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Study of inclusion prediction model for Ladle Furnace process in secondary steelmaking

철강 2차 정련 중 래들 퍼니스 공정의 개재물 예측 모델 개발

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Abstract

Strict control over various elements is required for the production of high quality steel, which in turn necessitates an understanding of the secondary refining processes which make it possible to control the mixing of the alloy elements and inclusions. The secondary steelmaking process is the deoxidation process which contains argon bottom bubbling to inclusion removal. To make simulation, flow, mass transfer of deoxidizer and other alloys, reaction of dissolved oxygen – deoxidizer in molten steel and its inclusion generation, inclusions collision – agglomeration and removal should consider. Proper understating of the mixing of alloy elements and their transfer route is important to enhance operations of process. Especially when alloy (or deoxidizer) is added, the local area of alloy addition site soars up to over ten times of equilibrium concentration. Before the end of mass transfer, this high and low concentration region is mixed all over the ladle. Understanding of alloy transfer is important because the quantity of inclusion generation is depending on that.

Bottom argon blowing in the ladle leads to the melt being exposed. The injected gas bubble moves up by its buoyancy force and pushes slag away. The exposed area is known as the “plume eye”. In this study, the equation which is able to predict plume eye area is proposed. Through several experiments and simulations, relationship between plume eye ratio and gas flow rates is proportional to the square root of the gas flow rate and inversely proportional to the square root of the slag thickness. The proposed equation is able to apply various size of ladle and slag properties to predict plume eye area.

The local equilibrium reaction is made to reveal the deoxidation behavior in the
ladle. To calculate equilibrium between deoxidizer and dissolved oxygen, associate model that is able to reduce interaction coefficients is applied. This feature is proper to calculate complicated reaction such as Calcium-Aluminum and Oxygen. The circulation point in the ladle is the lowest region of inclusion generation as a result of 10 minutes of process time. High Ca contents of Ca-aluminate is produced near the injection site of Ca. At the initial state of reaction, Al$_2$O$_3$ concentration decreases near the region of site of Ca injection. Independent on the Ca injection speed, CaAl$_2$O$_7$ and CaAl$_2$O$_4$ are produced after CaAl$_{12}$O$_{19}$ and Ca$_3$Al$_2$O$_6$ inclusions are produced. Ca wire injection speed is inverse proportional to the time of reaching equilibrium.

To develop the model of inclusion agglomeration, its collision frequency and apparent density are defined. To simulate over billions of inclusion particles, algorithmic technic is added. Through this model, major inclusion growth site and size are predictable. The major site of agglomeration is the circulation point in the ladle which inclusions gather by flow. This circulation point has the longest residence time of inclusion. The region of plume has the highest collision frequency but agglomeration is effected more by the residence time. In this study, inclusions grow to 15 um when reaction between Al 1000ppm and O 300 ppm for 10 minutes of process under 30m$^3$/hour.

In case of slag entrapment, the shape of slag is fixed as sphere. Entrapping of slag surface area and entrapping slag mass are calculated by the relationship between slag surface tension and turbulent kinetic energy. The range of slag droplet size is considered by turbulent and pressure difference. In this study, 5, 30, 70m$^3$/hour flow rate of Argon bottom bubbling cases are calculated. The result for 10 minutes process, the residual quantity of slag droplet is 0.2ppm, 10ppm, 35ppm each. The possible entrapment diameter is from 5um to 40mm in case of 70m$^3$/hour.
As mentioned above, this prediction program for ladle furnace (LD3D) can predict general phenomena such as bubbling process, deoxidation reaction, inclusion agglomeration behavior and slag entrapment. We hope to help designing secondary steelmaking process with this program.

**Keywords**: numerical analysis, ladle furnace process, plume eye, inclusion generation, inclusion agglomeration, slag entrapment

**Student number**: 2009-20632
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Chapter 1. Deoxidation process in Ladle Furnace (LF) system

Strict control over various elements is required for the production of high quality steel, which in turn necessitates an understanding of the secondary refining processes which make it possible to control the mixing of the alloy elements and inclusions. [1] The secondary steelmaking process is the deoxidation process which contains argon bottom bubbling to inclusion removal. Ladle Furnace (LF) process and RH vacuum degassing process are the most popular secondary refining processes to perform these operations. LF process usually use to remove dissolved oxygen and residual sulfur in molten steel after converter process. This operation mostly employs bottom bubbling to enhance inclusion rising, temperature homogenization and slag-metal reaction. [2]

The fluid flow driven by bottom bubbling governs the various phenomena in the ladle such as transport, slag entrapment and non-metallic inclusions removal. Therefore, the study of flow in LF is important for all subsequent research. Bottom argon blowing in the ladle leads to the melt being exposed. The injected gas bubble moves up by its buoyancy force and pushes slag away. The exposed area is known as the “plume eye”. In this study, the equation which is able to predict plume eye area is proposed. The relationship between plume eye ratio and gas flow rate is proportional to the square root of the gas flow rate and inversely proportional to the square root of the slag thickness.

From plume eye prediction model, flow profile of ladle could be obtained and we can predict mass transfer behavior over time. Especially when alloy (or deoxidizer) is added, the local area of alloy addition site soars up to over ten times of equilibrium concentration.
Before the end of mass transfer, this high and low concentration region is mixed all over the ladle. Understanding of alloy transfer is important because the quantity of inclusion generation is depending on that.

The calculation of inclusion generation reaction according to deoxidizer addition uses associate model which is adopted in FACTsage. Associate model can reduce interaction coefficient as one and this feature is proper to calculate complicated reaction such as Ca-Aluminum and Oxygen. With this model, inclusion generation reaction is able to simulate according to mass transfer and inclusion agglomeration also can calculate from the result of initial inclusion site.

To develop the model of inclusion agglomeration, its collision frequency and apparent density are defined. To simulate over billions of inclusion particles, algorithmic technic is added. Sum of inclusion particles agree before and after complex calculation. In case of slag, the range of slag droplet size is considered by turbulent and pressure difference. Terminal velocity of slag droplet is considered to calculate the quantity in the each ladle sites.

To simulate flow, mass transfer of deoxidizer and other alloys, reaction of dissolved oxygen – deoxidizer in molten steel and its inclusion generation, inclusions collision – agglomeration and removal should consider. Proper understating of the mixing of alloy elements and their transfer route is important to enhance operations of process. As mentioned above, this study focuses on the numerical simulation of deoxidation process in LF system which is objective procedure of secondary steelmaking. This prediction program for ladle furnace (LD3D) can predict general phenomena from bubbling process to slag entrapment which contains argon bottom bubbling, mass transfer of deoxidizer and other alloys, reaction of dissolved oxygen – deoxidizer in molten steel and its inclusion
generation, inclusions collision – agglomeration and removal by their terminal velocity.

To do this massive study, we made self-developed FORTRAN code instead of commercial code. Although many commercial programs that support the flow calculation module, most of these programs couldn’t have models that support inclusion generation and collision – agglomeration. The code includes flow module and other modules to simulate deoxidation procedure such as mass transfer, inclusion growth etc. In addition, slag entrapment module is also included to predict total mass ppm of inclusion. Self-developed code is more difficult than commercial program which is based on the graphic user interface, but calculation speed is much faster, less constraints of developing models and cheaper.
Chapter 2. Flow calculation model

2.1 Plume eye phenomenon

Bottom argon blowing in the ladle leads to the melt being exposed. The injected gas bubble moves up by its buoyancy force and pushes slag away. The exposed area is known as the “plume eye”. The plume eye affects not only on oxygen and nitrogen pick-up but also flow pattern. Also the plume eye leading to adverse phenomena such as slag entrapment or oxygen and nitrogen pick up. [3] The velocity field differs significantly depending on the presence of slag, so in order to precisely simulate mixing behavior and their reaction, prediction of the plume eye is very important.

Many studies have been performed regarding the plume eye behavior [4-12]. Yonezawa et al.[4] presented empirical formulas related to the Froude number in 1999. They suggested an empirical formula based on oil/mercury cold model experiments and applied it to industrial operations. In 2003, Subagyo et al. [5] modified the parameters of the equation presented by Yonezawa et al and obtained an improved formula for the 350 ton ladle used by Yonezawa et al. Mazumdar et al used Froude number and gas blowing angle to revise Yonezawa’s empirical Equation. [6] At 2006 and 2007, Krishnapisharody et al. [7, 8] calculated the slag and plume eye area ratio using the momentum balance of melt and slag. The area ratio is proportional to the Froude Number with the velocity values taken from an empirical formula. Maruoka et al. [9] used polystyrene particle to express slag layer and analyze plume eye area with the various bath heights and the number of nozzles and proposed empirical formula.

Each formulas well predicted at the conditions similar to the each experiments. However, the empirical formulas do not satisfactorily in agreement with the data obtained
from different conditions. To overcome these issues, some studies were presented in which numerical analysis was employed.

Han et al. [10] calculated the plume eye area by numerical simulation with volume of fluid method. The gas flow rate was 0.3 l/min to 1.0 l/min and the relationship between diameters of plume eye and gas flow rates were almost linear. In 2008, Li et al. [11] used volume of fluid method to perform numerical analysis for 3 cases regarding the plume eye, and verified the results through data obtained by Krishinapisharody and Yonezawa et al. Liu et al. [12] used a similar method to adjust the empirical formula presented by Yonezawa et al through numerical analysis for 7 different cases. However, these numerical analysis are limited to the narrow range of gas flow rate or fixed slag thickness or too small cases to reveal the relationship between plume eye behavior and various gas flow rates.

In this study, the prediction model for plume eye area is embedded into a numerical simulation program to simulate fluid flow for LF process. The eye area and flow vectors are verified by water model experiments with various slag thickness and gas flow rates. This simulation results show good agreement to the various experimental results of different configurations of water model or steel making field operations. The plume eye area does not increase in direct proportion to the gas flow rate because of slag recovery force. Slag recovery force is closely related to the slag height or potential energy of the slag and the values are able to calculate by Archimedes buoyancy principle.
2.2 Experimental method and numerical model

2.2.1 Experimental apparatus of water model

A cylindrical acrylic ladle with dimensions of 48 cm interior diameter and 50 cm height is used for the experiments. Nitrogen is injected into the ladle through a 6 mm diameter nozzle located at the center of the bottom of the ladle. The gas flow rate is changed from 1 liter / min to 10 liter / min using a mass flow controller. Considering the total specific energy input rate (W/kg) proposed by Mazumdar and Guthrie et al. [13, 14], 1 liter / min corresponds to values of 70 liter / min in a 300 ton ladle system. As shown in Fig. 2-1, the ladle is opened under 1atm and the temperature is kept at 25 °C. The water height is 40 cm. Paraffin oil is selected as the slag. The physical properties of each liquid are given in Table 2-1.

To analyze the effects of slag height, experiments were performed at various thicknesses of oil heights 0.7 cm, 1 cm, 1.2 cm, 3 cm and 5 cm.

To distinguish the paraffin oil from water, a small amount of black dye is added to the oil. The interface at the top of the plume eye and oil is not smooth because the plume eye areas fluctuate due to plume swirling [15] and its behavior is shown in Fig. 2-2. The area of the plume eye is measured by images from video recording and analysis of the area of water at the ladle surface through pixel counting. The oil area is converted to black and water area to white using MATLAB. Average values of 30 images, each image per second, are used for the area of each condition.
Figure 2-1 Schematic diagram of water model equipment

<table>
<thead>
<tr>
<th>Material</th>
<th>Kinematic viscosity (m²/sec)</th>
<th>Density (kg/m³)</th>
<th>Kinematic ratio (slag/melt)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water (25°C)</td>
<td>$1.0 \times 10^{-6}$</td>
<td>1000</td>
<td>-</td>
</tr>
<tr>
<td>Paraffin oil (40°C)</td>
<td>$9.14 \times 10^{-5}$</td>
<td>872</td>
<td>91.4</td>
</tr>
<tr>
<td>Molten Iron (1600°C)</td>
<td>$1.0 \times 10^{-6}$</td>
<td>7000</td>
<td>-</td>
</tr>
<tr>
<td>Slag (1600°C)</td>
<td>$8.85 \times 10^{-5}$</td>
<td>3000</td>
<td>88.5</td>
</tr>
<tr>
<td>N₂ (25°C)</td>
<td>-</td>
<td>1.14</td>
<td>-</td>
</tr>
<tr>
<td>Ar (1600°C)</td>
<td>-</td>
<td>0.26</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 2-1 Various physical properties for industrial model and water model equipment
Figure 2-2 (a) Side view: Bubbling water model equipment and its plume eye, (b) Top view: Paraffin oil (black) & plume eye area at water model in the analyzed region.
2.2.2 Velocity measurement through particle image velocimetry

The particle image velocimetry (PIV) equipment is the optical method of measuring velocity indirectly. This set of device measures the velocity of the glittering particles that are reflected by laser. Particles movement speed is almost same as fluid velocity because of its low terminal velocity, so the particle can represent the fluid velocity.

The general PIV system consists of several sub-systems. In most applications, some spoon of particles have to be inserted to the fluid. These particles are illuminated in a plane of the fluid by laser sheet beam. Laser sheet beam is made by an optical lens component and it converts the high power laser output to a thin light sheet. Images are recorded by the high-speed camera sequentially with a short time interval. The image analysis program evaluates displacement of the particles from a set of images and determine the velocity of desired region. In this study, a set of images received from camera with 0.005sec/pic for 10 seconds. The image data is processed using the commercial VidPIV 4 software. Multi pass correlation was calculated by an adaptive cross-correlation.

To quantitatively analyze interior flow velocities, Average 40 μm silver coated glass particle is used and its density is 500 kg/m3. The area subject to analysis is a region measuring 12 cm across and 9 cm high, at a location 6 cm away from the wall and 6 cm away from the water surface indicated in Fig. 2-1.
2. 2. 3 Ladle Furnace grid system

In the present study, we developed a 3D numerical model of a 300ton ladle and its 1/8 scale water model ladle. Calculations were performed using FORTRAN. We employ numerical analysis using Finite Volume Method (FVM) to simulate fluid flow. The liquid steel (or water) and slag (or paraffin oil) are assumed as Newtonian fluid. Cylindrical coordinates are used to calculate for the cylindrical type ladle.

A total of 210,000 cells are arranged in a grid with numbers of 42 in the azimuthal direction and 50 in the radial direction. In the height direction, 96 cells are arranged for the water or molten steel region, and 4 for the oil or slag region.
Figure 2-3 Schematic diagram of calculation grid (Industrial size)
2.2.4 Flow module

Mass conservation

Conservation of mass requires that the time rate of change of mass in a control volume be balanced by the net mass flow into the same control volume (outflow - inflow). This can be expressed as:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0 \]  

(2-1)

The first term on the left hand side is the time rate of change of the density (mass per unit volume). The second term describes the net mass flow across the control volume’s boundaries and is called the convective term.

Momentum conservation

Newton’s second law states that the time rate of change of the momentum of a fluid element is equal to the sum of the forces on the element. The x-component of the momentum equation is found by setting the rate of change of x-momentum of the fluid particle equal to the total force in the x-direction on the element due to surface stresses plus the rate of increase of x-momentum due to sources:

\[ \frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{V} \vec{u}) = \frac{\partial (-p + \tau_{xx})}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} + S_{Mx} \]  

(2-2)

Similar equations can be written for the y- and z-components of the momentum equation:
\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial (-p + \tau_{yy})}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} + S_{M_y}
\] (2-3)

\[
\frac{\partial (\rho \mathbf{w})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{w}) = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial (-p + \tau_{zz})}{\partial z} + S_{M_z}
\] (2-4)

In these equations, \( p \) is the static pressure and \( t_{ij} \) is the viscous stress tensor.

**Navier-Stokes equations**

The momentum equations, given above, contain as unknowns the viscous stress components \( t_{ij} \), therefore a model must be provided to define the viscous stresses.

