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Research Paper

Predicting transfer behavior of oxygen and sulfur in electroslag remelting process

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HIGHLIGHTS

- First developed a coupled model of oxygen and sulfur transfer in ESR process.
- Thermochemical and electrochemical reactions were included.
- Evolution of oxygen and sulfur concentration was demonstrated.
- An experiment was carried out to validate the simulation.

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ABSTRACT

A transient three-dimensional (3D) comprehensive mathematical model has been developed to understand oxygen and sulfur transfers in electroslag remelting process. The solutions of the mass, momentum, energy and species conservation equations were simultaneously carried out by finite volume method. The Joule heating and Lorentz force were taken into account. The thermochemical and electrochemical transfers of oxygen and sulfur were represented through the application of a metallurgical thermodynamic and kinetic module. In order to obtain the evolution of oxygen activity, the chemical reaction between dissolved aluminum and dissolved oxygen in the metal was included. The comparison between the measured and simulated data indicates that the model can predicate the transfer behavior with an acceptable accuracy. The thermochemical reaction always removes oxygen and sulfur from the metal, while the electrochemical reaction brings oxygen and sulfur back to the metal through the metal droplet-slag interface, and takes them away from the metal through the metal pool-slag interface. The oxygen removal ratio is about 60%, and the contribution of the electrochemical reaction is around 82%. The sulfur removal ratio is approximately 76%, and the contribution of the electrochemical reaction is around 39%.

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1. Introduction

Electroslag remelting (ESR) is a secondary refining process of metal, which has been widely employed to produce high grade steel for ocean, transportation and aeronautics [1]. A direct current, flowing from consumable electrode to baseplate, produces large amounts of heat in a highly resistive calcium fluoride-based molten slag layer. These heat then melts the electrode, and creates droplets at electrode tip. Subsequently, heavier metal droplets pass through the slag layer and form a liquid metal pool as shown in Fig. 1 [2].

Due to negative influences on ductility, strength and corrosion resistance of metal products, oxygen and sulfur are regarded as harmful impurities. With the development of metallic material, residual oxygen and sulfur in final metal products are only allowed for a few parts per million [3,4]. Efforts therefore have been devoted to understanding deoxidation and desulfurization in ESR processes. Shi et al. have experimentally studied the oxygen transfer path during the ESR process [5]. They found that the atmospheric oxygen significantly affected the oxygen content in the remelted ingot by reacting with the consumable electrode. Inert gas then was adopted to prevent the oxidation reaction. The decrease amplitude of the oxygen content however was smaller

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Nomenclature

A	specific surface area for reaction (m^{-1})
$a_{[Al]}$	activity of aluminum in the metal
$a_{(Al_2O_3)}$	activity of alumina in the slag
$a_{[O]}$	activity of oxygen in the metal
C_S	sulfide capacity of the slag
c	mass percent of element
D	diffusion coefficient of element (m^2/s)
F	Faraday law constant (C/mol)
$f_{[Al]}$	activity coefficient of aluminum in the metal
$f_{[O]}$	activity coefficient of oxygen in the metal
$f_{[S]}$	activity coefficient of sulfur in the metal
J	current density (A/m^2)
K_{Al}	reaction equilibrium constant
k_{AlS}	mass transfer coefficient of aluminum in the slag (m/s)
k_{AlM}	mass transfer coefficient of aluminum in the metal (m/s)
k_{OS}	mass transfer coefficient of oxygen in the slag (m/s)
k_{OM}	mass transfer coefficient of oxygen in the metal (m/s)
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_{Al}	aluminum partition ratio
L_S	sulfur partition ratio
M_{Al}	molar mass of the aluminum (kg/mol)
M_O	molar mass of the oxygen (kg/mol)
M_S	molar mass of the sulfur (kg/mol)
S_r	source term in Eq. (1)
S_{E-O}	oxygen transfer rate induced by electrochemical reaction
S_{E-S}	sulfur transfer rate induced by electrochemical reaction
S_{T-Al}	aluminum transfer rate induced by thermochemical reaction
S_{T-O}	oxygen transfer rate induced by thermochemical reaction
S_{T-S}	sulfur transfer rate induced by thermochemical reaction
t	time (s)
T	temperature (K)
$\vec{v}$	velocity (m/s)
$w[S]$, $w(S)$	mass percent of sulfur in the metal and in the slag (%)
$w[Al]$, $w(Al)$	mass percent of aluminum in the metal and in the slag (%)

