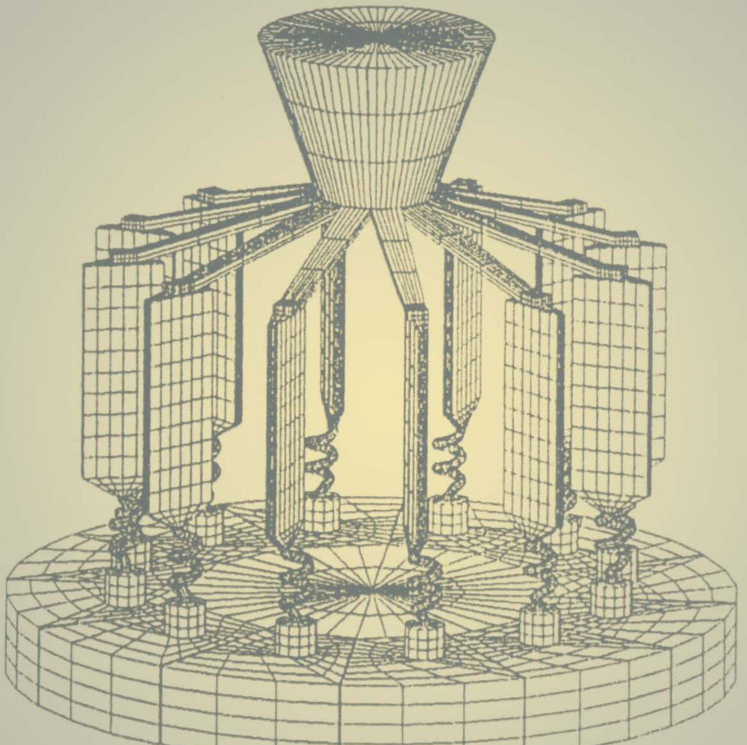
MODELING FOR CASTING AND SOLIDIFICATION PROCESSING



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CRC Press
Taylor & Francis Group
Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an **informa** business

CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742

Visit the Taylor & Francis Web site at
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Foreword

Modeling of casting and solidification processes, as we think of it today, can be traced back to the precomputer days of the first half of the twentieth century. To pick just a few examples, the first application of the error function solution to the solidification of ingots was in 1930. An elegant mathematical solution to the microsegregation problem was available in the 1940s. Simple fluid flow analyses were widely employed by foundrymen in the 1950s and thereafter. Of course, because of analytical and computational limitations, these models were necessarily highly simplified and therefore of only limited practical value.

With the advent of the computer and its development in the 1960s, the situation began to change quickly. The 1960s saw the development of quite detailed models for flow and solidification in complex sand castings and in continuous castings. From that point on, the steady and rapid advance of speed and power of computers has changed the world of design and production of cast metal parts. Today computation is an essential tool in modern foundries and cast shops for mold and process design and process control.

In a book I coauthored 40 years ago, we wrote that "metal casting has traditionally been an art and a craft, with secrets of the trade passed jealously from father to son. Only in the last century have science and engineering made noticeable in-roads on materials and processes of the foundrymen. But casting will always be one of the most economical routes from raw material to finished metal products, and it was inevitable the art of the founder would yield to the economy and precision of the engineering approach."

Those words were correct then, but this book shows how much truer they are today. The engineering "rules of thumb" of which we were so proud at mid-century have yielded to the precision of modern modeling. The guesses and the trials and errors we made in reaching suitable gating and risering processes have yielded to modern computational packages—with final results far better optimized than those we achieved with our mid-century "combination of art and science." Of course, in one sense the metal casting "art" of the future will survive; in using modeling in new and innovative ways to produce better components more inexpensively and quickly.

The combination of theory and application presented in this book represents the "new engineering" of casting processes. It is recommended reading for the experienced as well as for the newcomer to the metal casting field, to provide tools for the present as well as an understanding of the direction and power of this new engineering.

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Preface

Modeling is a method that uses mathematical equations and computer algorithms to represent certain physical phenomena. The application of modeling techniques to solve engineering problems provides many advantages over conventional trial-and-error methods. With the rapid advances in computer hardware and software, casting process modeling is being increasingly accepted by foundries and molten metal processing plants as a viable engineering tool to solve routine production problems. In order to effectively utilize modeling, process engineers need to have a thorough understanding of the principles of both casting/solidification processing and computer/numerical analysis.

Although numerous technical papers regarding casting process modeling are being published in technical journals and conference proceedings each year, very few books have attempted to provide a systematic introduction to the casting process modeling technology. The objective of this book is therefore to provide a comprehensive technical background as well as practical application examples regarding the technology. The ultimate goal is to increase the application of casting process modeling in production by enhancing the process engineer's understanding of this technology. It can be used as a reference book for process engineers in industry as well as casting/solidification researchers in academia and research institutes. In addition, it can also be used as a textbook for graduate and undergraduate students, the source of future process engineers in casting foundries and molten metal processing plants. This book includes three parts: Theoretical Background, Application to Shape Castings, and Application to Ingot Castings and Spray Forming. Presenting such an extensive amount of information constitutes a tremendous task. The approach that has been taken in the preparation of the book was to involve many experts with different backgrounds. Indeed, 26 dedicated experts from industry, research institutes, and academia contributed to this book.

I am grateful to the contributing authors for the time and effort they devoted to their respective chapters. I also appreciate the contributions of Dr. Francois Mollard, Mr. Patrick A. Russo, and Mr. Dun-Wei Yu, who assisted by proofreading and commenting on the text. Last but not least, I would like to acknowledge my secretary, Ms. Carol Muszik, who patiently prepared the manuscript.