In Newtonian flows, the viscous stresses are proportional to the deformation rates of the fluid element. The nine viscous stress components (of which six are independent for isotropic fluids) can be related to velocity gradients to produce the following shear stress terms:

\[
\tau_{xx} = 2\mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu (\nabla \cdot \mathbf{v})
\] (2-5)

\[
\tau_{yy} = 2\mu \frac{\partial v}{\partial y} - \frac{2}{3} \mu (\nabla \cdot \mathbf{v})
\] (2-6)

\[
\tau_{zz} = 2\mu \frac{\partial w}{\partial z} - \frac{2}{3} \mu (\nabla \cdot \mathbf{v})
\] (2-7)

\[
\tau_{xy} = \tau_{yx} = \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)
\] (2-8)

\[
\tau_{xz} = \tau_{zx} = \mu \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)
\] (2-9)
\[ \tau_{xc} = \tau_{cy} = \mu \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \]  

(2-10)

Substitution of the above shear stress terms into the momentum equations yields the Navier-Stokes equations:

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho \vec{V} u) = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[ 2 \mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu (\nabla \cdot \vec{V}) \right] + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] + S_{Mx}
\]  

(2-11)

\[
\frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho \vec{V} v) = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left[ 2 \mu \frac{\partial v}{\partial x} - \frac{2}{3} \mu (\nabla \cdot \vec{V}) \right] + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial v}{\partial y} + \frac{\partial w}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial x} \right) \right] + S_{My}
\]  

(2-12)

\[
\frac{\partial (\rho w)}{\partial t} + \nabla \cdot (\rho \vec{V} w) = -\frac{\partial p}{\partial z} + \frac{\partial}{\partial x} \left[ 2 \mu \frac{\partial w}{\partial x} - \frac{2}{3} \mu (\nabla \cdot \vec{V}) \right] + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial w}{\partial y} + \frac{\partial w}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial w}{\partial z} + \frac{\partial w}{\partial x} \right) \right] + S_{Mz}
\]  

(2-13)

By rearranging these equations and moving the smaller contributions of the viscous stress terms to the momentum source term, we can rewrite the Navier-Stokes equations in a more useful form:

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho \vec{V} u) = -\frac{\partial p}{\partial x} + \nabla \cdot (\mu \nabla u) + S_{Mx}
\]  

(2-14)

\[
\frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho \vec{V} v) = -\frac{\partial p}{\partial y} + \nabla \cdot (\mu \nabla v) + S_{My}
\]  

(2-15)
\[ \frac{\partial (\rho w)}{\partial t} + \nabla \cdot (\rho \vec{V}_w) = -\frac{\partial p}{\partial z} + \nabla \cdot (\mu \nabla w) + S_{Mz} \]  \tag{2-16}

In order to calculate the velocity, the pressure field should be known. However, the governing equation for the pressure does not exist. In this study, pressure is calculated by the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm as proposed by Patankar [16].

2.2.5 Turbulence module

Standard \( k-\varepsilon \) model

Ladle Furnace has a high Reynolds number because of bottom bubbling in a ladle. We use the standard \( k-\varepsilon \) model for turbulence calculation which is well known method to define turbulent as turbulent kinetic energy and its dissipation rate. In the model, the turbulent viscosity is expressed as:

\[ \mu_t = \frac{C_m \rho k}{\varepsilon} \]  \tag{2-17}

The transport equations for \( k \) and \( \varepsilon \) are,

\[ \frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho u_i k) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) - \rho u_j \frac{\partial u_i}{\partial x_j} - \rho \varepsilon \]  \tag{2-18}

\[ \frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho u_i \varepsilon) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) - C_{\varepsilon_t} \frac{\rho \varepsilon}{k} \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} - C_{\varepsilon_c} \frac{\rho \varepsilon^2}{k} \]  \tag{2-19}
In Table 2-2, the variable $\mu_l$ is the liquid dynamic viscosity, and $\mu_t$ is the turbulent viscosity. In addition, to calculate shear stress in turbulent flow, the turbulent Prandtl number of turbulent energy $\sigma_k$ and energy dissipation ratio $\sigma_\varepsilon$ are defined. These values are determined by the turbulent intensity and by the fluid properties. Values used in the present study are given in Table 2-2. [17]

The standard $k\cdot\varepsilon$ model is a high Reynolds model and is not intended to be used in the near-wall regions where viscous effects dominate the effects of turbulence. Instead, wall functions are used in cells adjacent to walls.

<table>
<thead>
<tr>
<th>$\Phi$</th>
<th>$u, v, w$</th>
<th>$K$</th>
<th>$\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma_\Phi$</td>
<td>$\mu_l + \mu_t$</td>
<td>$\mu_l + \frac{\mu_t}{\sigma_k}$</td>
<td>$\mu_l + \frac{\mu_t}{\sigma_\varepsilon}$</td>
</tr>
<tr>
<td>Constant</td>
<td>$C_\mu$</td>
<td>$C_{\varepsilon 1}$</td>
<td>$C_{\varepsilon 2}$</td>
</tr>
<tr>
<td>Value [17]</td>
<td>0.09</td>
<td>1.44</td>
<td>1.92</td>
</tr>
</tbody>
</table>

Table 2-2 Transfer constant and constant values for turbulent calculate
2.2.6 Boundary conditions

The turbulent boundary condition for the wall is needed to solve the fluid flow equation and other scalar equations (k, ε, Concentration, etc.). The wall boundary is the section of the wall where the melt makes contact with the ladle. The implementation of wall boundary conditions in turbulent flows starts with the following equation.

\[ y^+ = \frac{\rho \mu_{\text{ref}}^{1/4} \sqrt{k}}{\mu_1} y \]  

(2-20)

Where \( y \) is the distance from the near wall node to the solid wall. \( k \) is the value at the first grid point from the wall. The wall shear stress value \( (\tau_w) \) is obtained from

\[ y^+ \leq 11.63, \quad \tau_w = \frac{\mu u}{\mu_1} \]  

(2-21)

\[ y^+ > 11.63, \quad \tau_w = \frac{\rho \mu_{\text{ref}}^{1/4} K \sqrt{k u}}{\ln(Ey^+)} \]  

(2-22)

Where \( u \) is the velocity which is parallel to the wall at the grid node. \( K \) and \( E \) are constants of which the values are 0.4187 and 9.793 respectively. [18]
2.2.7 Calculation driving force of gas bubble

To simulate the velocity fields of the melt, the buoyancy force operated by blowing Ar gas must be calculated. The force operated by the gas in a liquid may calculate by drift flux model proposed by Graham[19]. The volumetric flow rate per unit area j is related to the local fraction of component and velocity as follows:

\[ j_1 = (1 - \alpha)v_1 \]  \hspace{1cm} (2-23)

\[ j_2 = \alpha v_2 \]  \hspace{1cm} (2-24)

where \( \alpha \) is the volume fraction of element which is occupied by component 2 and \( v \) is the velocity of each component.

The total flux is

\[ j = j_1 + j_2 \]  \hspace{1cm} (2-25)

Drift velocities are defined as the difference between the component velocities and the average as follows:

\[ v_{1j} = v_1 - \dot{j} \]  \hspace{1cm} (2-26a)

\[ v_{2j} = v_2 - \dot{j} \]  \hspace{1cm} (2-26b)

The drift flux represents the volumetric flux of a component relative to a surface moving at the average velocity

\[ j_{21} = \alpha(v_2 - \dot{j}) \]  \hspace{1cm} (2-27a)

\[ j_{12} = (1 - \alpha)(v_2 - \dot{j}) \]  \hspace{1cm} (2-27b)

Substituting Eq. 2-25 into Eq. 2-27a and using Eq. 2-24, the following equation is obtained.

\[ j_{21} = j_2(1 - \alpha) - j_1\alpha \]  \hspace{1cm} (2-28a)
\[ j_{12} = j_1(1 - \alpha) - j_2 \quad (2-28b) \]

Therefore, \( j_{21} \) is equal to \(-j_{12}\). This symmetry is an important and useful property of the drift flux. Substituting for \( j_1 \) and \( j_2 \) in Eq. 2-28b by using Eq. 2-23, the following equation is obtained.

\[ j_{12} = \alpha(1 - \alpha)(v_1 - v_2) = \alpha(1 - \alpha)v_{12} \quad (2-29) \]

Therefore, the drift flux is proportional to the relative velocity.

The momentum equations, equations of motion, for Newton’s law for the two phases can be written generally in three-dimensional vector form.

\[ \rho_1 \left( \frac{\partial v_1}{\partial t} + v_1 \cdot \nabla v_1 \right) = b_1 + f_1 - \nabla p \quad (2-30a) \]

\[ \rho_2 \left( \frac{\partial v_2}{\partial t} + v_2 \cdot \nabla v_2 \right) = b_2 + f_2 - \nabla p \quad (2-30b) \]

where \( b_1 \) and \( b_2 \) are the body forces per unit volume of that component, which act on each component. \( \nabla p \) is gradient of pressure and \( f_1 \) and \( f_2 \) is the average total force per unit volume containing the hydrodynamic drag, apparent mass effects during relative acceleration, particle-particle forces and so on.

\( F_1 \) and \( F_2 \) are defined as the equivalent of the \( f \)'s per unit volume of the whole flow field. Thus,

\[ F_1 = f_1(1 - \alpha) \quad (2-31a) \]

\[ F_2 = f_2\alpha \quad (2-31b) \]

If these forces are entirely equal due to mutual hydrodynamic drag, then

\[ F_1 = -F_2 = F_{12} \quad (2-32) \]

In case of one dimensional flow, Eq. 2-30 are resolved in the direction of motion
Drift-flux theory is convenient for analyzing flow regimes in which gravity or body force is balanced by the pressure gradient and the forces between the components. For vertical flow, Eq. 2-33 can reduce to

\[ 0 = -\frac{dp}{dz} - \rho_1 g + \frac{F_{12}}{1 - \alpha} \]  
(2-34a)

\[ 0 = -\frac{dp}{dz} - \rho_2 g + \frac{F_{12}}{\alpha} \]  
(2-34b)

Subtracting Eq. 2-34b from Eq. 2-34a, the following equation is obtained.

\[ F_{12} = \alpha(1 - \alpha) g (\rho_1 - \rho_2) \cdot V_j \]  
(2-35)

For gas-liquid system, the total force in the plume (immiscible mixture of gas bubble and melt) can be represented by following equation.

\[ f = \alpha(1 - \alpha) g (\rho_1 - \rho_2) \cdot V_{plume} \]  
(2-36)

Where \( V_{plume} \) is the volume of the plume and \( \alpha \) is the average volume fraction of gas. To calculate the buoyancy force using Eq. 2-36, the volume of plume and average gas fraction of the plume should calculate.

To estimate the shape of the plume that rises vertically, the Iguchi plume model [20] is applied. Iguchi proposed empirical equation that analyzed from perpendicular plume shape. To calculate vertical plume, \( \theta_c \) and \( y \) in Fig. 2-4 are assumed to 0 in the present
The following equations are function of ladle height that determine plume shape.

\[ b_\alpha = b_\alpha (z_0)(z/z_0)^a \]

\[ b_\alpha (z_0) = 0.26(G^2 / g)^{0.2} (\rho_l / \rho_g)^{0.07} \]

\[ z_0 = 0.77 d_m \left( \frac{\rho_l}{\rho_g} \right)^{0.28} Fr^{0.89(\rho_l / \rho_g)^{-0.16}} \]

\[ Fr' = \frac{\rho_g Q^2}{\rho_l gd_m^2} \]

\[ r_p = 1.7b_\alpha \] (2-37)

In Eq. 2-37, \( b_\alpha \) is the radial distance of the plume at the center line. \( Q \) is the gas flow rate (m\(^3\)/sec), \( \rho_l \) and \( \rho_g \) are the density of the melt and gas (kg/m\(^3\)). \( g \) is the gravity acceleration (m/sec\(^2\)). \( d_m \) is the diameter of nozzle(m) and \( r_p \) is the radius of plume area.

From Eq. 2-37, we can calculate \( V_{\text{plume}} \) in Eq. 2-36.

As mentioned above, \( \alpha \) is the average gas fraction, \( \alpha \) is defined as follows:

\[ \alpha = \frac{V_g}{V_{\text{plume}}} \] (2-38)

\[ V_g = \frac{Q}{(u_{\text{melt}} + u_{\text{slip}}) \cdot P_{\text{eff}}} \] (2-39)

Where \( u_{\text{melt}} \) is the melt velocity which is calculated from simulation and \( u_{\text{slip}} \) is the gas velocity relative to the liquid and a value of 0.3 m/s was used for the water, and 0.5 m/s for the steel melt [21]. \( P_{\text{eff}} \) is the effective pressure where the function of ladle height and melt density. \( P_{\text{eff}} \) can be defined as follows:

\[ P_{\text{eff}} = \frac{101325 + \rho_l \cdot g \cdot (h_{\text{melt}} - z)}{101325} \] (2-40)
In Eq. 2-40, 101,325 is the unit of Pascal at the top of the ladle and \( h_{\text{melt}} \) is height of melt from ladle bottom. \( z \) means the depth of the ladle. This equation indicates the relative pressure over depth. In Fig. 2-5 shows the relation of effective pressure and plume volume in case of 3.5m steel ladle.

Using equation from Eq. 2-37 to Eq. 2-40, we can calculate the buoyancy force of plume. In the ladle, gas bubble is assumed to rise vertically, the buoyancy force can calculate as the source term of w direction.
Figure 2-4. Schematic shape of perpendicular plume from Iguchi et al. [20]

Figure 2-5. The relationship of plume volume, effective pressure and ladle height.
2.2.8 Energy balance at plume eye boundary and its relationship

The center of the plume eye is called the ‘spout’ [15]. The spout is the area with the highest pressure in the ladle, and the height to which the slag may be displaced. The plume eye area is larger than the spout, which indicates kinetic energy is acting in the lateral direction which is induced from the melt’s uprising pressure. The relationship between the kinetic and potential energy of the slag and melt at the plume eye boundary can be defined as

\[
\frac{1}{2} \rho_m v_m^2 + \rho_m g \Delta h_m = \frac{1}{2} \rho_s v_s^2 + \rho_s g \Delta h_s
\]

(2-41)

In Eq. 2-41, the left term represents the sum of the melt energy and the right term is the sum of the slag energy. As illustrated in Fig. 2-6, the initial slag thickness is given as \( h_0 \). The base line is the melt surface, so \( \Delta h_m \) becomes 0. On the right (slag) term, the kinetic energy is nearly 0 because the value of \( v_s \) is much smaller than the velocity of melt at the plume eye boundary. Therefore, the melt velocity at the plume eye boundary, \( v_{b, \text{eye}} \) (\( v_m \) in Eq. 2-41) gives,

\[
v_{b, \text{eye}} \approx \sqrt{\frac{2 \rho_s g \Delta h_s}{\rho_m}}
\]

(2-42)

Here, \( v_{b, \text{eye}} \) represents the melt velocity required for plume eye expansion. As increased plume eye size means that space once occupied by slag is then filled with melt, so the slag thickness must increase. If we assume that the amount of slag entrapment is far
smaller than the total amount of slag, slag volume does not change during the process. The relation between the total slag thickness \( (h_{\text{all}}) \) and the plume eye area is as follows.

\[
   h_{\text{all}} = \frac{A_{\text{ladle}}}{(A_{\text{ladle}} - A_{\text{eye}})} \cdot h_0
\]

(2-43)

Here, \( A_{\text{ladle}} \) is the ladle area view from the top and \( A_{\text{eye}} \) is the plume eye area.

During bottom bubbling, the kinetic energy of melt strongly pushes slag. Due to slag’s own weight and melt / slag densities, slag may sink as in Fig. 2-6. The thickness of sunken slag may be derived from Archimedes buoyancy principle.

In an application of this principle to a bottom bubbling situation, the weight of slag which has descended to below the initial slag/melt interface is equal to the weight of melt with a volume equivalent to that of slag below the melt, which can be shown as

\[
   \rho_s V_{\text{slag}} = \rho_m V_x
\]

\[
   \rho_s A_{\text{ladle}} h_0 = \rho_m (A_{\text{ladle}} - A_{\text{eye}}) \cdot h_x \quad \Rightarrow h_x = h_{\text{all}} - \Delta h_s
\]

\[
   h_x = \frac{\rho_s}{\rho_m} \frac{A_{\text{ladle}}}{(A_{\text{ladle}} - A_{\text{eye}})} \cdot h_0 = \frac{\rho_s}{\rho_m} \cdot h_{\text{all}}
\]

\[
   \therefore \Delta h_x = h_{\text{all}} \cdot \left(1 - \frac{\rho_s}{\rho_m}\right) \quad (2-44)
\]

where \( V_x \) is the volume of melt which was occupied by slag at initial.

Since the slag volume is \( \text{(slag thickness)} \times \text{(slag area)} \), the thickness of slag above the base line can be derived from Eq. 2-44. The slag height increment \( \Delta h_s \) caused by plume eye expansion is related to the depth of descent \( h_x \).

Because the plume eye area is calculated using Eq. 2-42 – Eq. 2-44, the area is
affected by various parameters such as ladle size, slag height, density ratio of slag and melt
and velocity field in the melt. In particular, the velocity field is also affected by various
operating conditions and materials properties. As a result the plume eye area is affected by
various parameters and this model is incorporated in a numerical simulation program. The
plume eye area is determined by the following steps.

1. Calculate $v_{b_{,eye}}$ according to the slag thickness from Eq. 2-42 ~ Eq. 2-44.
2. Calculate velocity. Melt velocity in front of the slag is a cause of plume eye
   expansion. If melt velocity exceeds $v_{b_{,eye}}$, plume eye expands.
3. If melt is exposed, part of slag changes into melt. In other words, slag physical
   properties change into melt properties. If velocity value is less than $v_{b_{,eye}}$, melt
   properties change into slag properties.

