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## Postprint: Modeling and Simulation of Liquid Metal Cooling Directional Solidification and Process Principles for Nickel-Based Superalloy Castings

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### Abstract

By considering the dynamic convection boundary in the liquid metal cooling directional solidification process, a mathematical model of the temperature field for superalloy castings was established. The three-dimensional cellular automaton (CA) method and the KGT growth model were employed to develop a mathematical model for grain nucleation and growth during the solidification of nickel-based superalloys. By employing bidirectional synchronous coupling of macroscopic and microscopic models, numerical simulation of the temperature field and grain structure was achieved. Casting experiments were performed, and the accuracy of the mathematical model was verified using cooling curves and grain morphology. Research on the laws of liquid metal cooling directional solidification demonstrates that the withdrawal rate not only significantly influences the shape of the mushy zone, but also substantially affects the parallelism of grains and the fineness of the dendritic structure. At excessively low withdrawal rates, the mushy zone becomes convex upward, and the grain structure is prone to divergence; at excessively high withdrawal rates, the mushy zone becomes concave, the grain structure converges, resulting in coarsening of the dendritic structure; at an appropriate withdrawal rate, a flat mushy zone can be achieved, which improves the parallelism of grains and refines the dendritic structure.

## Full Text

### Modeling and Simulation of Directional Solidification by LMC Process for Nickel Base Superalloy Casting

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#### Abstract

Gas turbine plays an important role in energy and aviation, among which the turbine blades are the key components. Ni base superalloys are the preferred material to manufacture blades due to their high temperature strength, microstructural stability and corrosion resistance. As a conventional directional solidification method, high-rate solidification (HRS) is used to produce columnar grain and single crystal blades. However, there are several problems when HRS is scaled to cast industrial gas turbines (IGT) components. In recent years, several possible techniques are being proposed for large IGT blades. The liquid-metal cooling (LMC) is one of the best methods among them, which improves heat extraction by immersing the casting and the mold into a container of metal coolant with low melting temperature as they are withdrawn from the heating zone. Unfortunately, the trial and error method is time and money cost and lead to a long R&D cycle. Therefore, numerical simulation plays an important role to optimize the process, and enhance the productivity in LMC directional solidification.

In this work, mathematical models for dynamic heat radiation and convection boundary of LMC process are established to simulate the temperature fields. Cellular automaton (CA) method and KGT growth model are used to describe the nucleation and growth. The pouring experiments are carried out. The accuracy of the model is validated by the cooling curves and microstructure. Moreover, the liquid-metal cooling directional solidification process is discussed

in more detail, including primary dendrite arm space (PDAS), secondary dendrite arm space (SDAS), mushy zone and microstructure, etc.. Simulation and experiment results are compared in the work. This study indicates that simulation and experimental results agree with each other well. The maximum error of temperature is less than 5 percent and the morphologies of grains are similar. The withdrawal rate has an important influence on the shape of mushy zone and dendritic structure. A concave mushy zone is formed and the grain tends to convergent under an excessive withdrawal rate. However, the mushy zone has a convex shape and the grain is divergent under a smaller withdrawal rate. A proper withdrawal rate is found to obtain smooth mushy zone, improve the parallelism of grains, and refine the dendritic structure.

**KEY WORDS** liquid-metal cooling, mathematical model, directional solidification, numerical simulation

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## Introduction

Superalloys exhibit high temperature strength, excellent oxidation and corrosion resistance, as well as favorable fatigue, fracture, and plasticity properties, making them primarily suitable for hot-section components in aero-engines and gas turbines. Nickel-based single crystal superalloys offer even better comprehensive performance due to the elimination of grain boundaries and strict control of grain orientation.

Currently, the high-rate solidification (HRS) process is industrially applied to manufacture single crystal superalloy castings. This technique uses a baffle to separate the heating and cooling zones in a directional solidification furnace, creating a one-dimensional temperature gradient along the axial direction. The casting melts and superheats in the heating zone while being forcibly cooled in the cooling zone. By applying an appropriate withdrawal rate, the solid/liquid interface remains near the baffle, resulting in unidirectionally aligned solidification structures. Although mature and operationally simple, HRS is best suited for small castings such as aero-engine blades. However, with rapid industrial development, heavy-duty gas turbines demand larger superalloy blades. Traditional HRS technology faces numerous challenges when producing large-scale blades, including mold deformation and cracking, reactions between the mold and molten metal, and defects such as freckles, shrinkage porosity, and stray grains. These issues primarily arise from the low withdrawal rate in HRS processes, which creates a relatively low temperature gradient ahead of the solid/liquid interface.