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Introduction

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I. WHY MODELING?

The production of almost all metallic components involves melting and solidification processes. When a molten metal is poured into a mold to make a product with a specific shape, the process is called casting. However, in processes such as water, gas, vacuum, and centrifugal atomization, the molten metal is first disintegrated into small molten droplets which then solidify as powder.

Casting and solidification processing involves many physical phenomena such as fluid flow, heat transfer, electromagnetic force, thermal stress, defect formation, and microstructure evolution. The quality of the final product depends on the mechanisms of defect formation and microstructure evolution, which are controlled by heat transfer, fluid flow, and thermal stress. How to control processing parameters, such as metal superheat, pouring/casting speed, and mold preheat temperature/cooling condition, to provide proper solidification conditions and satisfactory quality castings, has been the subject of intensive investigations.

In production environments, process engineers typically use the trial-and-error method based on empirical relationships between processing parameters and the quality of the resultant castings. This method usually leads to long process development times and high production costs. Process modeling, on the other hand, enables process engineers to make virtual castings using computer techniques. As a result, the effects of processing parameters on the quality of the resultant castings can be evaluated without incurring the cost of actually making castings. The processing parameters can easily be modified until a set of processing parameters that will result in castings with satisfactory quality is found. By applying casting process modeling, the time and cost of developing new, and enhancing existing, processes can be significantly reduced.

As mentioned earlier, casting and solidification processing involve many complex physical phenomena. Developing a comprehensive model to represent all these phenomena is a very challenging task. From an engineering point of view, it is not always possible or even necessary to have a comprehensive model which simulates all the involved physical phenomena. In general, each casting and solidification processing process has its own unique characteristics which have a dominant effect on the quality of the resultant product. Thus, developing a model that provides an effective way to simulate these unique characteristics is often not only technically sufficient, but also cost effective. In this introduction chapter, a general description of the various metal manufacturing processes and their applications is first presented. The modeling approach used to effectively simulate the unique characteristics of each process is then discussed.

II. UNDERSTANDING METAL MANUFACTURING PROCESSES

The knowledge necessary to establish a model that effectively simulates a casting process is rooted in a general understanding of the various metal manufacturing processes relying on casting as one of their key steps.

There are three basic types of metallic products: cast, wrought, and those made by powder metallurgy (PM). Cast products are used in their as-cast form with little or no machining. The most important feature of the shape casting processes is the capability to produce near net shape components, resulting in significant savings in machining cost. In addition, castings also permit design simplification and parts count reduction. However, since no mechanical work is applied to the final casting to refine its microstructure, mechanical properties and microstructural uniformity are usually inferior to those of wrought products. Mechanical work such as forging, rolling, and extrusion is used to change the shape and refine the microstructures of cast products, resulting in wrought products which typically have finer microstructures and better mechanical properties than the original cast products. The major disadvantages of wrought products are the high machining cost and low material yield typical of the conversion of the input stock into the final products. PM products are made by consolidating metal powder into near net shape components. Conventional PM components usually have lower densities and mechanical properties than wrought products. On the other hand, advanced PM processes can produce fully densed materials which have mechanical properties that are equivalent to or better than those of wrought products.

A. Cast Products

Many different casting processes are used to make shaped components; the following sections briefly describe some of the most common.

1. Sand Casting

Sand casting is the most widely used shape casting process. It uses bonded sand as the mold material and can produce castings that weigh from only a few grams to more than a hundred tons. The sand casting process is applicable to a wide range of metals including aluminum, steel, cast iron, etc. Sand cast products are used by almost all industries, from the high volume, cost sensitive automobile industry to the high unit cost and top quality aerospace industry. Sand casting is always performed in air atmosphere, with the sand mold at room temperature. As a result, sand casting usually results in a relatively rough surface product; it also has only a limited capability to make thin wall components.

2. Investment Casting

The investment casting process uses ceramic molds and can be carried out in vacuum as well as in air. The ceramic molds may be preheated to very high temperatures (e.g., up to 1550°C for nickel-base superalloys), allowing for the producing of thin wall castings. Because of the high ceramic mold preheat temperatures, radiation heat loss from the mold surfaces strongly affects solidification conditions. The use of the vacuum environment enables the investment casting of superalloys and titanium alloys, which have a chemical composition otherwise difficult to control in air. On the other hand, aluminum alloys, steels, and cobalt alloys are typically cast in air. Investment castings are mostly used for aerospace and medical implant applications, which tend to have a relative low production volume but high unit cost. Recently, investment cast golf club heads have become an important nonaerospace application for titanium alloys.

3. Lost Foam Casting

The lost foam casting process has features of both investment casting and sand casting. It uses a coated polystyrene foam pattern imbedded in traditional unbonded sand. During mold filling, the foam pattern is decomposed by the heat of the molten metal. The metal replaces the foam pattern and duplicates all the features of the pattern. The permeable refractory coating on the pattern allows the gases from the decomposing foam to escape rapidly from the mold, yielding castings with a smooth surface. The major advantage of the lost foam casting process is that it can produce castings with a quality similar to that of investment casting, but at a cost close to that of sand casting. Lost foam castings (aluminum alloys and cast iron) are mostly used in the automobile industry.