These steps are repeated for every time step.
Figure 2-6. Schematic diagram of plume eye prediction model with Archimedes buoyancy principle.
2.3 Result and discussion

2.3.1 Velocity profiles in the water model

Fig. 2-7 shows simulation results corresponding to gas flow rates of 1, 3, 5, 7 L/min with oil at a thickness of 1.2cm. Results show water and oil have conical interface and vector is changed by gas flow rate. The center region of circulation flow marked as a white dot moves closer to the wall with higher gas flow rates and small circulation flow with opposite direction also appears near the wall. A higher gas flow rate results in a greater main circulation flow due to the plume eye area.

Fig. 2-8 shows velocity profiles for the same gas flow rates as in Fig. 2-7, but no oil. Results show the vector is similar. The circulation point marked as a white dot is almost equivalent for all the different gas flow rates.

Because the present model is based on the fluid flow, quantitative prediction of velocity values is very crucial. Hence, velocity field results from numerical simulation were compared with water model results.

Experiments were performed using Particle Image Velocimetry (PIV) experimentation and the results are well matched with the calculation as shown in Fig. 2-9.

Data obtained from cases with slag reveal lower velocities than those with no slag. The measured results are well matched with the calculation results. From these results, it is clear that velocity profiles are affected by the presence of slag. Therefore, accurate prediction of plume area is important to simulate LF fluid flow.
Figure 2-7 Simulation result of the water model with various gas flow rate (oil existence).

Figure 2-8 Simulation result of the water model with various gas flow rate (no oil).
Figure 2-9. Average velocity result of simulation and PIV image analysis at the measured region.
2.3.2. Effect of slag thickness on area of plume eye

Effects of gas flow rate and slag thickness on the area of plume eye are plotted in Fig. 2-10. As shown in Fig. 2-10, plume eye area decreases as slag thickness increases. In addition, increasing gas flow rates also increases the area. But the increment of the plume eye area decreases as gas flow rate increases. This phenomena appears to be due to the large value of $v_{b,\text{eye}}$ when the plume eye has a large area. $V_{b,\text{eye}}$ values calculated using Eq.2-42 ~ Eq. 2-44 are plotted in Fig. 2-11. The increase of $V_{b,\text{eye}}$ is accelerated as plume eye increases.

Thicker slag heights also need higher $V_{b,\text{eye}}$ to maintain the same plume eye area. For slag thickness of 0.7cm, to reach a plume eye radius of 20cm (plume eye area 0.126m$^2$) the water velocity at the oil interface must be at least 23 cm/sec. For the same plume eye radius with an oil thickness of 1.0cm, the water velocity must be 27cm/sec, and for an oil thickness of 1.2cm, the water velocity must be 30cm/sec.

The water model measurement results and the simulation results are compared in Fig. 2-12. All results show similar behavior for the effects of slag thickness and gas flow rates and all of the values are similar.
Figure 2-10. Simulation result of average plume eye area according to the various gas flow rate and oil thickness
Figure 2-11. Melt velocity in front of the plume eye boundary ($v_{b\_eye}$) according to the oil thickness (water model result).
Figure 2-12. The plume eye area of water model & simulation result.

(a) oil thickness: 0.7 cm, (b) oil thickness: 1.0 cm, (c) oil thickness: 1.2 cm,
(d) oil thickness: 3.0 cm, (e) oil thickness: 5.0 cm.
2.3.3. Comparison with other studies

Numerical analysis allows for flexible application to various different processing conditions and equipment systems. To confirm this flexibility, simulations are conducted and compared with research results presented in other studies. Krishnapisharody et al[7] proposed correlation between plume eye area and fluid height as follows:

\[
\frac{A_{\text{eye}}}{H^2} = \alpha + \beta \left( \frac{\rho}{\Delta \rho} \right)^{0.5} \left( \frac{U_p^2}{gh} \right)^{0.5}
\]

(2-45)

In this equation, H is fluid height, h is slag height, \(U_p\) is plume velocity and \(\alpha\), \(\beta\) are constants.

Plume velocity, \(U_p\) (m/sec), is given by Castello-Branco and Schwerdtfeger[22] et al:

\[
U_p = 17.4 Q^{0.244} \left( \frac{\rho_g}{\rho} \right)^{0.0218} H^{-0.08}
\]

(2-46)

where \(Q\) is the gas flow rate(cm³/sec), and \(\rho_g\) is the density of injection gas. In Eq. 2-45, Krishnapisharody et al proposed empirical constants for the water / oil system, \(\alpha\) : \(-0.15 \pm 0.1\) and \(\beta\) : \(0.574 \pm 0.12\).

Their experiments were based on the following conditions. The oil thickness was set at 1cm with ladle dimensions of 42cm diameter with 31.5cm height, and the nozzle located at the center.

Fig. 2-13 (a) shows, for the water model equipment used by Krishnapisharody et
al’s measured results, the predicted results from the empirical formula, and the simulation results of the present study. Under these conditions, the predictions from the present study are quite accurate. As shown in the figure, the curve presented by Krishnapisharody et al is in good agreement with their experimental results, but the prediction is not good for the present experiments as shown in Fig. 2-13 (b).

Figure 2- 13 (a)  Comparison of Krishnapisharody et al’s empirical line, experimental data and simulation result from current model (result of water / paraffine oil). Krishnapisharody et al’s water model measured data (Ladle diameter = 42 cm, Fluid height = 31.5 cm, oil density = 870 kg/m3, oil thickness= 1 cm, nozzle location : center, alpha = -0.15, beta = 0.574)
Figure 2-13 (b) Present water model measured data (Ladle diameter = 48 cm, Fluid height = 40 cm, oil density = 872 kg/m3, oil thickness = 1.2 cm, nozzle location: center).
2.3.4. Application to industrial ladle

Simulations on the Industrial size ladle were performed. At first, to verify the applicability of the model in a large ladle, calculation results were compared to the experiments by Yonezawa et al[4], who measured plume eye area with conditions of ladle diameter 4.4m, ladle height 3.5m and slag thickness approximately 5cm. Although the study explains that the gas nozzle is set away from the center, its exact location is not specified. In the present study we assume that the nozzle is located 40% of the radius away from the center, where material transfer occurs effectively[23].

Fig. 2-14 (a) shows a comparison between the experimental results of plume eye area presented by Yonezawa et al and the predictions of the present study. Simulation results are very similar to the experimental results. Fig. 2-14 (b) shows the plume eye area for a 300 ton ladle with slag thickness of 6cm and 10cm.

As shown in Fig. 2-14 (b) the effects of slag thickness and gas flow rates on the plume eye area are similar to the water model.

It should be very difficult to obtain a general equation which accurately predicts the plume eye behavior for various shapes of ladles and operating conditions. The predictive ability of reported equations [4, 7, 9, 15, 24] are very limited to conditions similar to those of each respective experiment. On the other hand the present numerical model can predict the plume eye area for various configurations of ladle systems, from water models to industrial sizes with steel melt.
Figure 2-14 (a) Comparison of Yonezawa et al’s experimental data and simulation result from current model (result of molten steel/slag). Yonezawa et al’s industrial ladle measured data (Ladle diameter = 4.4 m, fluid height = 3.5 m, slag density = 3000 kg/m³, nozzle location: 40% of radius away from center, slag thickness = 5 cm)
Figure 2-14 (b) Result of simulation on 300 ton industrial ladle according to the various slag thickness (Ladle diameter = 4.0m, fluid height = 3.41 m, slag density = 3000 kg/ m³, nozzle location : 40% of radius away from center, slag thickness = 6 cm and 10 cm).
2.3.5. General equation for plume eye prediction

At first, plume eye area may be assumed to be proportional to gas flow rate and inversely proportional to slag thickness $h_0$ as in Figure 8. Defining plume eye ratio ($AR_{plume}$) as $A_{eye}/A_{ladle}$ and combining these relationships of the plume eye ratio gives the following:

\[
\frac{Q}{h_0} \propto AR_{plume}
\]  

(2-47)

In Eq. 2-47, $Q$ is gas flow rate and unit is liter/min. $h_0$ is initial slag thickness and its unit is m. The relationship between two of Eq. 2-47 is shown in Fig. 2-15. Combining the 60 sets of simulation data from Fig. 2-12 shows that there is a regular relationship between the left and right terms of Eq. 2-47.

Fig. 2-16 plots simulation results for various ladle conditions in terms of $\sqrt{Q/h_0}$ and $AR_{plume}$. There are linear relationships between two terms and the slopes are different for steel ladle and the water model. We can summarize as follows:

\[
AR_{plume} = \beta \times \frac{Q}{h_0}
\]  

(2-48)

Even the values of $\beta$ are different at each conditions. However all results show linear relations between $AR_{plume}$ and $\sqrt{Q/h_0}$.

Additional research is needed regarding the factors which determine $\beta$. $\beta$ is likely a value related to ladle area, fluid height or material properties.
Figure 2-15 Relationship between plume eye ratio (ARplume) and gas flow rate related term (Q/h0) in water model. Radius 24 cm, height 40 cm, slag thickness: 0.7, 1.0, 1.2 cm, gas flow rate: 0.5-10 l/min. Total 60 simulation data.
Figure 2-16 (a) Relationship between plume eye ratio and for various result of water model and steel ladle. Simulation result of water model in this study and Krishnapisharody et al’s measurement data. H is fluid height, D is ladle diameter. (Krishnapisharody et al’s condition: D is fixed at 42 cm, H are 42 cm and 31.5 cm)
Figure 2-16 (b) Simulation data for 300 ton ladle condition and Yonezawa et al’s ladle condition.
2.4 Conclusion of flow calculation module

We developed a numerical model to simulate plume eye size. And this model is coupled with fluid flow simulations to predict fluid flow of ladle in LF processing. The simulation results are well matched to the results of present experiments and other group’s experiments. From the experiments and simulations, it is found that plume eye area is closely related to the slag potential energy and melt kinetic energy.

1) To calculate the velocity at the plume eye boundary, quantitative slag height is calculated according to the plume eye area. Slag height is related to Archimedes buoyancy principle and the value is increased with the plume eye area increases. But the increment of the slag height does not direct proportion to the size of plume eye. This means plume eye area is curvilinear increased with fluid flow velocity or gas flow rate.

2) The present numerical analysis model is applicable to various melts and ladle sizes. Previous plume eye prediction equations have been based on specific experimental conditions and were limited in predicting plume eye area for different conditions. However, the present model has been shown to be effective in predicting the plume eye area not just for the experiments of the present study, but also for the conditions presented in other studies.

3) In this study, we reveal the relationship between plume eye ratio and gas flow rate Q. Results indicate a linear relationship between the two terms, and solving for the two terms shows that the plume eye ratio is proportional to the square root of the gas flow rate Q and inversely proportional to the square root of the slag thickness $h_0$. 
Chapter 3. Deoxidation reaction model

3.1 Background study of oxide reaction

As mentioned above, LF process is very complex. It contains from argon bottom bubbling to inclusion removal. To make simulation program, we should consider flow, mass transfer, reaction and inclusion agglomeration. Proper understating of the mixing of alloy elements and their transfer route is important to enhance operations of process. From plume eye prediction model, flow profile of ladle could be obtained and we can predict mass transfer behavior over time.

Like Fig. 3-1, when alloy (or deoxidizer) is added, the local area of alloy addition site soars up to over ten times of equilibrium concentration. Before the end of mass transfer, this high and low concentration region is mixed all over the ladle. Understanding of alloy transfer is important because the quantity of inclusion generation is depending on that. Moreover in case of allotropy oxide such as Ca-aluminate, local alloy concentration makes un-wanted oxide. These reactions take place at the local high concentration region if the region is maintained for a period of time within the system. Therefore, an analysis of mixing behavior requires an understanding of the behavior.

When calculating inclusion generation, reaction calculation specialized program such as FACTsage [25] or ThermoCalc [26] can predict the quantity of inclusion under the equilibrium concentration or uniform distribution of reactants. However, these programs are difficult to calculate local reaction because of the imbalance of alloy concentration.

On the other hand, flow calculation specialized programs can predict the local behavior of alloy, but predicting inclusion generation reaction and inclusion tracking is
difficult. To overcome these problems, we developed inclusion generation model for LF.

In the present study, we choose associate model [25, 27, 28] that is used to FACTsage solution calculation. Unlike well-known Wagner formation [29], associate model needs only one self-interaction coefficient to calculate thermodynamics. This model is suitable to predict complex reaction like complex deoxidation inclusion such as Ca-aluminate. This model is also able to predict the alloy transfer and its reaction with flow calculation module. This integrated module will inform the initial location of inclusions for the inclusion agglomeration module -next calculation module-.

Simple reaction such as SiO$_2$ or Al$_2$O$_3$ generating reaction is developed based on the associate model that verified by Jung[27], Decterov[25], other FACTsage models that proposed by Bouchard and Bale [30], Heuzey and Pelton [31]. The model of inclusion generation in this program is verified comparing to FACTsage.

The concentration unit ‘ppm’ is weight unit, 1 ppm indicates 0.3 kg in the 300ton ladle in this study.
Figure 3-1. Mass concentration in a 300 ton ladle according to the 300ton flow calculation.

Gas flow rate is 30m$^3$/hour (500 liter / min). (a) 5 seconds after tracer addition

Figure 3-2. (b) 40 seconds after tracer addition
3. 2 Numerical model for deoxidation reaction

3. 2. 1 Reaction mechanism by Wagner formalism

Considering molten steel as solvent, M as metal solute of three phase Fe-M-O liquid solution, thermodynamic equilibria of steel are usually treated by the well-known Wagner formation [29]. For example x mole of dissolved metal [M], y mole of dissolved oxygen [O] makes pure MₓOₙ solid and if they exist as equilibrium state, the Gibbs free energy relationship between two is as follows:

\[ x \text{[M]} + y \text{[O]} = M_x O_y \text{ (solid)} \] (3-1)

\[ \Delta G = G_{MxOy} - [xG_M + yG_O] = 0 \]

\[ = \Delta G^0 + RT \ln \left( \frac{a_{MxOy}}{a_{M}^{x} a_{O}^{y}} \right) = 0 \]

(3-2)

\[ RT \ln \left( \frac{a_{MxOy}}{a_{M}^{x} a_{O}^{y}} \right) \] in Eq. 3-2, \( \frac{a_{MxOy}}{a_{M}^{x} a_{O}^{y}} \) is called as equilibrium constant K and this value is determined by the activities of reactants and product. Eq. 3-2 can simplify as follows:

\[ \exp \left( \frac{-\Delta G^0}{RT} \right) = \frac{a_{MxOy}}{a_{M}^{x} a_{O}^{y}} \]

(3-3)

When forward reaction occurs, reactants are consumed and similarly, backward reaction occurs, products are decomposed. These Gibbs energy relationships can be expressed as inequality.
Forward reaction:  \[ \exp \left( -\frac{\Delta G^0}{RT} \right) > \frac{a_{MxOy}}{a_{[M]}a_{[O]}} \]

Backward reaction:  \[ \exp \left( -\frac{\Delta G^0}{RT} \right) < \frac{a_{MxOy}}{a_{[M]}a_{[O]}} \]

(3-4)

If the product is pure solid and the reactant follows Henry’s law, equilibrium constant K can be written as

\[ K = \frac{1}{a_{[M]}a_{[O]}} = \frac{1}{(X_{[M]}f_{[M]}) \cdot (X_{[O]}f_{[O]})} \]

(3-5)

\[ f_{[M]} = \exp \left( \epsilon_{M}^O \cdot X_{[O]} + \epsilon_{M}^{M} \cdot X_{[M]} \right) \]
\[ f_{[O]} = \exp \left( \epsilon_{O}^M \cdot X_{[M]} + \epsilon_{O}^O \cdot X_{[O]} \right) \]

(3-6)

In Eq. 3-6, \( f_{[M]} \) and \( f_{[O]} \) indicate fugacities of dissolved metal and dissolved oxygen, Capital X indicates mole fraction of each component. \( \epsilon \) is the first order interaction coefficient. [32]

When defining interaction coefficient \( \epsilon \), it needs 4 constants (\( \epsilon_{A}^A, \epsilon_{A}^B, \epsilon_{B}^A, \epsilon_{B}^B \)) to calculate reaction between 2 reactants by Wagner formation. If 3 reactants exist, required interaction coefficients are 9 (\( \epsilon_{A}^A, \epsilon_{A}^B, \epsilon_{A}^C, \epsilon_{B}^A, \epsilon_{B}^B, \epsilon_{B}^C, \epsilon_{C}^A, \epsilon_{C}^B, \epsilon_{C}^C \)). If one reactant added, it needs 16 coefficients. Thus reactants add, required data also increases exponentially.