Greek symbols

α	volume fraction of metal
$\gamma_{Al_2O_3}$	activity factor of alumina in the slag
$\bar{\rho}$	density of mixture phase (kg/m^3)
ρ_M	density of metal (kg/m^3)
ρ_S	density of slag (kg/m^3)

than expected. The main reason was supposed to be the electrochemical reaction, which greatly influenced deoxidation behavior. Kato et al. measured the desulfurization rate in ESR processes with different current densities and oxygen partial pressures [6]. The desulfurization could be promoted by increasing the oxygen partial pressure, since the sulfur was oxidized into the sulfur dioxide. Yet the influence of the current density was still unclear, because the electromagnetic, flow and temperature fields all changed with the current density.

Unfortunately, the information provided by these experiments may not be sufficient to completely illustrate the thermochemical and electrochemical migrations of oxygen and sulfur during the ESR process because of the harsh environment and tough measurement. With the continuous increasing of the computation resources, numerical simulation is able to provide deep insights into the associated phenomena in this process. A transient axisymmetrical comprehensive mathematical model of the ESR process was developed by Weber et al. which included the coupled electromagnetic, flow and thermal fields [7]. The continuous growth of the remelted ingot was described by using a mesh-splitting method. An inward Lorentz force was created through the interaction between the current and the self-induced magnetic field. The melt was driven to move under the combined effect of Lorentz and buoyancy forces. The mass transfer however was not taken into account. In order to access performance of a forced convection air cooling system in a lithium-ion battery, Tong et al. established a coupled electrochemical and thermal-fluid model [8]. Electron transfer and electrochemistry energy were clarified by the electrochemical module, which was composed of conservation equations of charge and species in the solid-phase and the liquid-phase. Qiang et al. numerically studied the desulfurization in an ESR furnace [9]. The finite volume approach was used to solve the mass, momentum, energy and species conservation equations. A metallurgical thermodynamic module was introduced to define the desulfurization mechanism. Nevertheless, the oxygen activity in the metal, an important parameter for the desulfurization, was solved by a fitting function of temperature. And actually it is determined by the equilibrium between the dissolved aluminum and the dissolved oxygen in the metal.

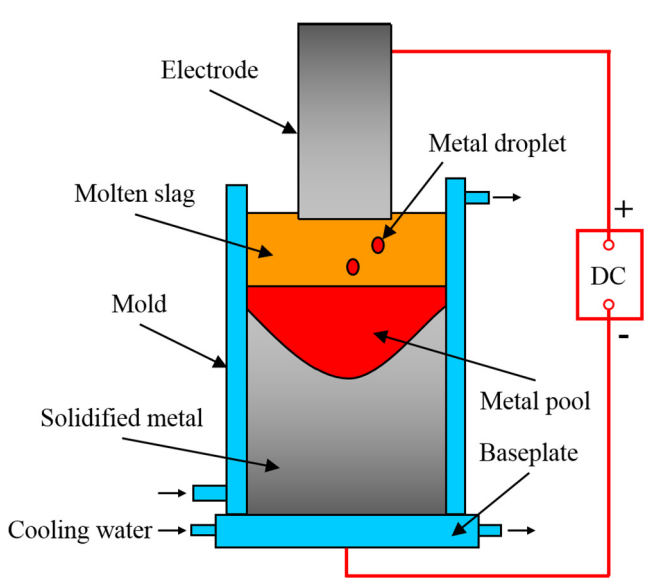

Fig. 1. Schematic of electroslag remelting process.

As discussed above, the thermochemical and electrochemical transfers of oxygen and sulfur in the ESR process require further investigation. Because of this, the authors were motivated to establish a transient 3D integrated model to understand the oxygen and sulfur transfer caused by the thermochemical and electrochemical reactions. The electromagnetic, flow and temperature fields were included. The transfer behavior of oxygen and sulfur was simultaneously solved through the application of a metallurgical thermodynamic and kinetic module. In order to calculate the oxygen activity in the metal, the chemical reaction between the dissolved aluminum and the dissolved oxygen was taken into

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