4. Permanent Mold Casting

Permanent mold casting uses metallic molds; cooling and/or heating channels are sometimes imbedded in critical locations of the mold to facilitate the control of the solidification process. Permanent mold casting process is particularly suitable for high volume production of castings with fairly uniform wall thickness and limited undercuts or intricate internal coring. Compared to sand casting, permanent mold casting can produce castings with more uniform wall thickness, closer dimensional tolerances, superior surface finish, and improved mechanical properties. Alloys that can be cast by the permanent mold casting process include aluminum, magnesium, zinc, copper, and hypereutectic gray iron. Because of the high cost of the metallic tooling, the permanent mold casting process is primarily used for making high-volume components such as those intended for automobile applications.

5. Die and Squeeze Casting

Die casting is another casting process using metallic dies/molds to make high-volume components that are particularly suitable for the automobile industry. However, instead of gravity mold filling as in the permanent mold casting process, die casting relies on pressure to provide very rapid filling of the metallic die. The jetting associated with the extremely rapid mold filling process can cause the entrapment of air in the resultant castings. The entrapped air will then expand to form bubbles during subsequent heat treatment. Because of this, die castings are typically not heat treatable and are limited to applications that do not require high mechanical strength. Recently, squeeze casting, one special form of die casting, has been developed to overcome this shortcoming by employing a slower and more controllable mold filling process to avoid the entrapment of air in the casting. Aluminum, zinc, magnesium, and copper alloys are most commonly made by either die or squeeze casting process.

6. Semi-Solid Metalworking

Semi-solid metalworking (SSM) also relies on a metallic die/mold; it bears some similarities to the die casting process. The two most important features of the SSM process are its reliance on input materials with a unique fine grain microstructure, and an operating temperature between the melt liquidus and solidus temperatures, i.e., in the mushy region. The unique fine grain microstructure of the input material is largely maintained in the final casting, resulting in mechanical properties superior to those of die castings. The major advantage of the SSM process is that it produces components with complex geometries similar to die casting, and yet with mechanical properties comparable to those of wrought products. SSM is a fairly new process and its products are primarily used in automobile and other high volume–high mechanical strength applications. Alloys that have been cast by the SSM process include aluminum, magnesium, and copper.

B. Wrought Products

The majority of metal components are made by making wrought products. For a long time, the input material for wrought processing was made by the conventional ingot casting process. Since the 1960s, continuous and semicontinuous casting processes have been gradually introduced into production. Now, with very few exceptions, most of input materials for wrought products are cast by either continuous or semicontinuous casting processes.

1. Conventional Ingot Casting

Ingots made by the conventional metal (mostly cast iron) mold casting process were the primary source for wrought processing before the 1960s. The productivity of the conventional ingot casting process is inherently low. Large ingots are usually octagon shaped and individually cast, whereas small ingots may have a square cross section and are cast in clusters. A thermally insulated or heated molten metal reservoir at the top of the ingot (called the hot top) is used to feed the solidification shrinkage and reduce the size of the shrinkage pipe or void. The hot top, and the part of the ingot with the shrinkage pipe, are cut off before subsequent forming (forging, rolling, and extrusion) operations, resulting in a significant material loss. Severe macrosegregation may also happen, which has a detrimental effect on ingot quality and hence limits the size of the ingot that can be cast. Today, the conventional ingot casting process is used primarily for small quantity production of certain specialty alloys.

2. Continuous Casting

The advantages of continuous casting in primary metals production have been recognized for more than a century. The dramatic growth of this technology, however, has only been realized since the 1960s. The principal advantages of the continuous casting process are high productivity, high material yield, good product quality, and low energy consumption. The primary purpose of continuous casting is to bypass conventional ingot casting and to cast a form that is directly rollable on finishing mills. The cross-sectional shapes of continuously cast blooms/billets/slabs can be round, square, or rectangular. The principle of the continuous casting process is to form the cast bloom/billet/slab in a continuously withdrawn water-cooled copper mold. To prevent sticking of the frozen casting surface to the copper mold, the mold is normally oscillating during the casting operation and a lubricant is added to the mold metal interface, resulting in a smooth as-cast surface. Beyond the mold, water spray is used to speed up the heat removal; this results in a fast cooling rate and a reduced degree of macrosegregation in the casting. The length of the casting can, in theory, be infinite. A vertical continuous casting machine is most commonly used. The solidifying casting is first curved from a vertical to a horizontal position. The completely solidified casting is then cut to length and subjected to subsequent rolling operations. Very little material is lost due to the hot top, and thus the material yield is high. In addition, the production rate of continuous casting is very high, typically in the hundreds of thousands or even millions of tons per year for steel. Continuous casting is primarily used for ferrous alloys, especially low carbon steels. Currently, most of the world's near 800 million tons of steel produced each year is made by the continuous casting process.

3. Direct Chill Casting

Compared to steel, aluminum and copper have a significantly higher thermal conductivity and thus solidify much faster. As a result, the curved continuous casting process cannot be used for aluminum and copper alloys. In addition, the quantity of metal to be produced for all nonferrous alloys is significantly lower than for steel. Thus, there is no economical incentive to use expensive continuous casting machines to cast nonferrous metals. Consequently, the principal continuous casting process for nonferrous alloys is the direct chill casting (DC casting) process. The vertical DC casting process is a semicontinuous process widely used for making aluminum and copper alloy billets and slabs. DC casting is similar to the ferrous continuous casting process, except that the resultant billets/slabs have a finite length, typically around 8–10 m. As a result, the slab/billet curving and cutting operations, which are important components of the ferrous continuous casting process, are not necessary in the DC casting process. Consequently, the capital cost for DC casting machines is significantly lower than for continuous casting equipment. Recently, horizontal DC casting process has been developed to cast large aluminum alloy slabs for rolling to plate and strip. In general, the withdrawal speed for DC casting is up to 0.2 m/min, significantly lower than that used for the continuous casting of steel (typically 1 m/min). For both DC and continuous casting processes, metal melting and billet/slab casting are uncoupled. Consequently, the molten metal superheat and the billet/slab casting speed can be controlled independently.