The weakness of the classical Wagner formalism lies in the assumption that the dissolved metal and O atoms are independent, randomly distributed particles. [3] Generally, negative cross-interaction parameters indicate attractive interaction between [M] and [O] such as deoxidizer and oxygen. By the associate model proposed by Jung et al. [27],
dissolved metal and oxygen are not independent particles, but should rather exist an “associates”.

3. 2. 2 Simple reaction by associate model

By the associate model, every deoxidizer has one self-interaction coefficient. Another reactants such as dissolved oxygen and associates self-interaction coefficients are fixed at 1.

\[
\ln f_{[M]} = \varepsilon_{M} X_{[M]}
\]

\[
f_{[O]} = f_{[M\cdot O]} = f_{[M2\cdot O]} = 1
\]  

(3-7)

For example, the reaction among dissolved [Al] and [O] in the molten steel, define \( G_{\text{initial}} \) as the sum of Gibbs free energy of 2 moles of [Al] and 3 moles of [O]. Also, \( G_{\text{final}} \) is the energy of 1 mole of Al\(_2\)O\(_3\). To take place spontaneous reaction, the value of \( G_{\text{initial}} \) must bigger than the value of \( G_{\text{final}} \). If define a reaction to form alumina as the forward reaction, alumina is created when \( \Delta G = G_{\text{final}} - G_{\text{initial}} < 0 \). From previous studies, \( \Delta G \) values for forming various inclusions are given in Table 3-1. [27] [33-36]
<table>
<thead>
<tr>
<th>Chemical Formula</th>
<th>ΔG (J/mol)</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) Al(l) + 1.5 O2(g) = Al2O3(s)</td>
<td>ΔG1 = G^0_{Al2O3} − 2G^0_{Al} − 1.5G^0_{O2}</td>
<td>[33-36]</td>
</tr>
<tr>
<td>2) Al(l) = [Al]</td>
<td>ΔG2 = RT * -15,280 /T + 3.5</td>
<td>[27]</td>
</tr>
<tr>
<td>3) O2(g) = [O]</td>
<td>ΔG3 = RT * -7,596.7/T + 1.2</td>
<td>[27]</td>
</tr>
<tr>
<td>4) 2 [Al] + 3[O] = Al2O3</td>
<td>ΔG4 = ΔG1 - 2 ΔG2 - 3ΔG3</td>
<td></td>
</tr>
<tr>
<td>5) [Al] + [O] = [Al*O]</td>
<td>ΔG5 = -108,614</td>
<td>[27]</td>
</tr>
<tr>
<td>(associate)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6) 2 [Al*O] + [O] = Al2O3(s)</td>
<td>ΔG6 = ΔG4 - 2 ΔG5</td>
<td></td>
</tr>
<tr>
<td>7) 2 [Al] + [O] = [Al2*O]</td>
<td>ΔG7 = -179,912</td>
<td>[27]</td>
</tr>
<tr>
<td>(associate)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8) [Al2*O] + 2[O] = Al2O3(s)</td>
<td>ΔG8 = ΔG4 - ΔG7</td>
<td></td>
</tr>
</tbody>
</table>

Table 3-1 Al2O3 reaction formula and ΔG by associate model
The products are Al*O Associate, Al₂*O associate and Al₂O₃. The equilibrium constants to create associate are as follows:

\[ K_{\text{Al}*O} = \frac{f_{[\text{Al}*O]}X_{[\text{Al}*O]}}{(f_{[\text{Al}]}X_{[\text{Al}]})^2(f_{[O]}X_{[O]})} = \frac{X_{[\text{Al}*O]}}{(f_{[\text{Al}]}X_{[\text{Al}]})X_{[O]}} \]  

(3-8)

\[ K_{\text{Al}_2*O} = \frac{f_{[\text{Al}_2*O]}X_{[\text{Al}_2*O]}}{(f_{[\text{Al}]}X_{[\text{Al}]})^2(f_{[O]}X_{[O]})^2} = \frac{X_{[\text{Al}_2*O]}}{(f_{[\text{Al}]}X_{[\text{Al}]})^2X_{[O]}} \]  

(3-9)

From various associates, the equilibrium constants to form Al₂O₃ are as follows:

\[ K_{\text{Al}_2O_3} = \frac{1}{X_{\text{Al}*O}^2X_{O}} \]  

(3-10)

\[ K_{\text{Al}_2O_3} = \frac{1}{X_{O}^2X_{\text{Al}_2*O}} \]  

(3-11)

The self-interaction coefficients and other various constants at 1873K are given in Table 3-2. [25, 27]
<table>
<thead>
<tr>
<th>Element</th>
<th>$\varepsilon_M^M$</th>
<th>$\Delta G_{M,O}^0$ (J/mol)</th>
<th>$\Delta G_{M2,O}^0$ (J/mol)</th>
<th>Stable Form</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>3802.7/T + 0.4</td>
<td>-108,614</td>
<td>-179,912</td>
<td>Al$_2$O$_3$</td>
</tr>
<tr>
<td>Ba*</td>
<td>0</td>
<td>-240,922 (&lt;1.5ppm)</td>
<td>-</td>
<td>BaO*</td>
</tr>
<tr>
<td>Ca*</td>
<td>0</td>
<td>-305,828 (&lt;17ppm)</td>
<td>-</td>
<td>CaO*</td>
</tr>
<tr>
<td>Ce</td>
<td>-29627.6/T</td>
<td>-192,464</td>
<td>-</td>
<td>Ce$_2$O$_3$</td>
</tr>
<tr>
<td>Cr</td>
<td>0</td>
<td>-38,650</td>
<td>-62,760</td>
<td>Cr$_2$O$_3$</td>
</tr>
<tr>
<td>La</td>
<td>0</td>
<td>-209,200</td>
<td>-</td>
<td>La$_2$O$_3$</td>
</tr>
<tr>
<td>Mg*</td>
<td>0</td>
<td>-218,272 (&lt;13ppm)</td>
<td>-</td>
<td>MgO*</td>
</tr>
<tr>
<td>Mn</td>
<td>0</td>
<td>-20,920</td>
<td>-</td>
<td>MnO</td>
</tr>
<tr>
<td>Nb</td>
<td>-27404.7/T</td>
<td>-43,368</td>
<td>-133,888</td>
<td>NbO$_2$</td>
</tr>
<tr>
<td>Si</td>
<td>4026/T + 10.25</td>
<td>0</td>
<td>-</td>
<td>SiO$_2$</td>
</tr>
<tr>
<td>Ti</td>
<td>3467.6/T</td>
<td>-96,145</td>
<td>-142,256</td>
<td>Ti$_3$O$_5$</td>
</tr>
<tr>
<td>V</td>
<td>-2768.9/T - 4.876</td>
<td>-49,371</td>
<td>-104,600</td>
<td>VO</td>
</tr>
<tr>
<td>Zr</td>
<td>0</td>
<td>-150,860</td>
<td>-251,040</td>
<td>ZrO$_2$</td>
</tr>
</tbody>
</table>

* : Ba, Ca, Mg stable phases are associate form. (BaO, CaO, MgO)

Table 3-2. Thermodynamic constant for associate model (at 1600 $^\circ$C)  [25, 27]
3. 2. 3 Formation of complex deoxidation inclusion

The type of complex oxide depends on the concentrations of the simple type inclusion, another type of complex inclusion and the element that has stronger affinity for oxygen. Complex inclusion has made to prevent nozzle clogging or removal, especially Al-killed steel. It is known as Ca changes the shape of alumina cluster into spherical shape. In case of making Ca-aluminate, the following reaction will take place.

**Reaction with Al₂O₃**

1) \( 1 \text{Ca} + 19/3 \text{Al}_2\text{O}_3 = 1 \text{CaAl}_{12}\text{O}_{19} + 2/3 \text{Al} \)

2) \( 1 \text{Ca} + 7/3 \text{Al}_2\text{O}_3 = 1 \text{CaAl}_3\text{O}_7 + 2/3 \text{Al} \)

3) \( 1 \text{Ca} + 4/3 \text{Al}_2\text{O}_3 = 1 \text{CaAl}_2\text{O}_4 + 2/3 \text{Al} \)

4) \( 3 \text{Ca} + 2 \text{Al}_2\text{O}_3 = 1 \text{Ca}_3\text{Al}_2\text{O}_6 + 2 \text{Al} \)

5) \( 1 \text{Ca} + 1/3 \text{Al}_2\text{O}_3 = 1 \text{CaO} + 2/3 \text{Al} \)

**Reaction with CaAl₁₂O₁₉ (Ca + 1CaO-6Al₂O₃)**

1) \( 12/19 \text{Ca} + 7/19 \text{CaAl}_{12}\text{O}_{19} = 1 \text{CaAl}_3\text{O}_7 + 8/19 \text{Al} \)

2) \( 15/19 \text{Ca} + 4/19 \text{CaAl}_{12}\text{O}_{19} = 1 \text{CaAl}_2\text{O}_4 + 10/19 \text{Al} \)

3) \( 51/19 \text{Ca} + 6/19 \text{CaAl}_{12}\text{O}_{19} = 1 \text{Ca}_3\text{Al}_2\text{O}_6 + 34/19 \text{Al} \)

4) \( 18/19 \text{Ca} + 1/19 \text{CaAl}_{12}\text{O}_{19} = 1 \text{CaO} + 12/19 \text{Al} \)

**Reaction with CaAl₄O₇ (Ca + 1CaO-2Al₂O₃)**

1) \( 3/7 \text{Ca} + 4/7 \text{CaAl}_4\text{O}_7 = 1 \text{CaAl}_2\text{O}_4 + 2/7 \text{Al} \)

2) \( 15/7 \text{Ca} + 6/7 \text{CaAl}_4\text{O}_7 = 1 \text{Ca}_3\text{Al}_2\text{O}_6 + 10/7 \text{Al} \)

3) \( 6/7 \text{Ca} + 1/7 \text{CaAl}_4\text{O}_7 = 1 \text{CaO} + 4/7 \text{Al} \)
Reaction with \( \text{CaAl}_2\text{O}_4 \) (\( \text{Ca} + 1\text{CaO} \cdot 1\text{Al}_2\text{O}_3 \)) \hspace{1cm} (3-15)

1) \( \frac{3}{2} \text{Ca} + \frac{3}{2} \text{CaAl}_2\text{O}_4 = 1 \text{Ca}_3\text{Al}_2\text{O}_6 + 1 \text{Al} \)

2) \( \frac{3}{4} \text{Ca} + \frac{1}{4} \text{CaAl}_2\text{O}_4 = 1 \text{CaO} + \frac{1}{2} \text{Al} \)

Reaction with \( \text{Ca}_3\text{Al}_2\text{O}_6 \) (\( \text{Ca} + 3\text{CaO} \cdot 1\text{Al}_2\text{O}_3 \)) \hspace{1cm} (3-16)

1) \( \frac{1}{2} \text{Ca} + \frac{1}{6} \text{Ca}_3\text{Al}_2\text{O}_6 = 1 \text{CaO} + \frac{1}{3} \text{Al} \)

Reaction formula Eq. 3-12 to Eq. 3-16 can simplify Eq. 3-17.

\[
\text{Ca} + \text{Al rich Ca-aluminate} = \text{Ca rich Ca-aluminate} + \text{Al} \\
\text{Reactant1} + \text{Reactant2} = \text{Product1} + \text{Product2}
\] \hspace{1cm} (3-17)

Various type of Ca rich Ca-aluminate (Product1 in Eq. 3-17) can produce by the concentrations of Ca (reactant1) and Al rich Ca-aluminate (reactant2). In this study, we ignored solid-solid reaction such as \( \text{CaO} + \text{Al}_2\text{O}_3 \) and assumed that most of Ca related reaction is taken place by dissolved Ca.

When some reactants makes any product, the difference of Gibbs free energy is as follows:

\[
\Delta G^0 = G^0_{\text{Amount of products}} - G^0_{\text{Amount of reactants}} + G^0_{\text{Remaining reactants after reaction}}
\] \hspace{1cm} (3-18)

Quantity of product is related on the quantity of reactants and its stoichiometric constant. Like Ca-aluminate, if two matters makes certain type of product, quantity of
product can be determined as follows.

\[ M_{\text{product1}} = \min \left[ \frac{M_{\text{reactant1}}}{s_{\text{reactant1}}}, \frac{M_{\text{reactant2}}}{s_{\text{reactant2}}} \right] \]  
 \hspace{1cm} (3-19)

In Eq. 3-19, \( s_{\text{reactant1}} \) and \( s_{\text{reactant2}} \) are the stoichiometric constants of reactants, \( M_{\text{reactant1}} \) and \( M_{\text{reactant2}} \) are the present mole number of reactants. And \( M_{\text{product1}} \) represents mole number of product.

By using Eq. 3-18 and Eq. 3-19, following Gibbs free energy differences can be obtained.

\[ \Delta G^0 = M_{\text{product1}} * G^0_{\text{product1}} + (M_{\text{product1}} * s_{\text{product2}}) * G^0_{\text{product2}} - (M_{\text{reactant1}} * G^0_{\text{reactant1}} + M_{\text{reactant2}} * G^0_{\text{reactant2}}) + (M_{\text{reactant1}} - M_{\text{product1}} * s_{\text{reactant1}}) * G^0_{\text{reactant1}} + (M_{\text{reactant2}} - M_{\text{product1}} * s_{\text{reactant2}}) * G^0_{\text{reactant2}} \]  
 \hspace{1cm} (3-20)

In Eq. 3-20, \( M_{\text{product2}} \) and \( s_{\text{product2}} \) mean [Al] mole number and stoichiometric constant among products. The first line of Eq. 3-20 represents \( G^0 \) amount of products in Eq. 3-18, second line represents \( G^0 \) amount of reactants, and last third, fourth lines represent \( G^0 \) remaining reactants after reaction.
Let’s assume that Al₂O₃ and Ca exist in the 1600 °C molten steel ladle. This system are made up of Al₂O₃ and Ca then reaction formula follows Eq. 3-12. There are 5 type of Ca-aluminate reaction by Ca + Al₂O₃ and the most stable phase can be calculated by Eq. 3-18 ~ Eq. 3-20.

1) Ca + 19/3 Al₂O₃ = CaAl₁₂O₁₉ + 2/3 Al

\( s_{\text{reactant1}} = 1, \ s_{\text{reactant2}} = 19/3, \ s_{\text{product2}} = 2/3 \)

\[ M_{\text{product1}} = \min[M_{\text{reactant1}}/s_{\text{reactant1}}, \ M_{\text{reactant2}}/s_{\text{reactant2}}] = 0.15789 \] (3-21)

2) Ca + 7/3 Al₂O₃ = CaAl₄O₇ + 2/3 Al

\( s_{\text{reactant1}} = 1, \ s_{\text{reactant2}} = 7/3, \ s_{\text{product2}} = 2/3 \)

\[ X_{\text{product1}} = \min[X_{\text{reactant1}}/s_{\text{reactant1}}, \ X_{\text{reactant2}}/s_{\text{reactant2}}] = 0.42857 \] (3-22)

3) Ca + 4/3 Al₂O₃ = CaAl₂O₄ + 2/3 Al

\( s_{\text{reactant1}} = 1, \ s_{\text{reactant2}} = 4/3, \ s_{\text{product2}} = 2/3 \)

\[ X_{\text{product1}} = \min[X_{\text{reactant1}}/s_{\text{reactant1}}, \ X_{\text{reactant2}}/s_{\text{reactant2}}] = 0.75 \] (3-23)

4) 3 Ca + 2 Al₂O₃ = Ca₃Al₂O₆ + 2 Al

\( s_{\text{reactant1}} = 3, \ s_{\text{reactant2}} = 2, \ s_{\text{product2}} = 2 \)

\[ X_{\text{product1}} = \min[X_{\text{reactant1}}/s_{\text{reactant1}}, \ X_{\text{reactant2}}/s_{\text{reactant2}}] = 0.33333 \] (3-24)

5) Ca + 1/3 Al₂O₃ = CaO + 2/3 Al

\( s_{\text{reactant1}} = 1, \ s_{\text{reactant2}} = 1/3, \ s_{\text{product2}} = 2/3 \)

\[ X_{\text{product1}} = \min[X_{\text{reactant1}}/s_{\text{reactant1}}, \ X_{\text{reactant2}}/s_{\text{reactant2}}] = 1.0 \] (3-25)
The values of $G^0$ for Ca-aluminates at 1600°C are in the Table 3-3. [33-35, 37-39].