To obtain larger temperature gradients and produce superalloy castings with better microstructure and properties, researchers have proposed several new directional solidification techniques, including gas-cooling casting (GCC), fluidized-bed quenching (FBQ), and liquid-metal cooling (LMC). Among these, the LMC process achieves higher temperature gradients and solidification rates by with-

drawing the casting and mold into a container filled with low-melting-point metal coolant.

The LMC process involves numerous influencing factors and complex heat transfer mechanisms, demanding sophisticated control technology. The influence patterns of its process parameters remain unclear and are still being explored experimentally. Researchers have employed numerical simulation to assist experimental studies, significantly improving efficiency and reducing costs. Elliott et al. used commercial software ProCAST to simulate the temperature field during LMC solidification and compared it with the HRS process, demonstrating that withdrawal rate significantly affects mushy zone shape. Kermanpur et al. developed secondary boundary conditions for ProCAST to simulate blade temperature fields and used the CAFE module to calculate actual blade grain structures, which were validated experimentally. Miller et al. simulated dendrite growth under LMC conditions from a microstructural perspective, showing that LMC permits higher withdrawal rates to produce finer dendritic structures, though excessive rates may cause transverse dendrite growth. Lu et al. used ProCAST to simulate temperature fields and microstructures of heavy-duty gas turbine hollow blades, optimizing the process to successfully produce columnar grain blades. Tang et al. developed dynamic composite boundary conditions for the immersion process through secondary ProCAST development, enabling numerical simulation of temperature fields and dendritic structures in single crystal blades under LMC conditions.

Building upon previous laboratory work, this study establishes a temperature field mathematical model considering dynamic convection boundaries during LMC solidification. A three-dimensional cellular automaton (CA) method combined with the KGT growth model is employed to develop a mathematical model for grain nucleation and growth in nickel-based superalloy solidification. Using temperature and enthalpy interpolation algorithms with bidirectional synchronous coupling between macroscopic and microscopic models, proprietary software was developed to calculate grain structures. Pouring experiments were conducted to validate model accuracy through cooling curves and grain morphology observations. The study investigates the formation patterns of primary and secondary dendrite arm spacings and examines the influence of withdrawal rate on mushy zone shape, grain structure, and dendrite morphology.

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## 1. Mathematical and Physical Models for the LMC Directional Solidification Process

[Figure 1: see original paper] shows a simplified schematic of the LMC directional solidification furnace, which includes a heating zone, fixed baffle, floating baffle, chill plate, and liquid metal pool. Before pouring, the mold shell is fixed on the chill plate and preheated for a period. The alloy is then poured into the mold and held for some time before being withdrawn at a specific rate into

the liquid metal pool, enabling convection heat transfer between the mold and liquid metal.

### 1.1 Temperature Field Model

The temperature field is governed by the nonlinear heat transfer equation:

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho c} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \frac{L}{c} \frac{\partial f_s}{\partial t} + \frac{Q_R}{\rho c}$$

where  $T$  is thermodynamic temperature,  $t$  is time,  $\rho$  is density,  $c$  is specific heat capacity,  $L$  is latent heat of crystallization,  $\lambda$  is thermal conductivity,  $f_s$  is solid fraction, and  $Q_R$  is heat flux density between the solid surface element and the environment.

The dynamic radiation and convection boundary conditions on the solid surface per unit area during the LMC process are:

$$q = \sigma \sum_{n=1}^N b_n (T_n^4 - T^4) \frac{S_n}{S} + \alpha(T_a - T) + \alpha_b(T_b - T)$$

where  $\sigma$  is the Stefan-Boltzmann constant,  $N$  is the number of rays in the ray tracing method,  $b_n$  is the energy weight of ray  $n$ ,  $T_n$  is the temperature at the endpoint of ray  $n$ ,  $e$  is the emissivity of the current surface,  $e_n$  is the emissivity at the endpoint of ray  $n$ ,  $S$  is the area of the current surface,  $S_n$  is the area of the entity patch at the endpoint of ray  $n$ ,  $\alpha$  is the convective heat transfer coefficient between the free surface and metal coolant,  $\alpha_b$  is the convective heat transfer coefficient between the free surface and floating baffle,  $T_a$  is the temperature of the medium outside the free surface,  $z$  is the Z-coordinate of the top face of the current element,  $h$  is the height of the liquid metal coolant, and  $h_b$  is the thickness of the floating baffle.

### 1.2 Microstructure Model

Microstructure simulation is based on the CA model with a continuous nucleation model to calculate nucleation density:

$$n(\Delta T) = N_{\max} \exp \left( -\frac{(\Delta T - \Delta T_N)^2}{2\Delta T_s^2} \right)$$

where  $\Delta T$  is undercooling,  $n(\Delta T)$  is nucleation density,  $N_{\max}$  is maximum nucleation density,  $\Delta T_s$  is standard deviation of distribution, and  $\Delta T_N$  is average nucleation undercooling.