4. *Vacuum Arc Remelting and Electroslag Remelting*

Vacuum arc remelting (VAR) and electroslag remelting (ESR) are two secondary remelting processes widely used for producing ingots of high performance alloys such as titanium (VAR) and nickel-base superalloys and specialty steels (VAR and ESR). These two processes are semicontinuous and bear some similarities with the DC casting process. The major characteristic of VAR and ESR is the use of a precast or prefabricated electrode as the input material. This electrode is then melted by vacuum arc (VAR) or slag joule heating (ESR). Molten metal droplets falling from the electrode tip accumulate in the water-cooled copper mold or crucible to form an ingot. High power input results in high electrode melting rate (i.e., high ingot casting rate) and high molten metal superheat. This coupled relationship between electrode melting and ingot casting results in a limited processing window yielding ingots with a desirable structure. Contrary to continuous casting and DC casting processes, the principal driving force for using VAR and ESR is ingot quality enhancement, rather than productivity improvement. In fact, the productivity of VAR and ESR is quite low. VAR and ESR ingots have a faster cooling rate, lower inclusion content, lower degree of macrosegregation, better grain structure, and improved forgeability than ingots made by conventional ingot casting process. Because of this, many segregation-prone alloys, which could not be made by conventional ingot casting processes, can now be produced routinely by VAR and ESR processes. Currently, some nickel-base superalloys and titanium alloys used for aerospace applications can only be produced by the VAR process.

5. *Electron Beam Melting and Plasma Arc Melting*

Electron beam melting (EBM) and plasma arc melting (PAM) are two relatively new secondary remelting processes used to improve the quality of titanium alloys by removing detrimental inclusions. EBM also produces nickel-base superalloy remelt stock. The heating source for EBM is an electron beam, and PAM is heated by a plasma arc generated by the ionization of helium and/or argon gases. Both processes use a water-cooled copper hearth to hold the molten metal. High density inclusions (HDI) such as tungsten carbide bits are removed since they sink to the bottom of the molten pool in the hearth. Refined clean molten metal then flows into an open mold to form a continuously cast ingot. EBM can cast both cylindrical ingots as well as rectangular slabs, whereas PAM currently can only cast cylindrical ingots. The application of EBM and PAM processed titanium alloys is primarily focused on the aerospace industry. EBM is also widely used to recycle commercially pure (CP) titanium.

C. Powder Metallurgy Products

Conventional and advanced powder metallurgy (PM) products have very different processing routes as well as properties. In addition, their intended markets are also different. Spray forming is a relatively new process derived from the advanced PM process.

1. Conventional Powder Metallurgy

The conventional PM process uses sintering to consolidate powders to form complex shaped components. Because sintering is not a melting and solidification process, the density of the resultant PM components is lower than the alloy theoretical density; these components contain porosity and are not fully dense. As a result, the mechanical properties of conventional PM products are lower than those of wrought products made from the same alloys. Sometimes a close die forging operation is used to forge PM preforms to produce components with improved mechanical properties. Powders are made by melt atomization as well as by hydrometallurgy processes. In general, conventional PM products are mostly used for high volume, complex shape, and relatively low mechanical property components. Both ferrous and nonferrous alloys are processed by conventional powder metallurgy.

2. Advanced Powder Metallurgy

The need for high mechanical properties is the primary driving force for using advanced PM products. For jet engine turbine disk applications, conventional superalloy disk alloys such as Inconel 718 and Waspaloy are produced by the VAR process. For alloys like IN100, MERL76, René 95, and René 88, a higher content of strengthening elements (aluminum and titanium) is used to develop superior mechanical strength and temperature capability. However, a higher strengthening element content also results in a stronger segregation tendency during solidification. The resulting ingots typically have an unacceptable forgeability for subsequent open die forging operations. As a result, these alloys cannot be produced by conventional secondary remelting processes (VAR and ESR); they have to be produced by advanced PM processes. In the advanced PM processing route, gas atomized or vacuum atomized powders are consolidated by hot compaction, hot isostatic pressing (HIP), or extrusion to produce fully dense billet material or disk preform. These billets or disk preforms have a forgeability that is significantly better than those of the wrought billets and can be easily close die forged to make the final disks. These disks have a uniform fine grain structure and no macrosegregation. Consequently, their mechanical properties are typically better than or equivalent to those of wrought products. The advanced PM process is primarily used for producing jet engine superalloy turbine disk materials, although some tool steels, high strength aluminum alloys, and titanium alloys are also amenable to this process.

3. Spray Forming

Although the advanced PM process can produce satisfactory products, its processing steps are complex and its production cost is high. Spray forming has the potential to make products with mechanical properties that are equivalent to those of advanced PM products, but at lower cost. The principle of spray forming is to use a mandrel or drum to catch molten metal droplets, produced by gas atomization, before they are completely solidified. The metal droplets hit the surface of the mandrel or drum, are flattened, and accumulate layer by layer to form billets or hollow cylindrical tubes/preforms. The billets can be used as input material for close die forging to make jet engine turbine disks. The tubes can be used in the as-sprayed condition whereas hollow cylindrical preforms can be ring-rolled to form engine frame components. Although superalloy components are the primary applications for spray forming, other high performance alloy components have also been produced by this process.

