Research and Application on Numerical Simulation of Heavy Rail Steel in Continuous Casting Process

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Abstract. According to the solidification process features of rail steel and continuous caster parameters, the solidification heat transfer mathematical model and grain growth models were established. The two models were coupled mathematical model called CA-FE model. Some parameters, such as superheat of molten steel, casting speed, specific water flowrate were researched. Tests show that Reducing super heat and specific water flowrate, improving the casting speed, were beneficial to the growth of the equiaxed grains, opposite to columnar grains. The superheat was 22℃ to 25℃, casting speed was 0.70 m/min to 0.75m/min and specific water flowrate was 0.22L/kg to 0.23L/kg that was benefit to the overall quality of rail steel.

Introduction

The organization of solidification numerical simulation has become one of the most active field of materials research in recent decades with increasingly urgent demand for performance prediction of material. Dendrite growth determines morphology at the end of solidification, the redistribution of the solute elements and solidification structure of two phase area in the continuous casting billet, thus it affects the quality of the final product. Oldfield proposed numerical simulation model for microstructure of graphite cast iron in 1966. The cooling curve was firstly applied for checking the model. Macroscopic and microscopic coupling model has tremendously developed from then on. Pang and Stefanescu[1,2] applied Cellular Automaton to microcosmically simulate the anisotropy and dendrite arm branching mechanism, then got dendrite morphology and grain group. On the basis of Dilthey’s research, Nastac proposed probability model to simulate the dendrite branching, equixed grain growth and columnar-to-equiaxed transition(CET). Li Qiang and Li Dianzhong simulate the dendrite growth of Fe-C alloy[5-8]. Wang Tongmin and Jin Junze proposed the CAMC model by using the computer to simulate the solidification structure in metal[9-10]. Chen Jin simulated the crystal structure in casting process by using the CA. The composition, degree of supercooling and interfacial energy were considered in the model. Huang Jianfeng simulated the solute diffusion and interfacial energy of grain growth by using the CA.

In recent years, the rail way steel is required to have safety, comfort and long life with the development of high speed railway. High purity, high surface and internal quality, high section size precision and straightness were required in rail steel. The composition and structure homogenization should be confirmed in the casting bloom. Based on macro solidification heat transfer of continuous casting bloom and grain nucleation theory, dendrite growth CAFD mathematical model of heavy rail steel in casting process was established. The growth process of solidification structure was predicted in different continuous casting process conditions. The influence factors of columnar grains size, equiaxed grains size and CET position in casting process were simulated quantitatively. The correct casting parameters were confirmed by using the model.

Mathematic Model

The main parameters of continuous caster were showed in tab11.the simulation steel grade was U75V steel.
Table 1. Parameters of the casting machine.

<table>
<thead>
<tr>
<th>Items</th>
<th>parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bloom transverse</td>
<td>280mm×380mm</td>
</tr>
<tr>
<td>Strand</td>
<td>6-straightener and 6-strand</td>
</tr>
<tr>
<td>Radius of caster</td>
<td>15000 mm</td>
</tr>
<tr>
<td>Height of crystallizer</td>
<td>850mm</td>
</tr>
<tr>
<td>Casting speed</td>
<td>Main 0.6~0.8 m/min</td>
</tr>
<tr>
<td>metallurgical length</td>
<td>40m</td>
</tr>
</tbody>
</table>

Heat Transfer Model in Solidification

On ideal condition, the mathematic model was established by using slice mobile method. The height direction of microelements was set as $dz$ from crystallizer meniscus to bloom center. The thickness and width direction of microelements were set as $dy$ and $dx$ respectively. Microelements move downward with bloom speed as shown in figure 1. Heat equilibrium of microelements was shown as following,

Heat accumulation of microelements = receiving heat of microelements - reduce heat spending of microelements

$$\rho C \frac{dT}{dt} \, dxdydz = \rho_C T dxdy - k_{eff} \left( \frac{\partial T}{\partial y} \right) dxdydz - k_{eff} \left( \frac{\partial T}{\partial y} \right) dydz - \rho_C \left( T + \frac{\partial T}{\partial z} \right) dxdy +$$

$$\left[ k_{eff} \left( \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial y} \left( k_{eff} \frac{\partial T}{\partial y} \right) \right] dxdy + \left[ k_{eff} \left( \frac{\partial T}{\partial z} \right) + \frac{\partial}{\partial z} \left( k_{eff} \frac{\partial T}{\partial z} \right) \right] dydz + S_o$$

(1)

