensional (3D) coupled mathematical model has been established to study the desulfurization behavior in electroslag remelting (ESR) process. The solutions of the mass, momentum, energy, and species conservation equations were simultaneously calculated by the finite volume method. The Joule heating and Lorentz force were fully coupled through solving the Maxwell's equations with the assistance of the magnetic potential vector. The movement of the metal droplet was described by the volume of fluid (VOF) approach. In order to include the influences of the slag composition and the electric current on the desulfurization, a thermodynamic and kinetics module was introduced. An experiment was conducted to validate the model. The completely comparison between the measured and simulated data indicates that the model can predicate the desulfurization with acceptable accuracy. The sulfur in the metal would be mainly transferred into the slag in the formation of the droplet. After the droplet enters into the metal pool, the sulfur would fast expand to the rest of the slag pool and move to the outer side of the mold along with the metal, and finally flows downward. The maximum calculated removal ratio during the whole process can reach up to 71%.

1. Introduction

Electroslag remelting (ESR) processes have been utilized to produce the ultralow sulfur nickel alloy for use in ocean, aeronautics, and pipeline [1]. Fig. 1 shows a schematic of the ESR process. In this process, a direct current is passed from the electrode to the baseplate, creating Joule heating in the highly resistive calcium fluoride-based molten slag. This heating is enough to melt the electrode. Molten metal film is then generated at the electrode tip, and a metal droplet is gradually formed with the continuous melting. The dense metal droplet sinks through the less dense molten slag to form a liquid metal pool in the water-cooled mold [2]. Sulfur dissolved in the metal would be transferred to the slag during this process [3]. The desulfurization behavior could be expressed:

$$[S] + 2e = (S^{2-}) \tag{1}$$

where [ ] and ( ) indicated that the matter was in the metal and slag, respectively.

Several experiments were conducted to measure the desulfurization rate [3–6]. The efficiency ranged from approximately 30% to 85% under different conditions. Unfortunately, the information provided by the experiments were limited because of the opaque reactor as well as the harsh environment. The electric current, velocity and temperature fields were unknown to us, which seriously influence the sulfur transfer. With the continuous increasing of the computation resources, numerical simulation is able to provide deep insights into the associated phenomena in this process.

Some efforts have been devoted to numerically investigate the electromagnetic field, two-phase flow and temperature distribution in the ESR process [7–11]. A magnetic field was induced by the current, and the interaction between the magnetic field and the current gave rise to an inward Lorentz force. The slag and the metal was driven to flow under the combined effect of Lorentz and buoyancy forces. However, the desulfurization, which occurs at the slag-metal interface, was not taken into account in the above works. Josson et al. [12] proposed a new coupled computational fluid dynamic (CFD) and thermodynamic module to describe the sulfur transfer between the slag and metal in a gas-stirred ladle. The desulfurization mechanism was represented by a metallurgical thermodynamic and kinetic module, and the relevant thermodynamic parameters such as sulfide capacity and oxygen activity,

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Nomenclature

A	specific surface area for reaction (m^{-1})
$\vec{A}$	magnetic potential vector (V·s/m)
$a_{[Al]}$	activity of aluminum in the metal
$a_{(Al_2O_3)}$	activity of alumina in the slagl
$a_{[O]}$	activity of oxygen in the metal
$\vec{B}$	magnetic flux density (T)
C_S	sulfide capacity of the slag
c	mass fraction of sulfur
$c_{p,m}$	specific heat of metal at constant pressure (J/(kg·K))
$c_{p,s}$	specific heat of slag at constant pressure (J/(kg·K))
D	diffusion coefficient of sulfur (m^2/s)
E	internal energy of mixture phase (J/m^3)
e_j^i	interaction coefficient of the element j with respect to the element i
F	Faraday law constant (C/mol)
$\vec{F}_e$	Lorentz force (N/m^3)
$\vec{F}_s$	solute buoyancy force (N/m^3)
$\vec{F}_{st}$	surface tension (N/m^3)
$\vec{F}_t$	thermal buoyancy force (N/m^3)
$f_{[Al]}$	activity coefficient of the aluminum in the metal
$f_{[S]}$	activity coefficient of the sulfur in the metal
I	current (A)
$\vec{J}$	current density (A/m^2)
K	reaction equilibrium constant
k_{ss}	mass transfer coefficient of sulfur in the slag (m/s)
k_{sm}	mass transfer coefficient of sulfur in the metal (m/s)
k_T	effective thermal conductivity (W/(m·K))
L	latent heat of fusion (J/kg)
L_S	sulfur partition ratio

