1. Introduction

Control of the solidification structures of a casting and ingot is important because the solidification structure has influences on the mechanical properties of final products. To predict the optimum conditions to obtain a desired solidification structure, it is important to clarify the effects of the process parameters on the solidification structure. However, many experimental works would be required to obtain optimum conditions. Hence, it is desirable to develop a mathematical model to simulate solidification structure formation in a casting and ingot. In the past two decades, several models for prediction of solidification structure formation have been developed. Stochastic models such as the Monte Carlo (MC) method and cellular automaton (CA) method and deterministic models such as the phase-field (PF) method have been presented, and many attempts have been carried out to simulate solidification structure formation of alloys using these methods.

However, there have been few attempts to simulate solidification structure formation in steel, which is the most widely used material in the world. For this reason, two factors might be considered. First, steels are mostly produced by the continuous casting process and solidification must proceed under flow in melt due to electromagnetic stirring (EMS) in the usual continuous casting process. This condition makes modeling of solidification structure formation in steel difficult. Second, during the solidification of steel, complex phase transformations such as peritectic reaction and subsequent peritectic transformation occur. These phenomena also make modeling of solidification structure formation in steel difficult.

The aim of this work was to develop a numerical model to simulate solidification structure formation during the continuous casting process of an Fe–0.7mass% C alloy. In this model, the cellular automaton method was combined with heat transfer calculation during the continuous casting process. The effect of electromagnetic stirring (EMS) during the continuous casting process was introduced as an increase in thermal conductivity in liquid. Furthermore, the effect of fragmentation of dendrites due to fluid flow during EMS was taken into account in the model as an increase in the formation of crystals. Simulations of grain structure formation in continuously cast billets with and without EMS were carried out, and the degree of fragmentation was evaluated from a comparison between experimentally observed and simulated macrostructures of the billets.

2. Numerical Model

In the present model, the cellular automaton method (CA) was combined with heat transfer calculation during the continuous casting process. The procedure for simulation by the CA method is basically the same as that by the CA technique developed by Rappaz and Gandin except for the nucleation model. The CA procedure in the present model was carried out under the temperature field obtained by heat transfer calculation.

2.1. Nucleation Model

The Gaussian distribution reported by Thevoz et al. has been widely used as a nucleation model in the CA method. In this nucleation model, if the mold wall and bulk liquid are considered as nucleation sites, six parameters must be
determined. This makes the model complicated and interpretation of the physical meaning of each parameter is difficult.

In the present work, a simple nucleation model was used, and the heterogeneous nucleation rate in undercooled melt, \(R_{Nu}\), is expressed as follows:

\[
R_{Nu}(\Delta T) = \frac{1}{\Delta t \cdot V_{CA}} \left( \frac{\Delta T}{a} \right)^n 
\] ..........................(1)

where \(\Delta t\) is the time step, \(V_{CA}\) is the area of a CA cell, \(\Delta T\) is undercooling, \(a\) is maximum undercooling for nucleation and exponent, \(n\), is the nucleation parameter. It has been demonstrated that the use of a combination of a fixed value of \(a\) and a variable \(n\) is effective for simulation of solidification structure formation.\(^{10}\) In this nucleation model, the fitting parameter is only the exponent, \(n\), for a constant value of \(a\).

Equation (1) expresses the rate of heterogeneous nucleation in the liquid CA regime, the imposed temperature gradient, \(\Gamma\), is related to the undercooling \(\Delta T\) at the dendrite tip and the growth velocity can be calculated from the Eqs. (2) and (3) by substituting an arbitrary value of the Pelet number for Eqs. (2) and (3).

To reduce the simulation time, the set of values for undercooling vs. growth velocity of the dendrite tip were calculated from Eqs. (2) and (3) in advance and then formulated as the form of Eq. (4) by using the least-square method.

\[
V(\Delta T) = 2.0 \times 10^{-4} \cdot \Delta T^4 + 4.6 \times 10^{-3} \cdot \Delta T^3 + 3.54 \times 10^{-3} \cdot \Delta T^2 + 7.56 \times 10^{-2} \cdot \Delta T 
\] ..............................(4)

where \(V(\Delta T)\) is the growth velocity of the dendrite tip (mm/s) and \(\Delta T\) is undercooling. The material properties used in the calculation are listed in Table 1.