After the reduction was equation(2).
\[
\rho c \frac{\partial T}{\partial t} = -\rho v_c \frac{\partial T}{\partial z} + \frac{\partial}{\partial y} \left( k_{\text{eff}} \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial x} \left( k_{\text{eff}} \frac{\partial T}{\partial x} \right) + S_o
\]  

(2)

If the coordinate system was put on the bloom, the microelements move downward with the bloom. The speed of height direction is zero. The heat transfer differential equation of two-dimensional slices in solidification process was shown as equation (3).

\[
\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial y} \left( k_{\text{eff}} \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial x} \left( k_{\text{eff}} \frac{\partial T}{\partial x} \right) + S_o
\]

in equation (3), \( T \) was temperature, °C. \( \rho \) was density, kg·m\(^{-3}\). \( c \) was heat capacity, J·kg\(^{-1}\)·°C\(^{-1}\). \( k_{\text{eff}} \) was coefficient of thermal conductivity, W·m\(^{-1}\)·°C\(^{-1}\). \( S_o \) was inner heat, W·m\(^{-3}\).

**Grain Growth Mathematical Model**

Continuous nucleation model was applied in CA-FE mathematic model. When the nucleation was heterogeneous, the nucleation was located in different position. The nucleation position was described by continuous discrete distribution function, that was Gauss function.

\[
\frac{dn}{d(\Delta T)} = \frac{n_{\text{max}}}{\sqrt{2\pi}\Delta T_o} \exp \left[ -\frac{(\Delta T - \Delta T_{\text{max}})^2}{2\Delta T_o^2} \right]
\]

(4)

In the equation, \( \Delta T_{\text{max}} \) was undercooling of nucleation, K. \( \Delta T_o \) was standard variance of undercooling, K. \( n_{\text{max}} \) was density of nucleation from 0 to infinite in normal distribution function. Gauss distribution function was described in heterogeneous cube and heterogeneous face nucleation as shown in fig. 3.

The parameters of Gauss distribution function interact with each other. It was influenced by some external factors, such as the shape of bloom, the casting temperature and the cooling condition. Nucleation parameters were chosen mainly referring to Fe—C alloy microstructure. Meanwhile, the microstructure tested by experiences was applied in the Gauss distribution function. The last parameters of Gauss distribution function was shown in Table 2.

**Table 2. Parameters of Gauss distribution function.**

<table>
<thead>
<tr>
<th>( \Delta T_s,\text{max}/K )</th>
<th>( \Delta T_s,\sigma/K )</th>
<th>( n_s,\text{max}/K )</th>
<th>( \Delta T_v,\text{max}/K )</th>
<th>( \Delta T_v,\sigma/K )</th>
<th>( n_v,\text{max}/K )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>0.1</td>
<td>1.2×10(^8)</td>
<td>8</td>
<td>1.5</td>
<td>2×10(^9)</td>
</tr>
</tbody>
</table>

**Initial Condition**

The initial condition was shown in Table3. On the condition, the simulation includes only one variable, such as superheat of molten steel, casting speed and water ratio in secondary cooling.
Through the simulation, the temperature field of bloom, the secondary dendrite arm spacing and
dendrite growth were calculated by every effective variable. Because of bloom symmetry, the
simulation was calculated 1/4 cross section.

<table>
<thead>
<tr>
<th>Superheat/°C</th>
<th>Casting speed/ (m·min⁻¹)</th>
<th>water ratio in secondary cooling / (L·kg⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.68</td>
<td>0.25</td>
</tr>
</tbody>
</table>

**Table 3. Initial condition.**

**Simulation Results and Discussion**

**Superheat**

On the initial condition as table 3 shown, the superheat was changed. The relationship between
superheat and solidification structure was presented by simulation. The characteristic value of
solidification structure was calculated by software ipp6.0. When the superheats were 15°C, 25°C and
35°C, the averages area of columnar grain in bloom were 2.01mm², 2.59 mm² and 3.14mm² respectively.
The averages radius of columnar grain in bloom were 0.58mm, 0.69 mm and 0.77mm respectively. The averages equiaxed grain area were 1.41mm², 1.35mm² and 1.33mm² respectively. The averages equiaxed grain radius were 0.85 mm, 0.83 mm and 0.82 mm respectively. The heat loosed a lot while the superheat was high in solidification process. The temperature of position in bloom is high with high superheat. On the position, the time to loss heat was more than that with low superheat. The secondary dendrite arm spacing increased. The equixed grain area was reduced with columnar grain area increased on the high superheat condition. Therefore, low superheat is benefit to equixed grain growth.