III. APPLICATION OF CASTING PROCESS MODELING

The application of casting process modeling in a production environment is not just a scientific exercise; it is an important technical step which can have a significant impact on the quality, yield, and hence, cost of the final products. To be successful in applying casting process modeling, process engineers need to have a good understanding of currently available technologies, and their capabilities and limitations, as well as their relevance to practical production issues. The following sections present general instructions on how to successfully apply casting process modeling in a production environment

A. Understanding the Role of Modeling

Modeling is a tool for helping engineers do a better job. As an engineering tool, modeling provides engineers with a way to understand the process dynamics and evaluate the quantitative effects of various process variables on the quality of the resulting products. Furthermore, casting modeling allows process engineers to make virtual castings and to optimize their casting process in terms of quality and yield without actually making castings. These capabilities make modeling more powerful than any other tools previously available to process engineers.

Because of its powerful capabilities, modeling is increasingly accepted as a technology which can improve quality and decrease cost in foundries and molten metal processing plants. For shape casting foundries, the combination of process modeling and rapid prototyping technology makes concurrent product and process development technologies a reality. The widespread use of casting process modeling has already made some positive impact on the production floors of foundries and molten metal processing plants. However, the powerful capabilities of process modeling also sometimes create a false understanding of the essence of modeling technology.

As powerful as it is, modeling is still just a tool. It is up to process engineers, not computers, to make the final decision. Modeling can be used to help process engineers develop new processes as well as optimize current production processes. However, the true power of modeling is in enhancing the engineer's understanding of process dynamics and ability to make a more intelligent judgment. The other important benefit of modeling is that it requires engineers to follow a strict discipline to define, as well as control, the process variables. This situation then results in lower variabilities in process control and product quality. Modeling should not be seen as providing a magic box where one can just push some buttons, and good results will automatically come out. Modeling should also not be treated as a panacea; not all the metal casting problems can be solved by modeling. The best way to apply casting process modeling is first to have a good understanding of the problem, and then to decide whether modeling can help. If the answer is yes, then the next step is to develop a suitable model to address that particular problem.

The justification for applying casting process modeling in foundries and molten metal processing plants is to provide process engineers with a better way to solve the complex technical problems they face in production. Thus, the usefulness of casting process modeling must be justified by its success in solving practical production problems. Having the capability to understand the heat transfer and fluid flow phenomena and to predict the mold filling sequence and molten metal pool profile is just a first step toward that goal. To be able to understand why, and predict when, defects will form is a further step in that direction, but it is still not enough. As one foundry manager once said: "We do not sell defects; we sell good castings." Process engineers have to demonstrate that they can use modeling results to develop a strategy for eliminating defects and producing good products quickly and cost effectively.

B. Possessing the Appropriate Technical Background

Casting and solidification processing involve many physical phenomena, such as fluid flow (mold filling, natural and forced convection), heat transfer, electromagnetic field, solidification, defect formation, and microstructure evolution. It is obvious that one who wants to perform casting process modeling needs a good understanding of the physical meaning as well as the mathematical representation of all these phenomena. In addition, one needs some background in the numerical analysis of differential equations and computer programming. However, it should be emphasized that, from an application point of view, process engineers should concentrate their efforts on understanding the problem, establishing an appropriate model to represent that particular problem, making sense out of the model prediction, and developing a strategy to solve the problem. Thus, process engineers should first have a very good understanding of the production process they are working on. They need just enough background in mathematical equations, numerical analysis, and computer programming techniques to allow them to effectively perform their own tasks. It is not necessary for process engineers to have a deep technical background in differential equation solving and computer code writing in order to perform casting process modeling.

C. Understanding Each Process's Unique Characteristics

Each casting and solidification process has its own unique characteristics that have a major influence on the quality of the resultant products. Understanding the unique characteristics of the particular process that one is using is the first step in establishing a proper model for successfully modeling that process.

1. Differences Between Shape and Ingot Castings

Shape casting processes involve complex shape components and require three-dimensional models to perform process simulation effectively. Model building activities, such as accurately, quickly, and cost effectively inputting the complex casting geometry into the model, as well as establishing a suitable finite element mesh, have a critical impact on the successful application of casting process modeling on the foundry floor. Electronic data interchange (EDI) and automated meshing technologies play major roles in these areas. On the other hand, ingot castings typically have simple geometries such as round, square, and rectangular cross-sectional shapes. In many instances, ingot casting processes can be effectively simulated by using two-dimensional models.

From the technical point of view, the mold filling events have a significant effect on the solidification conditions and structural integrity of shape castings. Once the mold is full, however, natural convection in the remaining molten metal plays only a minimal role in affecting casting quality. Conversely, the mold filling sequence generally has little effect on the structure of continuously or semicontinuously cast ingots, whereas the effect of natural convection can be significant, controlling the macrosegregation severity, especially in large size ingots. In addition, critical defects are also quite different for shape and ingot castings. For example, porosity (macroshrinkage and microporosity) is the most important defect in shape castings, but macrosegregation, which impacts ingot chemistry uniformity and formability in subsequent forging and rolling operations, is of primary concern for most ingots. Finally, shape castings are cast one by one, and always in a transient condition. As a result, true three-dimensional transient models are required. On the other hand, ingots are cast either in truly steady state conditions (continuous casting) or in quasi-steady state conditions (semicontinuous casting processes). In most cases, two-dimensional steady state models are adequate.