M_S	molar mass of the sulfur (kg/mol)
$\dot{m}$	melt rate (kg/s)
p	pressure (Pa)
Q_J	Joule heating (W/m^3)
R	gas constant (J/(mol·K))
S_r	source term in Eq. (14)
t	time (s)
T	temperature (K)
$\vec{v}$	velocity (m/s)
$w[S]$, $w(S)$	mass fraction of sulfur in the metal and in the slag (%)
$w(Al_2O_3)$, $w(FeO)$, $w(SiO_2)$	mass fraction of aluminum oxide, ferrous oxide and silicon dioxide in the slag (%)
x, y, z	Cartesian coordinates

Greek symbols

α	volume fraction of metal
$\bar{\mu}$	viscosity of mixture phase (Pa·s)
μ_0	permeability of vacuum (T·m/A)
$\bar{\rho}$	density of mixture phase (kg/m^3)
ρ_m	density of metal (kg/m^3)
ρ_s	density of slag (kg/m^3)
ξ	coefficient in Eq. (29) which represents the power efficiency
$\bar{\sigma}$	electrical conductivity of mixture phase ($\Omega^{-1}\cdot m^{-1}$)
φ	electrical potential (V)
$\bar{\phi}$	mixture phase property
ϕ_m	metal property
ϕ_s	slag property
Λ	optical basicity of the slag

affected by the flow pattern, were solved by the CFD module. Nevertheless, the temperature distribution, which is a critical part of the process, was assumed to be constant. Sen et al. [13] established a two-dimensional mathematical model for electrochemical magnetohydrodynamics. The Butler–Volmer model for the kinetics of the heterogeneous electrode reactions was used to obtain the faradaic current density, and moreover the interplay of Lorentz force, convection and redox species concentration distribution was studied.

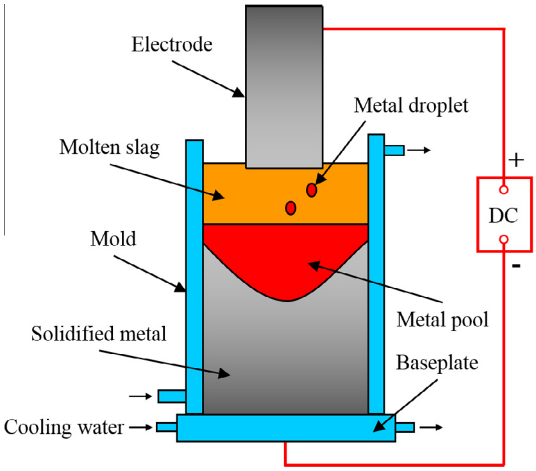

Fig. 1. Schematic of electroslag remelting process.

As discussed above, there have been no attempts to numerically investigate the desulfurization behavior in the ESR process. Because of this, the authors were motivated to establish a transient 3D comprehensive model to understand the sulfur transfer between the molten metal and the molten slag. The electromagnetic, flow and temperature fields were included. The desulfurization reaction rate was simultaneously solved using a thermodynamic and kinetic module. In addition, an experiment was carried out to validate the model.

2. Mathematical model

2.1. Assumptions

In order to keep the computational time reasonable, the model relied on the following assumptions:

1. The domain included the molten slag and the molten metal. The atmosphere and the solidified metal were ignored [14].
2. The growing of the solidified metal was not taken into account.
3. The two fluids were incompressible Newtonian fluid. The densities of the slag and the metal were a function of the temperature. The slag electrical conductivity depended on the temperature. The other properties of the slag and the metal were assumed to be constant [15].
4. The slag and the metal were assumed to be electrically insulated from the mold.
5. Other elements in the slag and the metal were ignored except the sulfur.