If $\text{Al}_2\text{O}_3$ and Ca make Ca-aluminate 1 mole by Eq. 3-21 ~ Eq. 3-25 and Table 3-3, $\Delta G^0$ values of each reaction formula are as follows:

<table>
<thead>
<tr>
<th>Type of products</th>
<th>$\Delta G^0$ (J/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) CaAl$<em>{12}$O$</em>{19}$</td>
<td>-23560.37</td>
</tr>
<tr>
<td>2) CaAl$_4$O$_7$</td>
<td>-60498.05</td>
</tr>
<tr>
<td>3) CaAl$_2$O$_4$</td>
<td>-91242.10</td>
</tr>
<tr>
<td>4) Ca$_3$Al$_2$O$_6$</td>
<td>-90778.47</td>
</tr>
<tr>
<td>5) CaO</td>
<td>-66978.26</td>
</tr>
</tbody>
</table>

Table 3-3. $G^0$ Values at 1600°C for Ca-Aluminate model

$G^0$ (J/mol)  | Reference |
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$G^0_{\text{Ca}}$ = -150918.108</td>
<td>[33]</td>
</tr>
<tr>
<td>$G^0_{\text{Al}}$ = -116275.101</td>
<td>[33]</td>
</tr>
<tr>
<td>$G^0_{\text{Al}_2\text{O}_3}$ = -1974008.777</td>
<td>[33-35, 40]</td>
</tr>
<tr>
<td>$G^0_{\text{CaAl}_2\text{O}_19}$ = -12726470.68</td>
<td>[37, 39]</td>
</tr>
<tr>
<td>$G^0_{\text{CaAl}_4\text{O}_7}$ = -4820582.823</td>
<td>[38, 39]</td>
</tr>
<tr>
<td>$G^0_{\text{CaAl}_2\text{O}_4}$ = -2827069.001</td>
<td>[38, 39]</td>
</tr>
<tr>
<td>$G^0_{\text{Ca}_3\text{Al}_2\text{O}_6}$ = -4440555.699</td>
<td>[38, 39]</td>
</tr>
<tr>
<td>$G^0_{\text{CaO}}$ = -798382.2898</td>
<td>[38, 39]</td>
</tr>
</tbody>
</table>
According to the result of 3-26, when \( \text{Al}_2\text{O}_3 \) and \( \text{Ca} \) exist 1 mole each, \( \text{CaAl}_2\text{O}_4 \) is the most effective way of reaction. As in the Eq. 3-12 (3), when produce 1 mole of \( \text{CaAl}_2\text{O}_4 \), consume 1 mole of \( \text{Ca} \) and \( 7/3 \) mole of \( \text{Al}_2\text{O}_3 \) and also, produce \( 2/3 \) mole of \( \text{Al} \). If \( \text{CaAl}_2\text{O}_4 \) is made, delta \( g_0 \) value also changes because the quantity of reactant will become change.

If various type of Ca-aluminates are in one cell, Gibbs free energy changes also able to calculate using Eq. 3-12 to Eq. 3-16 and Table 3-3.

In the Table 3-4, the second line ‘+’ means the type of inclusion that react with \( \text{Ca} \) and the first line ‘Type of Product’ means \( \text{Ca} \)-aluminate type. According to the Table 3-4, \( \Delta G^0 \) can have lowest value when \( \text{Ca} \) reacts with \( \text{Al}_2\text{O}_3 \). In contrary, when \( \text{Ca} \) react with \( \text{Ca}_3\text{Al}_2\text{O}_6 \), \( \Delta G^0 \) has smallest value.

<table>
<thead>
<tr>
<th>Type of products</th>
<th>Reactants, Ca</th>
<th>(+\text{Al}_2\text{O}_3)</th>
<th>(+\text{C1A6})</th>
<th>(+\text{C1A2})</th>
<th>(+\text{C1A1})</th>
<th>(+\text{C3A1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1A6</td>
<td>-134168</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>C1A2</td>
<td>-124532</td>
<td>-75102</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>C1A1</td>
<td>-103453</td>
<td>-75207</td>
<td>-32292</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>C3A1</td>
<td>-210155</td>
<td>-167786</td>
<td>-103413</td>
<td>-54975</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CaO</td>
<td>-43770</td>
<td>-36709</td>
<td>-25980</td>
<td>-17907</td>
<td>-8745</td>
<td>-</td>
</tr>
</tbody>
</table>


<table>
<thead>
<tr>
<th>Reaction priority</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
</table>

* \( \text{C1A6} : \text{CaAl}_1\text{O}_{19} \), \( \text{C1A2} : \text{CaAl}_4\text{O}_7 \), \( \text{C1A1} : \text{CaAl}_2\text{O}_4 \), \( \text{C3A1} : \text{Ca}_3\text{Al}_2\text{O}_6 \)

Table 3-4. \( \Delta G^0 \) (per \( \text{Ca} \)-Aluminate product 1mole) at 1600°C.
3.2.4. Assumption: Determining reaction speed and convergence

To determine whether the reaction end or not, this study uses equilibrium constant \( K \) and \( \Delta G^0 \).

\[
DCR = \exp \left( \frac{-\Delta G^0}{RT} \right) - \frac{a_{Product}}{a_{Reactant1}a_{Reactant2}}
\]  

(3-27)

In Eq. 3-27, DCR is a short term of Direction of Chemical Reaction. This constant is subtraction of \( \Delta G^0 \) term from activity term. If sufficient amount of reactants exist, more violent reaction occurs when the difference between the two terms is large. As the chemical reaction proceeds, DCR converges into 0 and the reaction is over.

Measuring reaction speed is very difficult in the steel melt. So we assumed that the speed of reaction is proportional linearly to DCR. Fig. 3-2 compares the reaction of 600kg of [Al], 90kg of [O] and 600kg of [Si], 90kg of [O] in 300 ton steel ladle. (1ppm is 0.3 kg in a 300ton ladle). Fig. 3-2 shows the amount of reactant, product and its DCR value. The distribution of reactants in a ladle are uniformed. The initial stage of reaction, [Al]-[O] reaction is more violent and DCR value decreases much faster than [Si]-[O] reaction.

The amount of reactant and product is determined by the following equations.

**Forward reaction:**

\[
X_{Product\_final} = X_{Product\_initial} + X_{Product\_initial} \times DCR \times N_{product}
\]

\[
X_{Reactant1\_final} = X_{Reactant1\_initial} - X_{Reactant1\_initial} \times DCR \times N_{react1}
\]

\[
X_{Reactant2\_final} = X_{Reactant2\_initial} - X_{Reactant2\_initial} \times DCR \times N_{react2}
\]
\textit{Backward reaction}:

\begin{align}
X_{\text{Product}_{\text{final}}} &= X_{\text{Product}_{\text{initial}}} - X_{\text{Product}_{\text{initial}}} \cdot DCR \cdot N_{\text{product}} \\
X_{\text{Reactant1}_{\text{final}}} &= X_{\text{Reactant1}_{\text{initial}}} + X_{\text{Reactant1}_{\text{initial}}} \cdot DCR \cdot N_{\text{react1}} \\
X_{\text{Reactant2}_{\text{final}}} &= X_{\text{Reactant2}_{\text{initial}}} + X_{\text{Reactant2}_{\text{initial}}} \cdot DCR \cdot N_{\text{react2}}
\end{align}

(3-28)

Subscript ‘initial’ and ‘final’ represent reaction before and after each. \(X_{\text{Product}}\) and \(X_{\text{Reactant}}\) represent mole fraction of product and reactant. \(N_{\text{product}}, N_{\text{react1}}, N_{\text{react2}}\) is stoichiometric constant, in case of Al\(_2\)O\(_3\), \(N_{\text{product}} = 1, N_{\text{react1}} = 2, N_{\text{react2}} = 3.\)

3.2.5 Algorithm of the module

The reaction module is calculated by the algorithm shown in Fig. 3-4. Based on the flow calculation module, reaction module calculates the concentration of deoxidizer, dissolved oxygen and quantity of inclusion production. The database of this module gives a lot of information. According to the deoxidizer name, the program load thermodynamic constants, self-interaction coefficients, stoichiometric constants for reactants and product. Then, reaction module calculates the concentration of deoxidizer and dissolved oxygen in each node. If the high concentration region such as deoxidizer addition site, have high value of inclusion concentration as we can imagine.
Figure 3. Average inclusion quantity in 300ton ladle and its DCR. Average inclusion quantities and their DCR of [Si] 2000ppm - [O] 300ppm and [Al] 2000ppm - [O] 300ppm calculated from associate model. The process temperature is fixed at 1600°C. Production quantity for each time step (1s) is DCR* 1/1000. Assuming to uniform distribution.
Figure 3-4 Algorithm of Reaction module for this study

Information

Plume shape
Gas volume fraction

Velocity (u, v, w), Pressure,
Turbulent kinetic energy,
Turbulent energy dissipation rate

Define metal names,
Define quantity of alloy addition
Metals concentration & mole fraction
Oxygen concentration & mole fraction
Inclusion concentration & mole fraction

Thermodynamic constant
Stoichiometric constant
Interaction constant
Mole weight of matters

Associate generation / decomposition
Inclusion generation / decomposition

Associate generation / decomposition
Inclusion generation / decomposition

Residual mole fraction of metals
Residual mole fraction of oxygen
Residual mole fraction of inclusion
Residual mole fraction of associates
3. 3 Result and discussion

3. 3. 1. Flow information

Alloy transfer and inclusion movement is depend on the flow. To simulate local concentration of reactant and movement of product, flow information is required that includes turbulence, flow vectors etc. Fig. 3-5 shows the simulation result of the 300 ton ladle under the condition of 30m³/hour Argon blowing. At the top view, red color means plume eye and Fe-melt located at the center pushes slag away. The plume eye area is approximately 1.54 m² when 30m³/hour Argon is injected. The average speed of the melt is 0.06m/sec.
Figure 3-5. Flow vector information of simulation ladle. (Radius: 2.0m, Fe-melt height: 3.41m, Slag height: 0.085m, Ar gas flow rate: 30m³/hour)
3. 3. 2 Reaction result of uniform distribution reaction

If dissolved oxygen and deoxidizer distributed uniformly, the calculation result of this module and FACTsage are shown in table 5 and Fig. 3-6. In the table 5, M*O and M₂*O represent metal associates. When the oxygen concentration is 100ppm (30kg in 300ton ladle), 8 kind of reactants (Al, Ba, Ca, Cr, Mg, Si, Ti, Zr) [27, 33, 35, 41-43] and their reaction results are similar as predicted by FACTsage. In this table, Calcium and Magnesium are assumed as closed systems cause of their vaporize temperatures are under 1600℃ at the pure states.

Fig. 3-6 is comparing to Al-O reaction of FACTsage and this module. Dissolved oxygen fixed at 300ppm and dissolved aluminum varies from 0 to 1000ppm. The difference of FACTsage and this module marks under ± 2 ppm.

Table 3-6 is comparing Ca-aluminate production quantity to FACTsage. If the value of [O], [Ca] and [Al] are defined, the maximum difference is 6ppm but the production type of Ca-aluminates are the same as FACTsage.

Figure 3-7 is calculation result of the 300 ppm [Al] - 50ppm [Ca] - 100ppm [O] over time. 50ppm (15kg) Ca is injected after the end of generating Al₂O₃ reaction. Al-O reaction occurs in stage 1 and in this stage, associate generation and inclusion generation are calculated. In the stage 2, equilibrium is calculated by Ca-Al₂O₃ reaction, Ca-O reaction and Al-O reaction. Stage 3, every Al₂O₃ transformed to Ca-Aluminate and the major reaction is Ca-CaAl₂O₇. In the Ca-CaAl₂O₇ reaction stage, the module calculates equilibrium of [Ca]-[O]-[Al]-CaAl₂O₄-CaAl₂O₇.
Figure 3- 6 Al-O reaction in Fe-melt comparing with Factsage & this study (Uniform distribution, 1600℃)
<table>
<thead>
<tr>
<th>Program</th>
<th>Metal (ppm)</th>
<th>Oxygen (ppm)</th>
<th>M^0O (ppm)</th>
<th>Inclusion (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Value</td>
<td>2000</td>
<td>100</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Metal</th>
<th>Oxygen</th>
<th>M^0O</th>
<th>Inclusion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>FactSage</td>
<td>1884</td>
<td>0.8343</td>
</tr>
<tr>
<td></td>
<td>This study</td>
<td>1883.8</td>
<td>0.7899</td>
</tr>
<tr>
<td>Ba</td>
<td>FactSage</td>
<td>1141</td>
<td>1.98e-3</td>
</tr>
<tr>
<td></td>
<td>This study</td>
<td>1141.67</td>
<td>7.26e-5</td>
</tr>
<tr>
<td>Ca</td>
<td>FactSage</td>
<td>1749.9</td>
<td>4.11e-5</td>
</tr>
<tr>
<td></td>
<td>This study</td>
<td>1749.41</td>
<td>6.20e-6</td>
</tr>
<tr>
<td>Cr</td>
<td>FactSage</td>
<td>1992</td>
<td>97.48</td>
</tr>
<tr>
<td></td>
<td>This study</td>
<td>1991.9</td>
<td>97.50</td>
</tr>
<tr>
<td>Mg</td>
<td>FactSage</td>
<td>1848.2</td>
<td>6.58e-3</td>
</tr>
<tr>
<td></td>
<td>This study</td>
<td>1848.19</td>
<td>3.69e-3</td>
</tr>
<tr>
<td>Si</td>
<td>FactSage</td>
<td>1999</td>
<td>99.59</td>
</tr>
<tr>
<td></td>
<td>This study</td>
<td>1998.8</td>
<td>98.98</td>
</tr>
<tr>
<td>Ti</td>
<td>FactSage</td>
<td>1822</td>
<td>4.549</td>
</tr>
<tr>
<td></td>
<td>This study</td>
<td>1821.8</td>
<td>4.381</td>
</tr>
<tr>
<td>Zr</td>
<td>FactSage</td>
<td>1697</td>
<td>0.1418</td>
</tr>
<tr>
<td></td>
<td>This study</td>
<td>1697.13</td>
<td>0.1293</td>
</tr>
</tbody>
</table>

Table 3-5 Systematic reaction result in Factsage & this study. Metal and Oxygen are 2000ppm and 100ppm fixed respectively and uniform distributed. The ladle temperature is fixed at 1600°C.
Figure 3- 7. Al-Ca-O reaction comparing with Factsage & this study

(Uniform distribution, 1600 °C)
<table>
<thead>
<tr>
<th>[Al]</th>
<th>[Ca]</th>
<th>[O]</th>
<th>Product</th>
<th>This study</th>
<th>Factsage</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>1000</td>
<td>300</td>
<td>1033.92 (CaO)</td>
<td>1034.08</td>
<td>(CaO)</td>
</tr>
<tr>
<td>1000</td>
<td>500</td>
<td>300</td>
<td>556.78 (C3A1)*</td>
<td>559.75</td>
<td>333.98</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>336.86 (CaO)</td>
<td></td>
<td>(CaO)</td>
</tr>
<tr>
<td>500</td>
<td>200</td>
<td>300</td>
<td>696.24 (C1A1)</td>
<td>695.73</td>
<td>36.777</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>36.771 (C3A1)</td>
<td></td>
<td>(C1A1)</td>
</tr>
<tr>
<td>200</td>
<td>100</td>
<td>300</td>
<td>316.13 (C1A2)</td>
<td>312.99</td>
<td>199.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>193.20 (C1A1)</td>
<td></td>
<td>(C1A2)</td>
</tr>
<tr>
<td>300</td>
<td>100</td>
<td>100</td>
<td>102.22 (C1A1)</td>
<td>101.88</td>
<td>150.58</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>150.33 (C3A1)</td>
<td></td>
<td>(C1A1)</td>
</tr>
<tr>
<td>300</td>
<td>50</td>
<td>100</td>
<td>94.847 (C1A2)</td>
<td>93.631</td>
<td>135.18</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>132.64 (C1A1)</td>
<td></td>
<td>(C1A2)</td>
</tr>
<tr>
<td>100</td>
<td>100</td>
<td>100</td>
<td>85.342 (C1A1)</td>
<td>82.091</td>
<td>161.85</td>
</tr>
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<td></td>
<td></td>
<td></td>
<td>153.66 (C3A1)</td>
<td></td>
<td>(C1A1)</td>
</tr>
<tr>
<td>100</td>
<td>20</td>
<td>100</td>
<td>77.965 (C1A6)</td>
<td>72.180</td>
<td>100.77</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>99.961 (C1A2)</td>
<td></td>
<td>(C1A6)</td>
</tr>
</tbody>
</table>

* C1A6 : CaAl$_2$O$_{19}$, C1A2 : CaAl$_4$O$_7$, C1A1 : CaAl$_2$O$_4$, C3A1 : Ca$_3$Al$_2$O$_6$

**Table 3-6.** Ca-aluminate reaction result in Factsage & this study. Distribution of dissolved oxygen and elements are uniform. Initial dissolved oxygen are 300ppm, 100ppm. Every number is expressed as weight ppm. (1ppm = 0.3kg)
3. 3. 3 Simple deoxidation based on local reaction module

When alloy is injected through plume eye, local high alloy concentration appears near the injection site. Fig. 3-8 shows the concentration of alloy transfer over time based on the flow calculation result expressed at Fig. 3-5. At the moment of alloy injection, the concentration soars up to over 600 times of equilibrium concentration and this high concentration region doesn’t disappear even after 60 seconds. To predict inclusion distribution, we should predict mass transfer trend together because un-equilibrium reaction occurs at the local high concentration region. The behavior of mass transfer becomes different by gas flow rate, nozzle position, the number of nozzles and site of alloy injection. In this study, we fix the injection site as plume eye center. The predicted result of local equilibrium reaction is different from systematic reaction.