2. Differences Among Shape Casting Processes

The characteristics of the various shape casting processes are quite different; thus, different models are needed to effectively simulate the unique characteristics of each process. For example, the sand casting mold can be treated as having a semi-infinite thickness, and the temperature of the mold outer surface can be considered to be a constant. Thus, the boundary condition for the sand casting mold can be simply a constant temperature. Conversely, preheat temperatures for investment casting molds are quite high and the radiation heat transfer rate at the mold surface has a significant effect on the casting solidification conditions. Consequently, radiation view factor calculation is a very critical step on modeling the investment casting process. In addition, because the mold and the molten metal temperatures are quite close to each other, or even identical in directional solidification and single crystal casting processes, mold filling analysis is not needed for investment cast columnar grains and single crystal superalloy turbine airfoils. For metallic mold/die casting processes (die/squeeze casting, permanent mold casting, and SSM), since the mold/die is used repeatedly, the quasi-steady state temperature distribution in the mold/die has important effects on the solidification condition and quality of the resultant castings. Consequently, knowing how to establish an accurate quasi-steady state mold/die temperature distribution is crucial for accurately modeling metallic mold/die casting processes.

3. Differences Among Ingot Casting Processes

Conventional ingot casting is a discrete process; thus, a true transient model is needed. On the other hand, the continuous casting process takes place under truly steady state conditions and hence, a steady state model is commonly used. For semicontinuous casting processes (DC casting, VAR, ESR, EBM, and PAM), both steady state and transient phenomena are important. At the top of the ingot, it is critical to know how to establish an effective hot top procedure to reduce the size of the shrinkage pipe and increase the material yield.

Thus, a transient model is needed to simulate the hot top procedure. However, in the middle portion of the ingot, where a quasi-steady state condition is reached, the shapes of the liquid metal pool and the mushy zone are relatively constant. Thus, a steady state model can be used to predict the liquid pool and mushy zone profiles, as well as their impact on the macrosegregation pattern in the resultant ingot.

In the continuous casting and DC casting processes, the molten metal superheat and ingot casting speed are not related and can be specified independently. On the other hand, in the VAR and ESR processes, electrode melting and ingot casting rates are coupled and usually cannot be controlled independently. This situation leads to narrow processing windows to produce ingots with a desirable structure. In addition, the strong electromagnetic field in VAR, ESR, and PAM processes has important effects on fluid flow behavior and macrosegregation formation tendency in these ingots. Because VAR and ESR processes are primarily used to melt high performance and high segregation tendency alloys, such as superalloys, titanium alloys, and tool steels, macrosegregation has a major effect on the quality of the resultant ingots. Thus, developing a model which can provide an accurate way to evaluate the ingot macrosegregation formation tendency has very practical benefits for the VAR and ESR processes.

4. Differences Between Spray Forming and Casting Processes

Spray forming is a free form deposition process and does not produce products with highly precise geometrical dimensions. Many physical phenomena and defects (e.g., mold filling, shrinkage pipe and macrosegregation) associated with regular casting processes are not present in the spray formed products. Thus, the modeling approach for the spray forming process is quite different from those of the regular casting processes. The major technical challenge for modeling the spray forming process is to predict the molten metal droplet size distribution during gas atomization, the individual droplet cooling/solidification rate before it hits the mandrel/drum, and the consolidation condition of the metal droplets during the deposition process. Porosity formation is primarily due to the entrapment of gas during deposition, not the volumetric change during solidification.

D. Developing a Suitable Model

A "suitable model" has two different meanings. First, as discussed in the above sections, a suitable model should include all the technical features necessary to simulate the unique characteristics of a particular process. Second, a suitable model must simulate the dominant effects that impact current product quality.

Shape castings typically exhibit many different types of defects. However, in practice, process engineers can develop a process based on their experience to produce a particular casting with only one or two defects which are difficult to eliminate. Thus, a suitable model need only be established to eliminate those defects without causing any other defects to form. For example, superalloy single crystal turbine airfoils exhibit many defects such as microporosity, hot tears, cold cracking, dimensional distortion, equiaxed grains, freckles, and recrystallized grains. When making turbine airfoils with one particular alloy, René N6, freckles tend to form. The best approach to solve this problem is to develop a casting process, based on past experience, that can produce castings without any other types of defects, except freckles. Then a suitable model must be developed to eliminate the freckle problem without causing any other defects to form.

E. Ensuring the Model's Accuracy

Model predictions should always be compared with experimental results to ensure the accuracy of the model. Two methods can be used. In the first one, melt temperatures recorded by thermocouples as a function of time are compared with model-predicted cooling curves to verify the casting thermal history. This method is time consuming, very costly, and hence is not always feasible. The second method compares model-predicted defect formation tendency with foundry inspection results. This method is easier to perform and most commonly adopted by foundries. In practice, an approach commonly employed by production foundries is to first establish a baseline simulation condition by comparing the model predictions with foundry experimental results, including both thermocouple data and defect inspection records. Once an appropriate baseline model is established, various process parameters are modified to evaluate their effects on the defect formation tendency. These process parameters are then optimized to develop a process that produces defect-free castings. Finally, actual castings are poured and their inspection results are compared to the model predictions.

It should be noted that only "relatively good" accuracy is needed to verify the model. It is not necessary to have model predicted cooling curves perfectly match experimental thermocouple data. The other point worth mentioning is that modeling is best used to compare the relative differences between different sets of processing parameters and to indicate in which direction they should be modified. Eventually, process engineers need to evaluate all model-predicted results, make sense out of them, and settle on the final casting process.

F. Using Models to Solve Practical Problems

As mentioned earlier, casting process modeling is not just a scientific exercise; it can have an important impact on a company's production performance. Thus, the success of casting process modeling should be judged by its ability to solve practical problems. In general, casting process modeling can be used by process engineers to develop new processes, as well as optimize existing ones. In practice, however, there are some differences in this regard between shape casting processes and ingot casting processes.