Grain growth is modeled using a simplified KGT model. The growth velocity  $v(\Delta T)$  at the dendrite tip is:

$$v(\Delta T) = a_1 \Delta T^2 + a_2 \Delta T^3$$

where  $a_1$  and  $a_2$  are growth coefficients.

### 1.3 Dendrite Arm Spacing Models

The primary dendrite arm spacing  $l_1$  is calculated using:

$$l_1 = M_1 G^{-1/2} v^{-1/4}$$

where  $M_1$  is a material constant and  $G$  is temperature gradient.

The secondary dendrite arm spacing  $l_2$  is calculated using:

$$l_2 = M_2 t_f^{1/3}$$

where  $M_2$  is a material constant and  $t_f$  is local solidification time, representing the time the current element spends in the mushy zone.

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## 2. Experimental Methods

Pouring experiments were conducted on a 25 kg HRS/LMC dual-purpose directional solidification furnace using DZ466 nickel-based superalloy with chemical composition (mass fraction, %): C 0.01-0.18, Cr 8.0-12.5, W 3.5-7.2, Al 3.0-5.5, Ta 5.0-7.0, Mo 0.8-3.2, Ti 0.5-4.0, Ni balance. The liquidus temperature is 1367 °C and solidus temperature is 1302 °C. Graphite chill plates and 5 mm thick mold shells were used. Temperature measurement employed W-Re thermocouples and an MV2000 data acquisition system, with thermocouple tips protected by 6 mm outer diameter quartz tubes. Grain structures were etched using a 90% HCl + 10% H<sub>2</sub>O<sub>2</sub> (volume fraction) solution and photographed with a digital camera. Dendritic structures were etched using a 15% HCl + 5% CuSO<sub>4</sub> · 5H<sub>2</sub>O + 5% HF + 75% H<sub>2</sub>O (volume fraction) solution and observed using an Imager A1m metallurgical microscope.

To validate the LMC directional solidification models and investigate solidification patterns, a double-plate sample geometry was used, with each plate measuring 50 mm × 10 mm × 200 mm. The three-dimensional model and thermocouple arrangement in the mold shell are shown in [Figure 2: see original paper], where the opposing faces of the two plates are inner surfaces. The mold preheat temperature was 1500 °C, pouring temperature 1450 °C, and pouring time 8 s. After pouring, the assembly was held for 2 minutes before withdrawal. Multiple experiments were conducted at withdrawal rates of 6, 8, 9, 12, and 15 mm/min, with temperature measurement performed at 8 mm/min.

### 3. Results and Discussion

#### 3.1 Cooling Curves

To validate temperature field accuracy, calculated temperature variations at thermocouple positions were compared with measured cooling curves. Cooling rates from simulations were also compared with experimental data. [Figure 3: see original paper] presents the simulated and experimental cooling curves, while [Figure 4: see original paper] shows the corresponding cooling rates.

The simulated cooling curves and rates agree well with experimental results. When the sample passes the floating baffle position, minor calculation errors occur near the chill plate due to baffle compression effects, but the overall error remains below 5%, satisfying requirements for both fundamental research and engineering applications. All four thermocouples were positioned away from the chill surface, so their temperature variations reflect vertical differences in LMC convective cooling. During preheating, the four points exhibit different temperatures, indicating non-uniform temperature distribution within the mold shell—points closer to the baffle in the heating zone show lower temperatures. Therefore, the temperature distribution after preheating must be considered when studying initial stage process effects. During pouring, all four points experience sudden temperature changes approaching the pouring temperature, confirming that temperature variation during pouring is minimal and can be simplified as instantaneous filling. Additionally, cooling rate variations near the chill plate depend primarily on chill plate heat dissipation and are also affected by coolant convective heat transfer, whereas regions far from the chill plate depend only on coolant convection. Consequently, heat dissipation rates near the chill plate exceed those in distant regions.

#### 3.2 Grain Structure

[Figure 5: see original paper] and [Figure 6: see original paper] compare simulated and experimental grain structures at different withdrawal rates, with [Figure 5: see original paper] showing the outer surface and [Figure 6: see original paper] the inner surface. The simulated grain structures match experimental results well across all surfaces, with close agreement in grain count, width, and grain angles at different locations. At 6 mm/min withdrawal rate, grains show slight divergence, while at 8 mm/min, divergence is minimal. This demonstrates that LMC permits higher withdrawal rates while maintaining good solidification structures. In production, higher withdrawal rates are desired to reduce mold-melt contact time and improve efficiency, but appropriate rates are essential for quality castings. Local grain convergence observed near the sample bottom results from rapid growth of numerous nuclei formed during initial solidification under chill plate effects. As withdrawal proceeds, competitive grain growth eliminates some grains, allowing those with preferred orientation to grow stably.