**Figure 4. Solidification structure of bloom with different superheat ((a).15°C, (b).25°C, (c).35°C)**

CET positions of bloom on three superheat conditions were shown as fig 5. when the superheat were 15°C, 25°C and 35°C respectively, the CET positions were located 27.8mm, 45.2 mm and 63.3mm under the surface of bloom respectively. The simulation results show that high superheat is benefit to columnar grain growth opposite to equixed grain growth. The columnar grain sizes increased with high superheat. The depths of supercooling reduced and the time of losing heat increased with superheat increasing. A lot of grains were remelted into the molten steel. Nucleation of equixed grains was dramatically restricted. The time to eliminate overheat increased while the time of columnar grains growth increased. The columnar grain sizes increased. The CET positions delayed.
The position of CET

Figure 5. Relationship between CET position and super heat.

Casting Speed

On the initial condition as shown in table 3, the casting speed was changed. The relationship between casting speed and solidification structure was presented by simulation.

When the superheats were 0.68 m/min, 0.75 m/min and 0.82 m/min, the averages area of columnar grain in bloom were 2.59 mm$^2$, 2.45 mm$^2$ and 2.35 mm$^2$ respectively. The averages radius of columnar grain in bloom were 0.69 mm, 0.65 mm and 0.63 mm respectively. The averages equiaxed grain area were 1.32 mm$^2$, 1.36 mm$^2$ and 1.37 mm$^2$ respectively. The averages equiaxed grain radius were 0.82 mm, 0.83 mm and 0.84 mm respectively. The averages equiaxed grain ratio in cross-sectional were 63.8%, 67.3% and 70.2% respectively.

Because residence time of molten steel in mould and secondary area reduced, the dissipation heat of molten steel reduced. The bloom temperature rose with casting speed rising. The microelements temperature rose at the same position. When the casting speed reached 0.82 m/min, the central bloom temperature at the end of mould is near the liquid line, the molten steel does not nucleate. Because residence time is short, the cooling intensity is not strong and the molten steel heat can not be removed by the cooling water. That led the temperature under bloom shell rose and temperature gradient of solidification front reduced. It is benefit to expanding the equiaxed grain area opposite to restraining columnar grain area.

Figure 6. Solidification structure of bloom with different casting speed ((a).0.68 m/min, (b).0.75 m/min, (c).0.82 m/min).

CET positions of bloom on three casting speed conditions were shown as fig 7. when the casting speeds were 0.68 m/min, 0.75 m/min and 0.82 m/min respectively, the CET positions were located 45.2 mm, 44.1 mm and 42.7 mm under the surface of bloom respectively. The simulation results show that high casting speed restrained columnar grain growth opposite to expanding equixed grains. The columnar grain sizes reduced with casting speed increasing. The CET position is shallow. Because casting speed increased, residence time of bloom in mould reduced. The cooling speed reduce too. That is benefit to expanding equixed grains. According to the dendrite tip growth kinetics equation, low degree of supercooling does not conducive to the growth of columnar crystal with columnar crystal size reducing. The simulation results show that high casting speed is benefit to CET convert. The central molten steel area increased when the casting speed increased at the same point. That would lead the casting bleed-out. The casting speed should be chosen appropriate to ensure expanding equixed grains and avoiding casting bleed-out.
The position of CET

Water Ratio in Secondary Cooling Area

On the initial condition as shown in table 3, the water ratio in secondary cooling area was changed. U75V is high carbon steel. Because the solidification temperature range is wide, the water ratio in secondary cooling is very strict. When the water ratio in secondary cooling area is strong, the temperature gradient in bloom increased, it is easy to form thermal stress and cracks in bloom internal. When the water ratio in secondary cooling area is weak, the bloom shell is thin, the bloom strength is very low, the bloom is easy to be out of shape. The simulation calculated the relationship between water ratio in secondary cooling area and nucleation structure when the water ratio in secondary cooling area were 0.22 L/kg, 0.24 L/kg and 0.27 L/kg respectively.

When the water ratio in secondary cooling area were 0.22 L/kg, 0.24 L/kg and 0.27 L/kg, the averages area of columnar grain in bloom were 2.13 mm$^2$, 2.59 mm$^2$ and 2.76 mm$^2$ respectively. The averages radius of columnar grain in bloom were 0.57 mm, 0.69 mm and 0.78 mm respectively. The averages equiaxed grain area were 1.38 mm$^2$, 1.36 mm$^2$ and 1.32 mm$^2$ respectively. The averages equiaxed grain radius were 0.84 mm, 0.82 mm and 0.81 mm respectively. The averages equiaxed grain ratio in cross-sectional were 72.3%, 66.6% and 56.4% respectively. The water ratio in secondary area increased, the columnar grains expanding area opposite to restraining equixed grains area. Low water ratio is benefit to expanding equixed grains area.