If the distribution of oxygen is uniform, inclusion generation depends on the mixing time of deoxidizer and the location of local high concentration. Also, inclusion moves along the fluid flow after generation. Additional generation quantity of inclusion would be different by the quantity of reactants in a calculation node. For example, according to the result of local reaction expressed at Fig. 3-9, the region of high [Al] concentration marks lower [O] than the result of uniform distribution. But inclusion production quantity marks higher than uniform distribution. By the low activity of oxygen, if additional aluminum is injected at the site, additional Al$_2$O$_3$ production is difficult.

In the Fig. 3-9, near the injection site has higher inclusion concentration than equilibrium. Inclusion generation is slow at the circulation point of the ladle. To reach equilibrium, over 600 seconds is needed. If no additional oxygen entrapment through plume eye and no inclusion removal, this prediction result have to same as the FACTsage result.
Figure 3- 8 Simulation result of high concentration region in a ladle according to the process time
Figure 3-9 Simulation result of Al-O reaction with local equilibrium reaction in Fe-melt.

([Al]: 1000 ppm, [O]: 300 ppm, fixed temperature at 1600°C)

(a) Dissolved oxygen and alumina distribution according to the process time.
Figure 3-9 (b) Concentration of each component according to process time
3.3.4 Ca Aluminate reaction

In the present study, Ca based inclusions such as CaAl$_{12}$O$_{19}$, CaAl$_2$O$_7$, CaAl$_5$O$_4$, Ca$_3$Al$_2$O$_6$, CaO can be appeared. Un-equilibrium reaction of Ca-Aluminate become severe by Ca injection speed. Fig. 3-10 shows CaO production quantity after the reaction of 1000ppm of [Al] and 300ppm of [O]. In this figure, Ca-aluminate reaction is suppressed. If Ca is added to the system from 0 to 1000ppm, initial Al$_2$O$_3$ decomposes by Ca. If 267 ppm Ca is added, 227 ppm of Al$_2$O$_3$ is decomposed and produces 357ppm of CaO. If 1000 ppm of Ca is injected, all Al$_2$O$_3$ is disappeared and only 1034 ppm of CaO is remained.

$$\text{Al}_2\text{O}_3 + 3\text{Ca} = 3\text{CaO} + 2\text{Al}$$

$$\Delta G^0 = 3G_{\text{CaO}}^0 + 2G_{\text{Al}}^0 - \left[G_{\text{Al}_2\text{O}_3}^0 - 3G_{\text{CaO}}^0\right] = -200933.2 \text{ J/mol}$$ (3-29)

When 1 mole of Al$_2$O$_3$ react with 3 moles of Ca and produce CaO, $\Delta G^0$ has – value like Eq. 3-29. From this, Ca oxygen affinity is stronger than aluminum oxygen affinity. In this model, the procedures of taking oxygen from Al$_2$O$_3$ by Ca are as follows:

i) If Ca is injected, [O] concentration marks lower than its concentration by Al can reach.


iii) Oxygen is supplied from Al$_2$O$_3$. Ca can react with oxygen from Al$_2$O$_3$ and become CaO.

iv) Reaching equilibrium by repeating procedure i)–iii).
Figure 3-10 $\text{Al}_2\text{O}_3 + \text{Ca}$ reaction calculation result based on average concentration.

(assume that no ca-aluminate is produced.)
Ca has the certain amount of solubility to molten steel. Fig. 3-11 shows Ca solubility in molten steel according to the static pressure. Ca solubility changes along to the depth. Solubility increment is 2.52ppm/cm. If molten steel static pressure has over 1.69atm at 2.48m from bottom, the Ca solubility is 426.2ppm.

Figure 3-11. Fe static pressure and Ca solubility in Fe-melt according to the ladle height.
The injection site of Ca makes Ca-aluminate that contains high contents of Ca. On the other hand, low Ca concentration region makes low Ca contents of Ca-aluminate. If putting some amount of Ca, the initial product of Ca-aluminate is made from Al$_2$O$_3$ and Ca reaction. The initial kind of Ca-aluminate is determined by Eq. 3-18 ~ Eq. 3-20. Fig. 3-12 is the distribution of inclusion by the reaction of 500 ppm [Al] – 300ppm [O] and 200 ppm [Ca]. The moment of Ca injection is the end of [Al] – [O] reaction. Inclusion removal is suppressed in this chapter. Fig. 3-12 (a) shows that the condition of injection Ca rate at 20ppm/sec and (b) shows injection rate at 2ppm/sec. The Ca injection location is plume eye center and 2 meters high from the ladle bottom. The average concentration of inclusion in the ladle is 695ppm of CaAl$_2$O$_4$ and 36.9 ppm of Ca$_3$Al$_2$O$_6$.

The initial state of reaction, Al$_2$O$_3$ concentration decreases near the region of site of Ca injection. Independent on the injection speed, high Ca contents of Ca-aluminate such as Ca$_3$Al$_2$O$_6$ and CaO are produced near the site of injection location. The concentration of [O] has lowest value at the Ca injection site. Also [O] concentration decreases along to the Ca diffusion.

60 seconds after Ca injection, Al$_2$O$_3$ decomposition can confirm from the distribution of Al$_2$O$_3$ and CaO. In case of 20ppm/sec, more CaO is produced than initial state. But 2ppm/sec case, concentration of CaAl$_{12}$O$_{19}$ and Ca$_3$Al$_2$O$_6$ are the highest value. The distribution of [O] is non-uniform because Ca-aluminate and CaO doesn’t reach equilibrium. This means inclusion production and decomposition occurs actively in the whole ladle. After 300 seconds, most of Al$_2$O$_3$ decompose except the circulation point and all of CaO is decomposed. Both two cases appear CaAl$_2$O$_4$ and Ca$_3$Al$_2$O$_6$ as equilibrium phase, but 2ppm/sec case is faster to reach equilibrium than 20ppm/sec case. This tendency appears at 600 seconds after Ca injection definitely. The [O] distribution is non-uniform at
20 ppm/sec case but 2 ppm/sec case occur reaction along to the distribution of CaAl$_4$O$_7$.

In the Fig. 3-12 (c) shows the average concentration of Ca-aluminate according to the process time. Total 15 minutes process, high Al contents of Ca-aluminate is decomposed both two cases. In the case of 20 ppm/sec, many CaO inclusions are produced at the initial stage of reaction. In 400 seconds, many CaAl$_{12}$O$_{19}$ and Ca$_3$Al$_2$O$_6$ inclusions are made and CaAl$_4$O$_7$ and CaAl$_6$O$_4$ are produced lately.
Figure 3-12 200ppm Ca - 500ppm Al - 300ppm O local equilibrium reaction in the ladle with various Ca-feeding speed. Ca feed location is at 2.0m from bottom and assuming that Al₂O₃ produced by 500ppm [Al] – 300ppm [O] has uniform distribution. Process time is 15min after Ca addition.

(a) 20ppm/sec

Ca addition after 2sec

![Chemical Analysis Images]

CaAl₂O₆
Ca addition after 60sec

Ca addition after 300sec
Ca addition after 600 sec

Al$_2$O$_3$
CaAl$_{12}$O$_{19}$ Eliminated
CaO

[O]

CaAl$_7$O$_7$
CaAl$_2$O$_4$
Ca$_3$Al$_2$O$_6$

83
(b) 2ppm/sec

Ca addition after 2 sec

\[ \text{Al}_2\text{O}_3 \quad \text{CaO} \quad \text{[O]} \]

\[ \text{CaAl}_2\text{O}_7 \quad \text{CaAl}_2\text{O}_7 \quad \text{CaAl}_2\text{O}_7 \quad \text{Ca}_4\text{Al}_2\text{O}_6 \]
(c) Average inclusion concentration as a weight ppm in the ladle according to the process time.
3.4 Conclusion of deoxidation reaction module

In this chapter, local equilibrium model is developed based on the flow calculation module. To calculate complex reaction, this program applied associate model. The result of this model and FACTsage are compared under 1600 ℃ molten steel case. This chapter can summarize as follows:

1) Associate model needs much less interaction coefficient than existing Wager formation. Each deoxidizer has only one self-interaction coefficient. By associate model, dissolved oxygen and associate’s self-interaction coefficient is fixed as 1.

2) Direction of Chemical Reaction (DCR) is the difference between ΔG₀ term and activity term. We are assuming that DCR determines reaction speed. If DCR reaches at 0, reaction is ended in a calculation node. If other deoxidizer inject, DCR changes and inclusion may decompose.

3) In this study, Ca-aluminate is produced by Al₂O₃ inclusion and dissolved Ca. The concentration of dissolved Ca, Al₂O₃ and Ca-aluminate determine Ca-aluminate type. Each calculation node calculates the most reducing Gibbs free energy to determine Ca-aluminate types.

4) Un-equilibrium reaction can calculate by this model. Initial state of alloy injection, over ten times of high concentration region appears near the injection site. Un-wanted reaction can occur at this time. In case of local equilibrium reaction of Ca-aluminate, CaO can appears at the initial reaction process which does not appear by average concentration.

5) High Ca contents of Ca-aluminate is produced near the injection site of Ca. At the initial state of reaction, Al₂O₃ concentration decreases near the region of site of Ca injection. Independent on the Ca injection speed, CaAl₄O₇ and CaAl₆O₁₄ are
produced after CaAl$_{12}$O$_{19}$ and Ca$_3$Al$_2$O$_6$ inclusions are produced.
Chapter 4. Inclusion agglomeration model

4.1 Background of studying inclusion agglomeration

There are many causes of production failure such as alloy precipitation, residual stress or grain size failure. In the secondary steelmaking area, failures are from alloy range failure, homogenization failure and large inclusion removal failure and so on. Especially, deoxidation inclusions have high hardness but brittle generally. If power loads into the product such as extrusion, these inclusions behave as stress concentration sources because they have different physical properties into the matrix.

In this chapter, we focus on the inclusion growth. This model can reveal where inclusion growth site is and where inclusions are. The inclusion agglomeration model is integrated to the chapter 2 and chapter 3. To define inclusion shape, we use fractal dimension constant[44]. Also, to define inclusion collision frequency, we uses some model of Forrest et al[45], Smoluchowski et al[46], Tozawa et al[47] and Nakaoka et al[48].

4.2 Numerical model for inclusion agglomeration

4.2.1 Collision frequency of inclusion

The inclusions in the steel melt are grown by collision and sintering. To simulate inclusion agglomeration, we modeled inclusion group as I and J. These groups exist in each calculation volume. So, calculation node is twice of flow calculation cells (I and J in one cell). When inclusion i in the I group and j in the J group collide, collision frequency by
their size can define as follows:

Inclusion collision frequency by turbulence [49]

\[
\beta_T(v_i, v_j) = 1.3 \left( r_i + r_j \right)^3 \left| \frac{\varepsilon}{\nu} \right|^{0.5}
\]  

(4-1)

Frequency by velocity difference

\[
\beta_V(v_i, v_j) = \frac{4}{3} \left( r_i + r_j \right)^3 \left| \frac{du}{dy} \right|
\]  

(4-2)

Frequency by terminal velocity difference[50]

\[
\beta_s(v_i, v_j) = \pi (r_i - r_j)^2 |V_i - V_j|
\]  

(4-3)

Total inclusion collision frequency

\[
\beta(v_i, v_j) = \beta_T + \beta_V + \beta_s
\]  

(4-4)

In the Eq. 4-1, \(v_i, v_j\) represent inclusion volume, \(r_i, r_j\) represent inclusion radius, \(\varepsilon\) means turbulent dissipation rate, \(\nu\) is kinematic viscosity. \(\frac{du}{dy}\) in Eq. 4-2 means velocity difference of unit distance. \(V_i - V_j\) in Eq. 4-3 is the difference between terminal velocities of two inclusions.

So, total collide inclusions from \(i\) number of inclusion and \(j\) number of inclusions can calculate by Eq. 4-4. The equation is the total value of these equations.

In the Fig. 4-1 shows the concept of inclusion agglomeration model. Two other groups in a cell can collide each other by its size.
Figure 4-1 Schematic diagram of basic and large particles crash and grow along the fractal dimension
4.2.2 Fractal dimension constant and apparent density

Fractal dimension constant is the constant that defines 3D-shape object to 2D-shape. [51] The new size of collided inclusion radius can calculate by its inclusion fractal dimension constant Df. The new size is as follows:

\[ R_{\text{new}} = \left( r_1^{D_f} + r_2^{D_f} \right)^{\frac{1}{D_f}} \]

(4-5)

If the inclusion is liquid at the process temperature, Df is 3.0 (spherical shape) because liquid tends to be sphere to reduce its interfacial area. 8 inclusions of 1um are required to grow 2um if Df is 3.0. On the other hand, if Df is 2.0 (cluster shape), 4 inclusions of 1um are required to grow 2um. Thus, required inclusions are different.

Terminal velocity is determined by inclusion size and its shape. In the Fig. 4-2, the sampling area of inclusion is expressed. In the black circle, Al\textsubscript{2}O\textsubscript{3} cluster fraction determines apparent density. If Df is high, inclusion fraction in the circle will increase then, apparent density will decrease. So, if inclusions tend to be sphere-like shape, they are easy to rise because of Fe fraction (black region in Fig. 4-2).

**Figure 4-2** Alumina cluster and its sampling region.
The apparent density can be calculated as follows:

\[
\rho_{\text{cluster}} = \rho_m \left\{ 1 - \left( \frac{r_0}{r} \right)^{3-D_f} \right\} + \rho_i \left( \frac{r_0}{r} \right)^{3-D_f}
\]

(4-6)

\(\rho_m\) is the molten steel density and \(\rho_i\) is the inclusion density that is in the physical property. \(r_0\) is the inclusion initial radius. In case of alumina, the initial radius is known as 1um.[44, 52] \(r\) is the present inclusion radius. Apparent density is the factor that determines the rising velocity of moving inclusion. According to Eq. 4-6, spherical inclusion (Df 3.0) has the same value of physical property’s density and apparent density. But cluster apparent density is different to its physical property’s density.

Terminal velocity varies by its apparent density. Terminal velocity is determined as follows:

\[
V_t = \frac{2gr^2}{9\mu} (\rho_m - \rho_{\text{cluster}})
\]

(4-7)

This equation is known as Stokes equation. This equation can be used in the creeping flow regime and we assume that inclusions don’t affect to the flow because inclusions are too small to create another flow. (1>>Re) In Eq. 4-7, \(\mu\) is the dynamic viscosity of molten steel, \(g\) is gravitational acceleration. The relationship between Df and terminal velocity is shown in Fig. 4-3.
Figure 4-3 The relationship between radius of inclusion and fractal dimension

Figure 4-4 Various shape of inclusion according to the fractal dimension.
Cluster shape inclusion has similar density with molten steel. Terminal velocity is determined by inclusion apparent density and molten steel density. Cluster shape inclusions are easy to grow but their rising speed are low. So inclusion removal is difficult.

4.2.3 Inclusion agglomeration simplifications

To calculate inclusion growth numerically, the model has to simulate various size of inclusions movement. However, the limitations of computer performance, tracing every inclusions are impossible. Moreover, calculation time is the cross product of inclusion size distribution and the number of grids. Size distribution increases as time goes by in progress, the more calculation time is required. If 1um basic particle grows to 30um of Df 3.0, 27,000ea 1um inclusions are required by Eq. 4-5. It means over 27,000ea grids are needed to express 30 um to simulate. Also, according to the concept of this inclusion agglomeration, possible numbers of collision are $27000^2$. Grids for flow calculation are $42 \times 50 \times 100$ as in the chapter 1, the required number of grids are over trillions to simulate 30um aggregate. (210,000 ea numerical grids x $27000^2$ ea possible way of collision)

To overcome these difficulties, inclusions are divided into small inclusions and large inclusions. The standard of dividing groups are 100 basic particles. If the inclusion constituted under 100 basic particles (small particle), numbering 100 inclusions each. But the inclusion constituted over 100 basic particles, inclusion is expressed as its average diameter. The large inclusion is atomized as 0.1 um. With this method, expressing 30um inclusion is required only 400ea enough. (30/0.1 + 100ea small inclusions) The virtue of this expression method is faster, have no errors and easy to express.