### Table 1. Materials properties of the Fe–C binary alloy used in the simulation.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(T_s)</td>
<td>1801 K</td>
</tr>
<tr>
<td>(m)</td>
<td>-65</td>
</tr>
<tr>
<td>(k_0)</td>
<td>0.353</td>
</tr>
<tr>
<td>(\Gamma)</td>
<td>(1.9 \times 10^3) (Km)</td>
</tr>
<tr>
<td>(D)</td>
<td>(2.0 \times 10^4) (m/s)</td>
</tr>
</tbody>
</table>

2.3. Heat Transfer Calculation during Continuous Casting

Equation (5) shows the governing equation for 2-dimensional heat transfer calculation.

\[
\frac{\partial T}{\partial t} = \frac{\kappa}{\rho C_p} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) 
\] ..............................(5)

where \(\kappa\) is thermal conductivity, \(\rho\) is density and \(C_p\) is specific heat. The evolution of latent heat during the solidification was incorporated to the calculation by using the effective specific heat method as shown in the following equation.

\[
C_p^e = C_p - L \left( \frac{df_s}{dT} \right) 
\] ..............................(6)

where \(C_p^e\) is the effective specific heat, \(L\) is latent heat and \(f_s\) is the solid fraction.

Figure 1 shows the boundary conditions of the heat transfer calculation of the continuous casting process of an Fe–C binary alloy billet.
transfer calculation during the continuous casting process. A billet was moving down from the mold, and the sample was first cooled in the mold by heat transfer from the sample to the mold. The sample was then cooled at the secondary cooling zone by spray, and this zone was divided into four zones with different heat transfer conditions to enhance the accuracy of the heat transfer calculation. Finally, the sample was cooled in air, and the heat extraction from the sample in this regime was calculated by radiation. In the heat transfer calculation, the heat flow condition at the surface of the billet was changed with lapse of time by synchronizing with the movement of the billet. The thermo-physical properties and the heat transfer coefficients in the mold and the secondary cooling zones used in the calculation are shown in Table 2.

### 2.4. Effect of EMS

Electromagnetic stirring (EMS) is generally used to reduce the centerline segregation in the continuous casting process. To evaluate the effect of the fluid flow due to EMS on heat flow in the billet, the accurate flow pattern in the molten steel melt must be known. However, at present, it is difficult to combine accurate calculation of fluid flow with heat transfer calculation and the CA procedure due to very large computational load.

A method has been reported for incorporating the effect of fluid flow into heat transfer calculation by changing thermal conductivity. In this method, apparent thermal conductivity in molten steel with EMS becomes larger than that without EMS. In the present study, this method was used to calculate the heat transfer in the billet with EMS. In the calculation, regions in which fluid flow can occur were determined according to the classification of solid–liquid coexisting zone proposed by Takahashi et al.

Figure 2 shows a schematic illustration of solid–liquid coexisting zone of a solidifying alloy. The solid–liquid coexisting zone was classified into three zones of \( q_2 \), \( q_1 \) and \( p \) based on the fluidity of interdendritic liquid. In the \( q_2 \) zone, primary crystals and liquid can flow concurrently, whereas only interdendritic liquid can flow among dendrites in the \( q_1 \) zone and the liquid is entrapped by solids and can not flow in the \( p \) zone.

In the present work, based on this concept of solid–liquid coexisting zone, the thermal conductivity in solid was used in the region of solid and the \( p \) zone, and the effective thermal conductivity in liquid with fluid flow was used in the region of liquid and the \( q_1 \) zone. In the \( q_1 \) zone, the thermal conductivity changes linearly from liquid to the \( p \) zone according to the fraction of liquid that can flow among dendrites as shown in Fig. 2.

