Intelligent Digital Simulation of Casting Process in Context of Materials Genome Engineering

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Abstract: Casting is a fundamental and irreplaceable method in advanced manufacturing. The design and optimization of casting processes are crucial for producing high-performance, complex metal structural components. Numerical simulation is the primary tool for achieving this optimization. The Materials Genome Engineering (MGE) aims to accelerate material design and development and has shown significant potential in enhancing numerical simulations of casting processes. This article reviews the impact of material genome engineering on numerical simulation technology in casting and forecasts future trends in intelligent digital simulation for casting processes.

Keywords: Casting,Numerical simulation,Materials Genome Engineering, Machine Learning

1 Introduction

In recent years, the MGE has significantly transformed materials design and manufacturing, particularly in developing new materials and optimizing processes. MGI aims to accelerate material development by integrating high-throughput computing, experimental databases, and materials informatics. This innovative approach has profoundly influenced traditional manufacturing.Casting involves complex multi-stage processes, including the flow and solidification of molten metal, which present significant challenges due to the interplay of multiple scales and physical fields. The introduction of material genetic engineering has opened new opportunities for enhancing numerical simulation in casting.Traditional simulation methods, such as Finite Element Analysis (FEA) and Computational Fluid Dynamics (CFD), can predict macroscopic results but are computationally intensive and often struggle with complex microstructure evolution and multi-scale coupling. Material genetic engineering has improved the accuracy and efficiency of numerical simulations by leveraging big data and machine learning technologies.A key advancement of MGI is the introduction of data-driven models that allow machine learning to capture complex physical relationships in casting processes. The material genome database offers extensive data on material composition, processing techniques, and performance relationships, providing a solid foundation for simulations. By employing machine learning and deep learning techniques, researchers can quickly develop accurate predictive models, enhancing simulation precision. Overall, material genetic engineering has accelerated the optimization of casting processes and advanced intelligent digital simulation technology. This article will explore the latest developments in numerical simulation for casting within the context of material genetic engineering and provide insights into future advancements.

2 Employing MGEto expedite numerical simulation

Material genetic engineering reverses the traditional product development process by starting with application requirements and deriving the necessary material composition and structure to meet those functional needs. This approach significantly bridges the gap between academic research and industrial production, driving innovation in new materials.

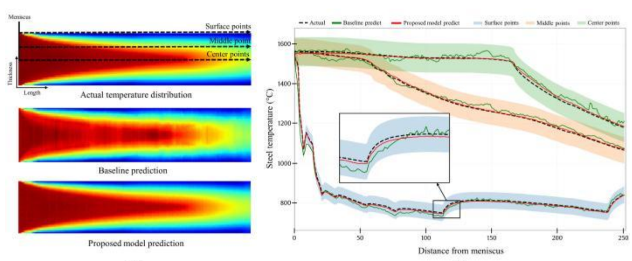

Figure 1 An example of temperature predictions of the solidifying steel [1]

Traditional physics-based computational simulation methods face limitations in efficiency and accuracy due to the precision of thermal property parameters, model complexity, and high-performance computing devices. In contrast, data-driven models, characterized by "data + artificial intelligence," focus on data generation and processing, representing the core direction of material genetic engineering.The predictive power of machine learning can enhance traditional numerical simulations by significantly reducing computation time while maintaining accuracy. Current data-driven methods to accelerate numerical simulations include solving equations more efficiently, rapidly predicting thermal properties parameters, and establishing alternative models for metallurgical changes. Additionally, machine learning models can replace traditional simulations, exemplified by deep learning techniques for predicting shrinkage porosity, the temperature distribution (as shown in Figure 1) [1]and generating microstructures.

3 Integrated Computational Materials Engineering (ICME)

The connection between ICME and MGE is evident in their data sharing and model complementarity: MGE provides extensive material data, while ICME leverages computational models to optimize manufacturing and processing. Additionally, MGE can refine ICME models. MGE has expanded ICME's philosophy across the entire materials science, technology, and engineering chain. A notable example of ICME in the casting process is the Virtual Aluminum Casting (VAC) manufacturing process developed by Allison et al. from Ford Motor Company in 2006. Furthermore, the casting ICME framework proposed by Alan A. Luo et al. [2] (shown in Figure 2) parallels the industrial product development process that utilizes various CAD-CAE-CAM tools, including microstructure and performance simulations for local casting positions.

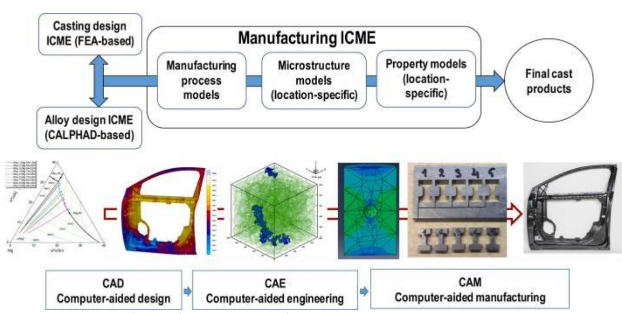

Fig. 2 ICME framework for casting design and process development as compared to industrial CAD-CAE-CAM approach [2]

4 Establishment of relevant databases

Currently, there is extensive research on material databases, such as the Thermocalc thermodynamic database, AFLOWLIB, and the Materials Project calculation database. However, studies on casting-related databases are relatively scarce and typically limited to specific categories, like casting process databases, generative process databases, or material databases. Cho et al. [3] proposed an integrated database system for casting production, which includes shape databases, material physical properties (melting point, solidus line, liquidus line, etc.), process databases, and expert systems. Despite this, the high flexibility, complexity, and variability of casting production processes, along with organizational challenges and isolated departmental data, result in difficulties in data storage, retrieval, and application. To advance digital casting technology, integrate process design, ensure casting quality, and predict lifecycle, it is imperative to establish a standardized key material performance database. This database should store information about the relationships between processing technology and microstructure, microstructure and material properties, and thermal properties parameters to support the development and validation of computational models.

5 Conclusion

The Materials Genome Initiative (MGI) has introduced significant innovations to the numerical simulation of casting processes. Material genetic engineering has enhanced the efficiency of traditional numerical simulations. Moreover, the integration of Integrated Computational Materials Engineering (ICME) with material genetic engineering has further improved the multi-scale coupling capabilities of these simulations. This advancement allows for more accurate predictions from microstructure to macroscopic performance, offering comprehensive optimization solutions for casting processes. Future development trends in numerical simulation of casting within the framework of material genetic engineering include:

1) A rich and perfect database of material thermophysical parameters used to improve the calculation accuracy, as well as a technology to synergistically improve the accuracy and efficiency of numerical simulation.
2) The establishment of special database for casting and the improvement of process data quality evaluation and control technology.
3) The deep integration of data drive, simulation software and ICME, and the construction of digital platform based on digital twins throughout the life cycle.

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