In the program, the way of expression is shown in below.
In case of Al$_2$O$_3$ (Df 2.0), the size of 100 basic particles is $100^{1/2.0}$ that is, 10um. Thus, small inclusion can be categorized until 9um. Over 10um, the program recognizes inclusion as large inclusion. In case of SiO$_2$ (Df 3.0), the standard size of categorize is 4.64 um ($100^{1/3.0}$) and large inclusion diameter is started from 4.7um. In the Fig. 4-5, I, J, K are the index of location in the ladle. Last one or two numbers in the coordinates represent size information. Before 100 basic particle collision number, the program categorize as small inclusion and the number of coordinate is same as collision number. Over 100, program converts its collision number as size of inclusion diameter and the coordinate (L,M) is same as diameter, not collision number. For example, 10.0 um in the Fig. 4-5, is expressed as (10, 1). (The starting number is 1 at FORTRAN.) Like this, 10.9um can be expressed as (10, 10) and 11um is (11, 1).

In this way, one problem can find. For example, there are two inclusions in a calculation cell. The two are (I, J, K, 1) and (I, J, K, 4) as small clusters. If the two are colliding, new inclusion collision number is 5 and its index is (I, J, K, 5). Also, there are...
two sets of large inclusions (I, J, K, 10, 1) and (I, J, K, 11, 1) can make (I, J, K, 14, 10) by the Eq. 4-5 if their Df is 2.0. However, in case of collision between small cluster and large cluster, it can’t calculate right away because the unit is not matched because the array INCLUSION(I, J, K, X), the unit of (X) is ‘ea’. In the CLUSTER(I, J, K, L, M), the unit of (L, M) is ‘um’. So, this program adopts ‘Mean size of inclusion’ concept. The mean size of inclusion in a calculation grid can be defined as follows:

\[
\frac{A \text{ (um)} \times a \text{ (ea)} + B \text{ (um)} \times b \text{ (ea)}}{a \text{ (ea)} + b \text{ (ea)}}
\]

(4-8)

In Eq. 4-8, units are expressed in the parenthesis. For example, 8ea of 9.0 um inclusions and 10ea of 9.1 um inclusions exist, the mean size of inclusion is 9.056um. The ‘Mean size of inclusion concept’ can be used in the following example. In case of SiO\(_2\) (Df 3.0), a 5.0 um agglomerated inclusion collide with INCLUSION(I, J, K, 3), the index of new inclusion is still (5, 1) because the \((5^3+3)^{1/3.0}\) is still 5.039 um. But the inclusion is certainly grown. If this 5.039um inclusion collide with INCLUSION(I, J, K, 78), the real size is 5.906um but if CLUSTER(5, 1) collide with particle that consist of 78, calculated size is 5.877um. To reduce these errors, Mean size of inclusion is required. According to this method, mean size coordinates saved the real size of (5, 1) as 5.039um. So 5.039um is expressed as CLUSTER(I, J, K, 5, 1) and MEAN_SIZE(I, J, K, 5, 1) remember the real size of CLUSTER(I, J, K, 5, 1).

The collision frequency is proportional to the number of inclusions. In the initial state, small inclusions lead inclusion growing. In the final state, large inclusions lead inclusion growing. In the present study only 10 sorts of inclusions that have highest
collision potential are considered to reduce calculation time. Because of long calculation time is required when considering whole size distribution. The collision potential is set as the cross product of collision frequency and the number of inclusions. According to the inclusion size, this model can be divided into three steps of growth mode.

1) small-small inclusion collision
2) large-small inclusion collision
3) large-large inclusion collision

In each time step after collision, inclusion movement is calculated. The governing equation is as follows:

$$\frac{\partial \rho \phi}{\partial t} + \nabla \rho (u + V_t) \phi = S$$

(4-9)

In the Eq. 4-9, $\frac{\partial \rho \phi}{\partial t}$ is the quantity of accumulation in the unit time, $\nabla \rho (u + V_t) \phi$ is the quantity of transferring by convection in the controlled volume, $u$ means velocity, $V_t$ means terminal velocity of inclusions. $S$ is the source term in the controlled volume. Eq. 4-9 has no diffusion related term because inclusions don’t solute in the molten steel.
Figure 4-6 The number of inclusions as the size distribution in the molten steel according to the process time.
4. 2. 4. The algorithm of inclusion agglomeration module

This inclusion agglomeration program starts from particle location & concentration from deoxidation reaction module. From the sort of deoxidizer, database module determines its Df and apparent density. Collision frequency is also calculated before the beginning of particle collision module. In the subroutine ‘agglomeration’in Fig. 4-7, set collision order by collision potential and set the collision mode. Repeating above through whole calculation grids then, inclusion location is calculated by the Eq. 4-9 according to the terminal velocity. If inclusion location is at the interface between slag and molten steel, inclusion can remove if the conditions are met.

Figure 4-7 Algorithm of inclusion agglomeration module.
4.3 Result and discussion

4.3.1 Comparing with Si-O reaction and Al-O reaction

The condition of inclusion generation reaction is same as flow information in the chapter 2. The alloy transfer and inclusion movement depend on the flow. The alloy injection site is set as plume eye center. Slag is covered on the molten steel and its height is 10cm. The composition of slag is CaO 50% - SiO₂ 50% and its physical properties are same as Table 4-2. 30m³/hour Ar gas is injected through nozzle and its location is set at the center on the ladle bottom. Initial [O] is set as 300ppm. In this chapter, we put the Si 5000ppm or Al 1000ppm as deoxidizer. To calculate reaction, associate model and its self-interaction coefficient is used. The reaction results from FACTsage are shown in the Table 4-1. Also various conditions for calculating inclusion agglomeration are shown schematically in the Table 4-2.

<table>
<thead>
<tr>
<th>Deoxidizer</th>
<th>Initial</th>
<th>Equilibrium</th>
</tr>
</thead>
<tbody>
<tr>
<td>5000 [Si]</td>
<td>1000 [Al]</td>
<td>4791 [Si]</td>
</tr>
<tr>
<td>Oxygen</td>
<td>300 (dissolved)</td>
<td>62.96 (dissolved)</td>
</tr>
<tr>
<td>Inclusion</td>
<td>0 (SiO₂)</td>
<td>0 (Al₂O₃)</td>
</tr>
</tbody>
</table>

Table 4-1. Information of additional alloys and its chemical reaction result from FACTsage.
Fig. 4-8 shows average inclusion weight concentration after 10 minutes of alloy addition. Assuming basic particle diameter is 1.0 um, 3um inclusion (consist of 27 basic particles to 63 particles agglomerate) weight average concentration has 212.2 ppm. 1um inclusion (consist of 1 basic particle to 7 particles agglomerate) marks 45.3 ppm. Until 140 seconds, 1um inclusions are dominantly generated in the ladle, and after, its concentration is reducing. This means inclusion agglomeration speed is faster than inclusion generation speed after inflection point in Fig. 4-8. Total weight ppm of inclusion concentration is 443ppm. This value is almost same result of FACTsage result in the Table 4-1. This result shows there are no errors after complex calculation.

Fig. 4-9 is the same condition after Al addition. As shown in Table 4-1, 1000 ppm of [Al] and 300ppm of [O] makes 627ppm of Al₂O₃ and the total agglomerated inclusion marks same value of reaction result. The agglomeration result is significantly different from Fig. 4-8. The largest inclusion was 5um when using Si as deoxidizer but in case of using Al, the largest inclusion is over 25um. The reason why is that the difference of Df values. For example, 4um SiO₂ has minimum 27 basic particles to maximum 63 particles. But same diameter of Al₂O₃ has minimum 16 particles to maximum 25 particles. In case of SiO₂ includes wide range of collision number. Also, Al₂O₃ has wide surfacial area and easy to collide than sphere.

Fig. 4-10 is the basic particle concentration in the ladle in case of Si injection and Al injection. In each figure, (a) is the weight concentration of SiO₂ and (b) is the Al₂O₃ concentration. Both figures show that inclusion agglomeration locations are the circulation point of the melt. The circulation point in the ladle is the latest mass transfer site. However, inclusions accumulate and agglomerate here because of the residence time. Plume has the highest collision frequency because of its turbulence and du/dy value. But from these
figures, main inclusion agglomeration site is not the plume which has high turbulence but the high numbers of inclusions exist.

1. Physical properties & Process condition

<table>
<thead>
<tr>
<th>Elements</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molten Iron (Fe)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature</td>
<td>1600</td>
<td>°C</td>
</tr>
<tr>
<td>Density</td>
<td>7000</td>
<td>Kg/m³</td>
</tr>
<tr>
<td>Injection Gas (Ar)</td>
<td>Density</td>
<td>0.26 Kg/m³</td>
</tr>
<tr>
<td>Injection rate</td>
<td>30.0</td>
<td>m³/hour</td>
</tr>
<tr>
<td>Slag (CaO 50%, SiO₂ 50%)</td>
<td>Density</td>
<td>2600 Kg/m³</td>
</tr>
<tr>
<td>Thickness</td>
<td>10</td>
<td>cm</td>
</tr>
</tbody>
</table>

2. Ladle shape condition

<table>
<thead>
<tr>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ladle Radius</td>
<td>2.0  m</td>
</tr>
<tr>
<td>(Grids)</td>
<td>J = 50</td>
</tr>
<tr>
<td>Fluid Height</td>
<td>3.51 m</td>
</tr>
<tr>
<td>(Grids)</td>
<td>K = 100</td>
</tr>
<tr>
<td>Nozzle Location</td>
<td>Center</td>
</tr>
</tbody>
</table>

3. Alloy addition condition & Chemical properties

<table>
<thead>
<tr>
<th>Elements</th>
<th>Concentration</th>
<th>Unit</th>
<th>note</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>5000</td>
<td>ppm</td>
<td>add to plume eye</td>
</tr>
<tr>
<td>Al</td>
<td>1000</td>
<td>ppm</td>
<td>add to plume eye</td>
</tr>
<tr>
<td>Oxygen</td>
<td>300</td>
<td>ppm</td>
<td>Initial oxygen</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ΔG</th>
<th>ΔG = 0</th>
<th>ΔG = -333,300</th>
<th>J/mole</th>
<th>3.0(Sphere)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si + O₂</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Al + O₂</td>
<td>ΔG = -108,614</td>
<td>ΔG = -551,457</td>
<td>J/mole</td>
<td>2.0(Cluster)</td>
</tr>
</tbody>
</table>

Table 4-2. Various conditions for calculating inclusion agglomeration.
Figure 4-8. SiO$_2$ inclusion oxygen contents and their distributions over time.

At about 140 sec
Basic particle generation almost complete.
(Alloy mass transfer is almost complete)

Figure 4-9 Al$_2$O$_3$ inclusion oxygen contents and their distributions over time.

At about 95 sec
Basic particle generation almost complete.
(Alloy mass transfer is almost complete)
Figure 4-10. Total inclusion concentration & major growth location

(a) Total inclusion concentration in the ladle

(b) Basic particle concentration in the ladle.
4.3.2 Calculation result including inclusion removal

If inclusions are removed only by slag, the boundary condition can set as follows:

i) The cell beneath the slag (internal interface), inclusion can remove when cell velocity has positive. The cell velocity is the sum of melt velocity and inclusion terminal velocity.

ii) The cell beside of the slag (eye interface), molten steel which is located at the top attach to the melt / slag interface.

In the present study, we assume that if inclusion attaches to the slag, inclusion is melted to the slag right away. As mentioned above, slag and melt have two interfaces that remove inclusions. The one is eye interface. Molten steel at the surface pushes slag away. Inclusions in the molten steel have to attach slag by its flow. And the other is internal interface. Molten steel flows along the interface but the inclusions in the melt tend to rise by its density difference. Large inclusions can have large terminal velocity then it can be removed into the slag. Especially, if no flows in the ladle such as waiting or moving time to tundish, internal interface removal is very important. The following calculation results are the results of many modules. The program contains from plume eye prediction module to inclusion removal module.

Fig. 4-11 compares the result of removal module and non-removal module of the Al-O reaction. In the initial state, dissolved oxygen drops radically by the transfer of [Al] and total Al$_2$O$_3$ concentration rise. Total O is the sum of oxygen contents in the inclusions and dissolved oxygen. It starts from 300 ppm and this value is the same of initial dissolved oxygen concentration. As time goes by, dissolved oxygen reaches equilibrium. Total
Al₂O₃ and Total O decreases gradually. Comparing with no inclusion removal result, total 74% of inclusions are removed during 10 minutes after Al injection. Total O has similar tendency to the Total Al₂O₃ because the residual [O] concentration in the ladle is quite low.

**Figure 4-11.** Average weight ppm of inclusion, Total O and dissolved oxygen in the ladle according to the process time.
Fig. 4-12 shows inclusion concentration changes by size according to the process time. The black bars are non-removal result and red bars are the concentration assuming that inclusion removal. (a) is the result of 1 minute after alloy addition. As expected, small inclusions such as 1um or 2um appears dominantly. However, (b) (10 minutes after alloy addition) appears various kind of inclusion size. Moreover, inclusion distributions differs between removal and non-removal result. Because of the total number of inclusions. If inclusion removes well, suppressing inclusion growth can achieve.

Inclusion distribution in the ladle can confirm in Fig. 4-13. (a) is the concentration of Total O. At the circulation point in the ladle, inclusion concentration shows higher value than other site like Fig. 4-10. 1um inclusion concentration including basic particle is shown in Fig. 4-13 (b). 1um inclusion concentration decreases over time by means of growing inclusions as basic particle. However, the speed of decreasing is faster at the non-removal side because there are more inclusions in the ladle. Fig. 4-13 (c) shows 3um inclusion growing location. If assuming inclusion removal, the growing speed is low as we expected. 3um inclusions also disappear by removal or growing over time.
Figure 4-12. The results of inclusion removal module off (black bars) and on (red bars).

The size distribution of Al$_2$O$_3$ and its weight ppm of concentration.

(a) 1 minute after alloy addition, (b) 10 minute after alloy addition
Figure 4-13. The cases of removal and non-removal models of inclusion distribution in the ladle at 240sec after alloy addition according to the inclusion size.

(a) Total O distribution

(b) 1μm inclusion distribution

(c) 3μm inclusion distribution
4.4 Conclusion of inclusion agglomeration module

In this chapter, we can calculate what is the major size of inclusion according to the process time and shows main growth site in the ladle. We assume that inclusion growth is determined by its own collision frequency according to the fractal dimension constant (Df) as the characteristic value of inclusion. Fractal dimension constant is depends on the inclusion melting point. If the inclusion is liquid at the process temperature, its fractal dimension constant is 3.0 because liquid tends to be sphere to reduce its interfacial area. Generally, Al₂O₃ grows as cluster and its fractal dimension constant is known as 2.0. Terminal velocity is determined by inclusion size and its shape. If Df is high, inclusion fraction will increase in the sampling region then, apparent density will decrease. So, sphere-like inclusions are easy to rise. To reduce calculation time, simplified model is used. At first, two other groups in a cell collides each other by its size. The collision frequency is determined by the value of cell turbulence, velocity difference and terminal velocity differences. And then we divide calculation section into small inclusions and large inclusions. The standard of these groups are 100 basic particles. Small inclusion group is numbered as particle collision number and large inclusion group is categorized by its diameter and atomized as 0.1 um. According to the inclusion size, this model can be divided into three steps of growth mode. (Small-small, large-small and large-large inclusion collision)

In the two cases of calculation show that inclusion agglomeration locations are the circulation point of the melt. The circulation point in the ladle is the latest mass transfer site. However, inclusion is gathering at this point, accumulate and agglomerations occur. Plume has the highest collision frequency because of its turbulence and du/dy value. But the most affected factor is the number of inclusions according to the
simulation results. Generally, sphere shape inclusion grows slower and cluster shape inclusion grows faster. Sphere shape inclusion requires more basic particles than cluster shape inclusion to grow.
Chapter 5. Slag entrapment modeling

5.1 Background study of slag entrapment modeling

During steelmaking process, a huge number of nonmetallic inclusions are generated in the ladle and have harmful effect on the quality of steel especially when agglomerated large-size inclusions remain in steel products. The inclusion removal from molten steel becomes critical to improve the cleanness of molten steel. The efficiency of the inclusion removal and mixing in the ladle has become the main objectives in steelmaking process for the high quality steel. [53] The possibility of slag entrapment will become high if bubbling control cannot be properly applied, and thus the molten steel will become dirtier. [54]

Slag doesn’t soluble to the molten steel and the density is about 1/3 of the molten steel. So, slag makes layer on the molten steel. Therefore Navier-Stokes equation can be simplified for the water-oil relationship

\[
\frac{\partial (\rho_1 \alpha_1)}{\partial t} + \nabla (\rho_1 U \alpha_1) = 0
\]
\[
\frac{\partial (\rho_2 \alpha_2)}{\partial t} + \nabla (\rho_2 U \alpha_2) = 0
\]

(5-1)

The equation above is the governing equation of Volume of Fluid (VOF) that widely uses to multiphase flow. In Eq. 5-1, \( \alpha_i \) is the oil or slag volume in the cell and \( \alpha_i \) is the water or molten steel volume.
The following assumptions have been made in the establishment of the mathematical model for flow in the ladle with argon blowing.[55]

(1) The flow in the ladle is incompressible and turbulent.