CET positions of bloom on three water ratio in secondary cooling area were shown as fig 9. When the water ratios were 0.22 L/kg, 0.24 L/kg and 0.27 L/kg respectively, the CET positions were located 40.7 mm, 45.2 mm and 47.7 mm under the surface of bloom respectively. The simulation results show that weak water ratio restrained columnar grain growth opposite to expanding equixed grains. Because the weak water ratio increased while the cooling intensity increased. The bloom surface temperature reduced that led the temperature gradient of bloom internal increasing. The simulations results show that reducing the water ratio is benefit to expanding equixed grains.
Parameters Chosen

The CET position in bloom should be controlled to expanding equixed grains in rail producing process. On the one hand, the equixed grains area is bigger, the rail performance is more homogeneous. On the other hand, the biggest shear stress of rail is located under the surface of rail tread from 10mm to 15mm. Serious composition segregations did not be allowed existed at that area. Comparing casting bloom with rolling rail, the same positions were 10 to 15 mm area under rail head tread and 25 to 40mm under bloom surface. Therefore, bloom CET position should not be controlled in these areas by modifying the continuous casting parameters.

The simulation results show that CET positions were more than 40mm under the bloom surface while superheat was more than 22 ℃. Therefore, the superheat should be controlled more than 22 ℃. When the casting speeds were ranged from 0.66m/min to 0.82m/min, the CET position under the surface of bloom is located from 25mm to 40mm. However, the high casting speed was benefit to expanding equixed grains with adding risk of bloom bleed-out. Therefore, casting speed should be chosen the middle line at 0.70 m/min to 0.75 m/min. Whatever were the water ratio in secondary cooling area from 0.22L/kg to 0.27L/kg, the CET positions did not locate at 25 to 40mm under the bloom surface. To get more equixed grains, the water ratio should be chosen from 0.22 L/kg to 0.23 L/kg.

Testing Results

The bloom macrostructures were shown in fig10 between the optimization. The columnar grain areas in fig10 (b) were bigger than that in fig10(a). The CET position under the bloom surface was not located from 25mm to 40mm.

Conclusions

The solidification heat transfer model and grains growth model were established on the basis of rail steel character and caster performance. The superheat, casting speed and water ratio in secondary cooling were calculated in the simulation. The results are shown as following.

(1) Reducing superheat and water ratio in secondary cooling, improving casting speed were
benefit to equiaxed grains growth opposite to columnar grains growth. CET position moved into the bloom center with superheat improving and water ration improving.

(2) When the superheats was 25℃, the CET position is 27.8mm under the bloom surface, the averages area of columnar grain in bloom was 2.59 mm$^2$. The average radius of columnar grain in bloom was 0.69 mm. The average equiaxed grain area was 1.35mm$^2$, the average equiaxed grain radius was 0.83mm, the average equiaxed grain ratio in cross-sectional was 68.2%.

(3) When the superheats was 0.75 m/min, the average area of columnar grain in bloom was 2.45 mm$^2$. The average radius of columnar grain in bloom was 0.65 mm. The average equiaxed grain area was 1.36mm$^2$, the average equiaxed grain radius was 0.83 mm, the average equiaxed grain ratio in cross-sectional was 67.3%.

(4) When the water ratio was 0.22 L/kg, the CET positions was located 40.7mm under the bloom surface. When the water ratio in secondary cooling was 0.22 L/kg, the average area of columnar grain in bloom was 2.13mm$^2$. The average radius of columnar grain in bloom was 0.57mm. The averages equiaxed grain area was 1.38mm$^2$, the averages equiaxed grain radius was 0.84 mm, the average equiaxed grain ratio in cross-sectional was 72.3%.

(5) The best continuous casting parameters were as following, superheat should be controlled 22℃ to 25℃, casting speed should be controlled 0.70 m/min to 0.75m/min, the water ratio in secondary area should be controlled 0.22L/kg to 0.23L/kg. The practices test show that the parameters after optimization were benefit to bloom. CET positions were not located from 25mm to 40mm under bloom surface. The CET positions avoided the biggest shear stress, it is good to rail performance.

References