### 3.3 Mushy Zone

To further explore solidification patterns under LMC conditions, temperature fields at various withdrawal rates were simulated to investigate mushy zone curvature changes, as shown in [Figure 7: see original paper]. At different withdrawal rates, the mushy zone curvature in the initial stage transitions from convex to concave with increasing solid/liquid interface height, eventually stabilizing as chill plate heat dissipation dominates initially. [Figure 7: see original paper] also reveals that when withdrawal rate exceeds 15 mm/min, increased rates cause more severe mushy zone concavity, while rates below 9 mm/min produce convex mushy zones. This suggests an optimal withdrawal rate between 9-15 mm/min yields a flat mushy zone.

[Figure 8: see original paper] illustrates mushy zone evolution at 24 mm/min withdrawal rate during the initial stage. Analysis shows that when chill plate heat dissipation dominates, the mushy zone is convex; as withdrawal proceeds, lateral heat transfer becomes significant. Excessive withdrawal rates cause mushy zone concavity, and the slowest solidification front advancement during the convex-to-concave transition leads to dendrite coarsening, which should be avoided.

### 3.4 Dendrite Arm Spacing

To investigate dendrite size variations, primary dendrite arm spacing distributions were simulated and experimentally studied at 8 mm/min withdrawal rate. [Figure 9: see original paper] shows the simulation results. Two vertical lines were selected at the mid-thickness longitudinal section: one at the center and another 5 mm from the edge. During experiments, cross-sections at different heights were sampled, and metallographic images were taken at intersections with the two vertical lines to measure primary dendrite arm spacing. [Figure 10: see original paper] compares simulated and experimental primary dendrite arm spacing at 8 mm/min. The calculated values agree well with experimental results. During the initial stage, regions closer to the chill plate experience larger temperature gradients and solidification rates due to chill plate effects, resulting in smaller primary dendrite arm spacing averaging approximately 150  $\mu\text{m}$ . Above 30 mm from the chill surface, chill plate effects weaken, temperature gradients and solidification rates decrease, local solidification time increases, and dendrites coarsen slightly, with average primary spacing of about 250  $\mu\text{m}$ .

Secondary dendrite arm spacing was similarly investigated, with results shown in [Figure 11: see original paper] and [Figure 12: see original paper]. The calculated secondary spacing along vertical lines matches experimental data well. Within 20 mm of the chill surface, higher solidification rates produce shorter local solidification times and smaller secondary dendrite arm spacing of approximately 30  $\mu\text{m}$ . At about 30 mm from the chill surface, the convex-to-concave transition causes the slowest solidification front advancement, resulting in maximum secondary spacing of about 65  $\mu\text{m}$ . Subsequently, secondary spacing

decreases and stabilizes at approximately 45  $\mu\text{m}$  beyond 50 mm from the chill surface. During stable growth, secondary spacing at the edge is smaller than at the center because lateral radiation heat transfer at the edge exceeds that at the center. Both heating flux above and cooling flux below the baffle gap are substantial, creating larger longitudinal temperature gradients at the edge near the baffle gap, which produces narrower mushy zones. Since solidification front advancement rate approximates withdrawal rate during stable stages, narrower mushy zones correspond to shorter local solidification times and finer secondary dendrite arm spacing.

Cross-sectional dendrite morphologies at withdrawal rates of 9, 12, and 15 mm/min are shown in [Figure 13: see original paper]. Within a certain range, increasing withdrawal rate shortens local solidification time, refining both primary and secondary dendrite arm spacing. At the critical withdrawal rate of 12 mm/min, the finest dendritic structure is obtained; beyond this critical rate, both primary and secondary spacing coarsen with increasing withdrawal rate. The 12 mm/min rate produces dense, fine dendritic structures, confirming the optimal rate range of 9-15 mm/min determined previously.

[Figure 14: see original paper] compares simulated and experimental grain morphologies at 12 mm/min withdrawal rate. The simulation matches experimental results well, showing excellent grain parallelism without significant defects such as broken grains or stray grains, further validating the conclusions.

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## Conclusions

This study establishes temperature field and grain nucleation-growth models for the LMC directional solidification process and develops proprietary simulation software. Model accuracy is validated through temperature measurement experiments and grain morphology observations, demonstrating that numerical simulation can effectively optimize directional solidification process parameters. Primary and secondary dendrite arm spacing calculations show good agreement with experimental results. The LMC process permits relatively high withdrawal rates, but excessive rates cause mushy zone concavity while insufficient rates produce convex mushy zones. Appropriate withdrawal rates between 9-15 mm/min yield flat mushy zones, improved grain parallelism, and refined dendritic structures. Through comparative study of plate sample experiments and simulations, optimal LMC directional solidification process parameters were identified, enhancing grain parallelism and refining dendritic microstructures.

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