(2) The top surface is flat, and no tangential stresses are present.

(3) The shape of droplet is spherical because of its melting temperature and its size will not change during rising in the ladle.

(4) The domain is occupied by a single-phase fluid.

This method can only use to no solubility with each other. In this study, to reveal the slag’s physical behavior, the reaction between slag and molten steel is ignored.

The slag droplet rises automatically because of its density difference with molten steel. The rising velocity (terminal velocity in chapter 4) and this value depends on the size of the droplet. If the slag droplet is sphere in the molten steel, the velocity can express according to the flow regime : [56]

\[ V_t = \sqrt{\frac{4gd}{3Cd}} \left( \frac{\rho - \rho_s}{\rho_s} \right) \]

(5-2)

G is gravitational accelerate, d is diameter of slag droplet, Cd is drag coefficient and \( \rho \) and \( \rho_s \) are the density of molten steel and slag. In this case, we assume that the droplet is sphere, \( C_d \) is fixed at 0.47. Terminal velocity according to the droplet size is as follows.
Figure 5-1. Terminal velocity according to the droplet diameter under normal flow regime. ($P_{ke} > 10$)
X axis represents droplet size and its unit is um. Y axis represents terminal velocity and its unit is cm/sec. Terminal velocity has approximately 7 cm/sec at 100um. In case of this droplet, it needs about 50 seconds to reach top from ladle bottom.

The Reynolds number can be defined for several different situations where a fluid is in relative motion to a surface. These definitions generally include the fluid properties of density and viscosity, plus a velocity and a characteristic length or characteristic dimension. For a sphere in a fluid, the characteristic length-scale is the diameter of the sphere and the characteristic velocity is that of the sphere relative to the fluid some distance away from the sphere, such that the motion of the sphere does not disturb that reference parcel of fluid. The density and viscosity are those belonging to the fluid. Note that purely laminar flow only exists up to Re = 10 under this definition. Under the condition of low Re, the relationship between force and speed of motion is given by Stokes’ law. [57]

\[ V_t = \frac{g d^2}{18 \mu} (\rho_s - \rho) \]

(5-3)

Comparing to the Fig. 5-1 and Fig. 5-3, the particle Reynolds number (P\(_r\)) belongs to the creeping flow regime, terminal velocity is approximately 10 times smaller than normal flow regime.
Figure 5-2. Qualitative behaviors of fluid flow over a cylinder depend to a large extent on Reynolds number. [58]

Figure 5-3. Terminal velocity according to the droplet diameter under normal flow regime. (Pr<1)
The Particle Reynolds number is defined as

\[ P_{Re} = \frac{\rho d V}{\mu} \]

(5-4)

V represents flow velocity (m/sec) and d is droplet diameter (m). In this study, we assume that creeping flow regime occurs under 0.1 of droplet Reynolds number and it means a droplet doesn’t affect to the fluid flow. According to the above equations, the required velocity of creeping flow regime for 10 um droplets have to 10 times lower than the 1um droplets. Therefore, large droplet follows to the Eq. 5-2, large slag droplet removes much faster than small droplets.

5.2 Various theories of slag entrapment conditions

Slag entrapment can occur by various interfacial conditions. Slag entrapment phenomena can be divided into physical entrapment and chemical entrapment. Bubble breakups, turbulent of surface, the differences of shear force at the steel/slag interface or vertical downward flow belong to the physical entrapment. Slag re-oxidation or release harmful element to the molten steel belongs to the chemical entrapment. In this study, we focus on the physical entrapment and analysis the behavior at the LF process.

When bubble pass through the interface of slag and molten steel, the bubble which is located at the interface become unstable because of the fluids density and
surface tension differences. Using this, critical bubble size ratio of slag and steel can be calculated. [59]

\[
\text{Bubble size ratio} = \frac{R_s}{R_m} = \frac{\sigma_s}{\sigma_m} \frac{\sqrt{\rho_s}}{\sqrt{\rho_m}} = 0.3
\]

(5.5)

In Eq. 5.5, \(R_s\) is the bubble radius in the slag and \(R_m\) is the radius in the molten steel. \(\sigma_s\) and \(\sigma_m\) are the surface tensions of slag and molten steel.

From above equation, the bubble in the slag can have much smaller size than in the molten steel. By this reason, if bubble in the molten steel goes to the slag layer, bubble would breaks up and the slag can be entrapped.

When plume eye is opened by bubble, the very first bubble can breakup. But generally, most of the bubbles are confined in the plume eye area and vaporize at the surface of the plume eye, so the effect of bubbles breakup are negligible.

The other theory of slag entrapment is Kelvin-Helmholtz instability at the interface.[60] The viscosities differ between two fluids, the slag and molten steel show different behavior. If the velocities differ, surface or interface rocks oneself. At this point, if the ones horizontal velocity is much faster than other, the other fluid doesn’t overcome shear forces and separates from its matrix. In this case, if molten steel moves faster than slag, slag can entrap to the molten steel. These rocking phenomena by viscosity differences and velocity differences are called as Kelvin-Helmholtz instability. The velocity of instability is as follows:
\[ v_c = \sqrt{\frac{\rho_m + \rho_s}{\rho_m \rho_s} \left[ (\rho_m - \rho_s) \frac{g}{k} + \sigma_m k \right]} \]

(5-6)

The \( k \) in the Eq. 5-6 is the wave number which is the reciprocal number of wave length. \( k \) is proportional to the frequency and inverse proportional to velocity.

\[ k = \frac{1}{\lambda} = \frac{f}{v} \]

(5-7)

In the Fig. 5-4 shows the critical molten steel velocity to shear slag layer. The x-axis is the interface wave number and y-axis is the shear velocity (horizontal velocity) to entrapment. According to the Fig. 5-4, the minimum horizontal velocity of molten steel is 0.38m/sec. The simulation result marks maximum 0.05m/sec of horizontal velocity at 70Nm^3/hour and this means entrapping slag requires very high velocity of molten steel. So, interface instability also be able to ignored.
Figure 5-4. The shear velocity for slag entrapment by Kelvin-Helmholtz instability.
Finally, the effect of turbulent at the slag and melt interface is noticeable. Slag droplet entrap to the molten steel side by turbulent, maximum entrapment depth $y$ can be calculated through the kinetic energy balance and surface tension balance.

$$\rho_s vy'' = (\rho_m - \rho_s) g vy - \sigma A$$

(5-8)

The equation above can be summarized to the quadratic equation for $y$.

$$\left(\frac{\rho_m}{\rho_s} - 1\right) g y^2 - y'' y - \frac{\sigma}{\rho_s} = 0, \quad y_{max} = \frac{9}{2} r$$

(5-9)

If the shape of interface is cylinder at just before entering the slag into the molten steel, required cylinder length is $9/2r$ to have spherical type droplet. Substituting calculated length to Eq. 5-9, the condition of spherical slag droplet can get.

$$\frac{81}{4} \left(\frac{\rho_m}{\rho_s} - 1\right) g r^2 - \frac{27}{2} kr - \frac{\sigma}{\rho_s} = 0$$

(5-10)

In Eq. 5-10, k represents turbulent kinetic energy ($m^2/sec^2$) and $r$ is the radius of slag droplet. Obtainable slag droplet size from Eq. 5-10 is described in the Fig. 5-5.
**Figure 5-5.** The simulation result of turbulent kinetic energy and its maximum slag droplet under 300 ton ladle. 30Nm$^3$/hour is applied.

Fig. 5-5 shows the information of turbulent energy, plume eye size and the maximum size of entering slag droplet size. The blowing condition is 30Nm$^3$/hour at the 300 ton ladle.
5.3 Result of slag entrapment simulation and its condition

In the previous session, slag entrapment is depends on the turbulent kinetic energy. Turbulent kinetic energy is proportional to the velocity square and describes as:

\[ k \propto \frac{1}{2}(u^2 + v^2 + w^2) \]

(5-11)

Slag makes new interface when molten steel gives some energy. To get the new interfacial area by the energy from molten steel, we use surface tension. Surface tension is the elastic tendency of liquids which makes them acquire the least surface area possible. [61] It also called as interfacial tension. Surface tension is the required energy to make 1m².

Surface tension is the unique value of matter. In this study, the surface tension of CaO 50%-SiO₂ 50% is already revealed. [62] The unit of surface tension is Joule/m² and its SI unit is kg/sec². From the definition of surface tension, surface tension can be write as:

\[ \sigma = \frac{dW}{dA} \]

(5-12)
That is, applied energy $dW$ and the new area $dA$ has 1 dimensional relation and these values are connected to the surface tension. And also, surface tension has the relationship between turbulent as follows:

\[
\text{surface tension} = \text{kg} \times \text{kinetic energy} / \text{area}
\]

Unit: $\text{kg} / \text{sec}^2 = \text{kg} \times \frac{m^2}{\text{sec}^2} / m$

\begin{equation}
(5-13)
\end{equation}

The new area at the slag interface can be calculated according to applied energy from Eq. 5-13.

\[
\text{new}_\text{area} (m^2) = \frac{k \times \text{mass}}{\sigma}
\]

\begin{equation}
(5-14)
\end{equation}

The new area ($m^2$) represents the area at the slag / molten steel interface made by turbulent. Entrapped slag mass can calculate from total new area and slag droplet size. If user defines slag size, slag mass is:

\[
\text{entrainment} (\text{kg}) = \frac{\text{new}_\text{area}}{4\pi r^2} \times \frac{4}{3} \pi r^3 \times \rho_s
\]

\begin{equation}
(5-15)
\end{equation}

In the Eq. 5-15, $r$ means the radius of slag droplet that is defined by user.
The minimum droplet radius under the given pressure and surface tension can calculate from Young-Laplace equation. [63]

\[ \Delta P = \frac{2 \sigma}{r} \]  

\( (5-16) \)

By the Eq. 5-16, minimum slag droplet radius is determined by the molten steel pressure because the surface tension is constant. Pressure is inverse proportional to the radius, strong pressure makes small radius and weak pressure makes large radius. This is the same principle of making soap bubble. For example, when we make soap bubble through straw, weak blowing on the breath makes large bubble. If blow hard on the breath to the straw, many small bubble is made. This is the same as the bubble making. Therefore slag inclusion radius range is determined by the power of turbulent kinetic energy and pressure. But the definite radius is unknown. In this case, the radius is selected randomly and the random function frequency is fixed at 100 times per 1 sec of process time. The condition of simulation is same as chapter 4, 10cm slag and 300ton ladle. The blowing conditions are 5Nm³/hour, 30Nm³/hour and 70Nm³/hour respectively.

Slag entrapment quantity according to process time is shown in Fig. 5-6.
Figure 5-6. Slag entrapment quantity according various gas flow rates over process time.
(diagram)
Figure 5-7. Slag entrapment quantity according various gas flow rates over process time.
(ladle cross section view)

a) blowing after 10 seconds

b) blowing after 100 seconds
c) blowing after 240 seconds

In the Fig. 5-6 and Fig. 5-7, there are some fluctuations over time. This means active slag entrapping and removal is occurring during process time. Generally, slag droplet (approx. over 20um) is larger than de-oxidation inclusion (approx. 1um~30um) and it is the result of reflecting slag terminal velocity.
5.4 Conclusion of slag entrapment

In this chapter, we try to quantify slag entrapment and their behavior. The slag layer doesn’t diffuse to the molten steel and Volume of Fluid (VOF) method that widely uses to multiphase flow is used. The shape of slag droplet is sphere because of its melting temperature and we assume that its size will not change in the ladle. Terminal velocity has two options according to the slag droplet size and its flow regime. The standard of this regime is defined as particle Reynolds number. Turbulent kinetic energy and pressure at the steel / slag interface determine range of the slag droplet size. Random number is used to define the size of droplet in this study. During the process time, some fluctuation of slag concentration is observed at the simulation. Active slag entrapping and removal is occurring. The range of slag droplet is generally over 5um to 40mm, so its terminal velocity is much faster than the result of chapter 3. (De-oxidation inclusion removal)
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고급강의 수요가 늘어 강에 요구되는 물성도 상향 평준화 됨에 따라 2차정련 공정의 중요성도 커지고 있다. 2차 정련은 레들 유동을 위한 Argon-bubbling 공정부터 탈산제 투입, 개재물 형성 및 제거에 이르는 매우 복잡한 공정으로써 이를 예측하는 시뮬레이션 프로그램을 제작하기 위해서는 유동, 물질전달, 반응 및 개재물 성장, 제거 등을 고려해야 한다. 특히 탈산제 혹은 합금 원소 투입 시 투입 위치에서의 물질 농도는 평형농도의 수십 배 혹은 수백 배까지 차단되어 물질 전달이 완료되기 전까지는 레들 내의 각 부분에는 농도 불균형이 영역이 존재한다. 그에 따라 레들 각 부분에서 생성되는 개재물의 양도 달라진다.

Argon-bubbling을 실시하면 편연적으로 아르곤의 부력에 의해 상단의 슬래그는 옆으로 밀려나고 내부의 용강이 드러나게 되는데 이 현상을 나탕 (plume eye)이라고 한다. 본 연구에서는 유속과 아르키메데스의 부력원리를 이용하여 나탕의 크기를 예측할 수 있는 수식을 제안하였다. 여러 번의 시뮬레이션과 수모델 실험을 통해 나탕의 크기는 주입되는 가스의 양에 비례하고 슬래그의 두께에 반비례하며 이들 변수는 나탕의 크기의 1/2승에 정비례한다. 본 연구에서 제안된 식을 이용하여 다른 크기의 레들이나 다른 조건의 슬래그에 대해서도 적용이 가능하다.

레들 내부 탈산 거동을 알아보기 위해 국부적 평형 반응 모델을 제작하였다. 열역학적 평형을 계산하기 위하여 상호작용계수를 줄일 수 있는
associate model을 사용하였으며 이를 통해 Ca-aluminate와 같은 복잡한 반응도 모사할 수 있다. 탄산 개재물의 생성은 10분 공정 모사결과 레들 내부의 환류 지점에서 가장 느리게 발생하는 것으로 나타났다. Ca-aluminate의 경우 Ca이 투입된 지점 근처에서 Ca 함유량이 높은 Ca-aluminate가 형성되었으며 이 지점 근처의 암투미나는 가장 먼저 제거된다. Ca-aluminate 반응은 투입지점의 Ca 농도에 따라 평형에 도달하는 시간이 달라지며 본 모사에서는 느린 속도로 Ca wire를 공급할수록 평형에 더 빨리 도달하였다.

국부적 평형 반응모델을 통해 초기 개재물의 생성 위치를 계산하고 개재물의 충돌 성장을 모사할 수 있다. 개재물의 크기별 거동 모사를 위해 본 연구에서는 충돌 반도를 정의하고 개재물의 접보기 밑도에 따른 종속을 계산하였다. 수 억개 이상의 개재물 충돌을 모사하기 위하여 알고리즘적인 기법이 사용되며 이를 통해 개재물의 성장에 가장 큰 영향을 미치는 개재물의 크기와 주요 성장 위치를 추정할 수 있다. 개재물의 주요 성장 위치는 개재물이 모이는 레들 내부의 환류 지점이다. 이 환류 지점은 개재물의 잔류 시간이 가장 긴 위치이다. 따라서 충돌반도는 플럼 영역이 가장 크지만 개재물의 성장은 개재물의 잔류 시간에 더 큰 영향을 받는 것을 알 수 있다. 본 연구에서 Al 1000ppm - O 300ppm으로 30m³/hour로 10분 공정 시 개재물은 약 15um 수준까지 성장하였다.

슬래그 혼입은 구형 슬래그 혼입을 전제로 하였다. 슬래그의 혼입 표면적을 슬래그의 표면장력과 난류 에너지의 관계에 의해 구했으며 이를 통해 슬래그의 혼입량을 결정하였다. 구형 슬래그의 크기를 결정하기 위해 난류에
너지와 계면에서의 압력구배를 이용하였다. 본 연구에서 5, 30, 70m³/hour의 유량으로 Argon을 투입한 결과 10분 공정 시 슬래그 혼입량은 각각 0.2ppm, 10ppm, 35ppm으로 나타났으며 이 때 용강 내로 혼입이 가능한 슬래그 입자 의 크기는 5μm~40mm이다.

본 레들 퍼니스 예측 프로그램(LD3D)은 물질의 전달, 탈산반응, 탈산 개재물의 충돌 거동 및 크기 별 거동 예측, 슬래그의 혼입까지 레들 퍼니스 공정 전반에서 일어나는 다양한 현상들을 모사할 수 있어 추후 공정 설계에 도움이 될 것으로 기대한다.

주요 단어 : 수치해석, 레들 퍼니스 공정, 나탕, 탈산 반응, 개재물 성장, 슬래그 혼입

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