Mizikar used a 7.5-times higher thermal conductivity in liquid with fluid flow due to EMS. Although the exact value of the thermal conductivity in liquid with EMS is not clear because the value changes depending on flow velocity in the liquid, a 10-times higher thermal conductivity was assumed as the effective thermal conductivity in liquid with EMS in comparison with the thermal conductivity in liquid without EMS.

### 3. Calculation Procedure

#### 3.1. Experiment and Simulation Model

To examine the effectiveness of the present model, simulation was carried out under the same conditions as those used in a continuous casting experiment. Figure 3 shows a schematic illustration of the continuous caster used in the experiment.

In Table 3, a vertical type test continuous caster with a machine height of 8 m was used to produce a billet with a size of 120 mm×120 mm, and EMS was applied in a mold. Figure 4 shows solidification structures in the cross sec-

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**Table 2.** Thermophysical properties and heat transfer coefficients used in the simulation. \( h_{\text{mold}} \) is the heat transfer coefficient at the mold wall, and \( h_{S1} (0–0.1 \text{ m}) \), \( h_{S2} (0.1–0.9 \text{ m}) \), \( h_{S3} (0.9–2.2 \text{ m}) \) and \( h_{S4} (2.1–4.4 \text{ m}) \) are the heat transfer coefficients at the secondary cooling zone. Figures in parentheses are distances from the bottom of the mold. \( z \) is the distance from the top of the mold, and \( v \) is casting speed.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
</tr>
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<tbody>
<tr>
<td>( \kappa )</td>
<td>28.55W/mK</td>
</tr>
<tr>
<td>( \rho )</td>
<td>7000kg/m³</td>
</tr>
<tr>
<td>( C_p )</td>
<td>0.645J/kgK</td>
</tr>
<tr>
<td>( L )</td>
<td>0.268J/kg</td>
</tr>
<tr>
<td>( h_{\text{mold}} )</td>
<td>( 1256 \times \exp(1.31 \times z / (v \times \text{60})) ) W/m²K</td>
</tr>
<tr>
<td>( h_{S}(0-0.1 \text{m}) )</td>
<td>1248W/m²K</td>
</tr>
<tr>
<td>( h_{S}(0.1-0.9 \text{m}) )</td>
<td>758W/m²K</td>
</tr>
<tr>
<td>( h_{S}(0.9-2.2 \text{m}) )</td>
<td>582W/m²K</td>
</tr>
<tr>
<td>( h_{S}(2.1-4.4 \text{m}) )</td>
<td>427W/m²K</td>
</tr>
</tbody>
</table>

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**Fig. 2.** Schematic illustration of solid–liquid coexisting zones during the solidification of an alloy.

**Fig. 3.** Schematic illustration of the continuous caster used in the experiment.
tions along with casting direction of continuously cast billets with and without EMS. In the case without the EMS (Fig. 4(a)), columnar grains were formed from the mold surface to the center of the ingot. On the other hand, in the case with EMS (Fig. 4(b)), the region of equiaxed grains was extended due to the effect of EMS.

3.2. Calculation Conditions

To solve Eq. (5) by using the finite difference method, the cross section perpendicular to the casting direction of the billet was divided into rectangular grids with 1.2 mm on x- and y-coordinates. Since the shape of the sample is axisymmetric, a quarter of the cross section was divided as shown in Fig. 5, and calculated thermal field in the quarter was transferred to the other three quarters.

An explicit finite difference method was used, and the time step was determined to be 0.0025 s by considering the stability of the numerical computation. A network of square CA cells was laid on the cross section of the billet, and the heat transfer grids were superimposed on the CA cells as shown in Fig. 5. One heat transfer grid contains 16 CA cells, and the size of a CA cell was 0.3 mm.

It should be noted that the simulated area of the billet was a cross section perpendicular to the casting direction, whereas the observed macrostructure of the billet in Fig. 4 was a section parallel to the casting direction. However, it is no difficulty for comparison of the simulated and observed microstructures of the billet.