For shape casting foundries, each component has its own unique geometry configuration and quality requirement, and hence each requires a unique process to obtain good castings. It is common for a foundry to have 30–50 different parts in production at the same time. As time goes on, some of the old parts drop out and new parts come in. As a result, developing a new casting process for a new part happens all the time. Consequently, the application of casting process modeling in shape casting foundries puts more emphasis on developing new processes than on enhancing existing ones.

In ingot casting, due to the simple geometry and large volume production rate, enhancing existing processes happens more frequently than developing new processes. For example, Inconel 718 and Waspaloy are two nickel-base superalloys which are widely used for jet engine turbine disk applications. For the last 30 years, these two alloys have been produced by the VAR process. The industry standard process is to melt a 432 mm (17 in.) diameter electrode in a VAR furnace to make a 508 mm (20 in.) diameter ingot. It can be seen that the need for developing a new process for this product is minimal. However, there are two separate requirements for enhancing the existing process. First, since the electrode is produced by the conventional ingot casting process, longitudinal shrinking pipe and horizontal cracks are sometimes present. During VAR processing, the shrinkage pipe and the cracks can cause arc instability and result in variability in ingot quality. The combination of process modeling and experimentation can provide an insight into understanding and developing a way to minimize this variability. Second, the current process needs to be modified to make ingots that are larger than the current 508 mm diameter. However, as the ingot diameter becomes larger, so does the tendency to form freckle-type defects. Process modeling is an effective way to simulate ingot solidification conditions and provide information for developing a modified process. One possible approach is to develop a modified process for the large diameter ingot, which has a similar Local Solidification Time (LST) as the currently produced 508 mm diameter ingot. Because the formation of freckles is related to the ingot LST, similar LST for both ingot sizes will increase the probability to produce freckle-free, large diameter ingots.

IV. SUMMARY

A general overview regarding the application of various casting and solidification processing processes in metal manufacturing, as well as instructions on how to effectively model these processes, has been presented. The following chapters will first introduce the general background on casting process modeling. The application of modeling to each specific process will then follow.

2

Fundamentals of Casting Process Modeling

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I. INTRODUCTION

Casting process modeling involves the simulation of mold filling and solidification of the cast metal. At the macroscopic scale, these processes are governed by basic equations which describe the conservation of mass, momentum, and energy. This chapter focuses on fundamentals of casting process modeling. Special emphasis will be placed on heat transfer (which is of obvious importance in solidification simulation), fluid dynamics (which is necessary to model mold filling and the natural convection which may occur during solidification), and general procedures for performing casting process modeling. Thermal-mechanical modeling (stress analysis) is described in Chapter 3. The modeling of microstructural evolution (micromodeling) is discussed in Chapter 5.

The chapter is outlined as follows. The fundamentals of heat transfer are first described in Sec. II and then applied to solidification heat transfer modeling in Sec. III. Next, the principles of fluid dynamics are presented in Sec. IV and applied to mold filling simulation in Sec. V. General numerical methods and special techniques used to solve the governing equations are then discussed in Secs. VI and VII. The types of commercially available software are described in Sec. VIII, and step-by-step modeling procedures are explained in the last section of the chapter.

II. HEAT TRANSFER

Heat transfer is perhaps the single most important discipline in casting simulation. The solidification process depends on heat transfer from the part to the mold and from the mold to the environment. There are three possible modes of heat transfer: (1) *conduction*, (2) *convection*, and (3) *radiation*. Conduction refers to the heat transfer that occurs as a result of molecular interaction. Conduction is important in modeling heat transfer in the cast part (both liquid and solid states) and is the primary mode of transfer through the mold (solid state only). Convection refers to heat transfer that results from the movement of a fluid. Convection heat transfer is important to the liquid metal both during mold filling (forced convection) and after the mold is filled (natural convection) as well as cooling of the mold exterior to the atmosphere. Radiation heat transfer refers to the transfer of electromagnetic energy between surfaces, a process which does not require an intervening medium. Radiation heat transfer is most important in investment casting processes. The different modes of heat transfer are described in the following subsections. The interested reader may consult one of several textbooks, such as Ref. 1, for additional details.

A. Conduction

The temperature at any point in a medium is associated with the energy of the molecules in the vicinity of the point. When molecules collide, energy is transferred from the more energetic (higher temperature) molecules to the less energetic (lower temperature) molecules. Thus conduction heat transfer must occur in the direction of decreasing temperature. The rate of heat transfer by conduction is given by Fourier's law:

$$\mathbf{q} = -k\nabla T \tag{1a}$$

In Cartesian coordinates,

$$q_x = -k\frac{\partial T}{\partial x} \qquad q_y = -k\frac{\partial T}{\partial y} \qquad q_z = -k\frac{\partial T}{\partial z} \tag{1b}$$

The above expression simply states that *heat flux* (heat transfer rate per unit area) is proportional to the temperature gradient. The proportionality constant k is the *thermal conductivity* of the material. The minus sign indicates that heat is transferred in the direction of decreasing temperature.