4. Results and Discussion

4.1. Simulation without EMS

Figure 6 shows the simulated macrostructure of the continuously cast billet without EMS. Fine equiaxed grains, i.e., chill crystals, were formed near the mold surface, and columnar grains grew up to the center of the billet. The structure shown in Fig. 6 was composed mostly of columnar grains, whereas a region of equiaxed grains was observed in the center of the billet obtained by the experiment as shown in Fig. 4(a).

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this means that constitutional undercooling in front of columnar grains hardly occurs. As a result, the formation of equiaxed crystals in front of columnar grains is difficult and columnar grains can grow up to the center of the billet.

The disagreement between simulated and experimentally observed solidification structures might be ascribed to the presence of fluid flow in the solidifying billet due to pouring of molten steel and convection in the experiment. The presence of concentrated heterogeneous nucleation catalysts in the center region of the billet at the final solidification stage might be the reason of the formation of an equiaxed crystal region observed in the experiment.

4.2. Simulation with EMS

Figure 8 shows the simulated macrostructure of the continuously cast billet with EMS. The same nucleation parameters as those used in the simulation without EMS were used in the simulation. In the simulation with EMS, higher thermal conductivity in liquid due to fluid flow was used to introduce the effect of EMS, and a region of equiaxed grains was formed in the center of the billet as shown in Fig. 8. Increased thermal conductivity in liquid ahead of the columnar crystals reduced the temperature gradient in liquid, which enhanced the constitutional undercooling in liquid and resulted in the formation of equiaxed crystals in front of columnar crystals. However, the simulated region of equiaxed crystals at the center of the billet was smaller than that in the experimentally observed solidification structure shown in Fig. 4(b). These results suggested that the effect of EMS is not only change in thermal conductivity in liquid but also promotion of fragmentation of dendrites due to fluid flow.

To take into account the accurate effect of the fragmentation of dendrites, it is necessary to understand the mechanism of fragmentation due to fluid flow. However, at present, it is difficult to make such model.

In the present work, the contribution of fragmentation of dendrites to the multiplication of equiaxed crystals was incorporated into the nucleation model. Total crystal formation rate, \( R_c \), was defined as the sum of the contribution of heterogeneous nucleation in liquid and the contribution due to the fragmentation of dendrites, \( R_{v_f} \).

\[
R_c = R_{v_0} + R_{v_f}
\]

(7)

The value of \( R_{v_f} \) was assumed to be independent of the undercooling in melt because the fragmented crystals were moved by the fluid flow, and the number of fragmented crystals could not be related to the undercooling at the position to which the crystals were carried. Figure 9 shows the relationship between the undercooling, \( \Delta T \), in melt and the total crystal formation rate, \( R_c \), used in the simulation with consideration of the fragmentation of dendrites.

Figure 10 shows the simulated macrostructure of a continuously cast billet taking into account the effect of the fragmentation of dendrites due to EMS. A large region of equiaxed grains that was the same as that observed in the experiment was simulated. This result demonstrates the potential of the present model to simulate solidification structure formation during the continuous casting process of steel.

5. Conclusions

A numerical model to simulate solidification structure formation during the continuous casting process of an Fe–C binary alloy was developed by combining heat transfer calculation and the cellular automaton (CA) method. To avoid the difficulty in modeling peritectic transformation, an Fe–0.7mass%C binary alloy without peritectic reaction was chosen as the target alloy. The effect of the fluid flow due to electromagnetic stirring (EMS) was introduced into the model by considering enhanced thermal conductivity in liquid and crystal multiplication due to the fragmentation of...
Simulations of solidification structure formation during continuous casting with and without EMS were carried out, and the results of simulation were compared with experimental results. In the simulation without EMS, columnar grains grew from the chill zone to the center of the billet, whereas a small region of equiaxed crystals was observed in the experiment. In the simulation with EMS, a solidification structure similar to that observed in the experiment could be simulated by considering both the effects of enhanced thermal conductivity in liquid and the contribution of fragmentation of dendrites due to fluid flow.

REFERENCES