The differential equation describing heat conduction is given by

$$\rho c\frac{\partial T}{\partial t} + \nabla\cdot\mathbf{q} = \dot{Q} \tag{2a}$$

where $\dot{Q}$ is a heat generation term, ρ is the *density*, c is the *specific heat*, and t represents time. In Cartesian coordinates, the heat conduction equation is

$$\rho c \frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) - \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) - \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z}\right) = \dot{Q} \tag{2b}$$

The solution of the above equation in a given domain (region of space) requires knowledge of initial and boundary conditions. The *initial conditions* define the temperature distribution throughout the domain at some initial point in time. The *boundary conditions* describe the conditions that must be satisfied on the boundary of the domain. For equations such as Eq. (2), boundary conditions must be specified on the entire boundary. These conditions may describe (1) the value of the dependent (unknown) variable, (2) the value of the spatial derivative of the variable in a direction normal (perpendicular) to the boundary surface, or (3) a combination of these conditions. When applied to the heat conduction equation, these conditions become (1) prescribed temperature, (2) prescribed normal heat flux (which is a condition on the spatial derivative), and (3) a convection and/or radiation condition discussed in the following sections.

B. Convection

In addition to the energy transfer due to random molecular motion, energy is transferred by the bulk motion of a fluid. Convection heat transfer can be categorized as either forced or natural (free). The term *forced convection* is used when the flow is caused by some external means, such as a fan. The term *natural convection* is used when the flow is caused by buoyancy forces in the fluid.

Of particular interest is the heat transfer that occurs between a fluid (i.e., liquid metal) in motion and a stationary surface, such as the mold surface. In casting, liquid metal is in contact with the mold's interior surface and air (or possibly water) is in contact with the mold's exterior surface. In addition to a velocity boundary layer, a thermal boundary layer exists where the temperature varies from the surface temperature to the fluid freestream temperature. Heat transfer at the mold exterior could be determined by modeling the fluid dynamics and heat transfer in the fluid (air or water) in conjunction with the heat transfer in the solid (mold). Such an approach is fundamentally sound but requires a great deal of computational effort. The most common approach in this case is to approximate the heat flux at the solid surface using Newton's law of cooling:

$$q = h(T_s - T_\infty) \tag{3}$$

Here the *heat flux* (normal to the surface) is taken to be proportional to the difference between the surface and freestream fluid temperature. The proportionality constant h is the *convection heat transfer coefficient*. The value of this parameter depends on the nature of the fluid flow as well as the properties of the fluid and the solid.

Empirical relationships for the convection coefficient are frequently expressed in terms of certain dimensionless groups. For forced convection, the *Nusselt* number (Nu) is typically a function of the *Reynolds* (Re) and the *Prandtl* (Pr) numbers, defined as

$$\mathrm{Nu} = \frac{hL}{k} \qquad \mathrm{Re} = \frac{LV\rho}{\mu} \qquad \mathrm{Pr} = \frac{c\mu}{k} \tag{4}$$

where L is a characteristic length of the problem and V is the freestream velocity. The conductivity k, density ρ, specific heat c, and the viscosity μ are fluid properties. The convection coefficient for natural convection is generally given in terms of the *Grashof* number:

$$\mathrm{Gr} = \frac{g\beta\rho^2(T_s - T_\infty)L^3}{\mu^2} \tag{5}$$

where g is the gravitational acceleration and β is the coefficient of thermal expansion:

$$\beta = -\frac{1}{\rho}\left(\frac{\partial\rho}{\partial T}\right)_p \tag{6}$$

C. Radiation

Thermal radiation is energy emitted by all matter at temperatures above absolute zero. The energy of the radiation field is transported by electromagnetic waves and therefore does not require a material medium. The radiative heat flux emitted from a surface is given by

$$q = \varepsilon\sigma T_s^4 \tag{7}$$

where σ is the Stefan-Boltzmann constant ($\sigma = 5.67 \times 10^{-8}\ \mathrm{W/m^2\,K^4}$) and the *emissivity* ε is a radiative property of the surface. A perfect emitter (blackbody) has an emissivity value of unity. In many cases heat transfer due to radiation is negligible compared to convection. In other cases, such as vacuum investment casting processes, radiation is the dominant (perhaps the only) mode of heat transfer.

The above expression describes the radiation emitted by a surface. Determination of the net rate at which radiation is exchanged between surfaces is much more complicated. A rigorous approach involves determining a *radiosity* value for each surface element. The radiosity includes direct emission from the surface as well as the reflected portion of irradiation received by the surface. This method requires the simultaneous solution of radiosity values for each surface element. Since each element interacts with many other elements, this approach can be very computationally demanding for three-dimensional problems.

A frequently used alternative approach is to approximate the radiative heat flux from a surface element to the surrounding environment as

$$q = F\varepsilon\sigma(T_s^4 - T_\infty^4) \tag{8a}$$

where F (radiation view factor) is the fraction of radiation leaving the surface which reaches the surroundings. The view factor F is necessary in order to account for obstructions in the view path. The above expression may be cast in the following convective form:

$$q_{\text{rad}} = h_{\text{rad}}(T_s - T_\infty) \tag{8b}$$

by defining a radiation coefficient as

$$h_{\text{rad}} = F\varepsilon\sigma(T_s^2 + T_\infty^2)(T_s + T_\infty) \tag{9}$$

III. SOLIDIFICATION

Solidification modeling involves the application of the heat transfer concepts described in the previous section along with techniques to account for the release of latent heat during solidification. The mold and any other solid materials (chill, insulation, etc.) are modeled using the standard heat conduction equation (2). For the solidifying metal, special procedures are required to accurately model the latent heat release.

A. Fraction of Solid

The extent of solidification at any location within the casting is represented by the *fraction of solid* f_s. At temperatures greater than or equal to the *liquidus* temperature, the cast metal is in a completely liquid state with a solid fraction value of zero. As the latent heat is removed, the fraction of solid increases and reaches a value of unity when the metal is in a completely solid state. The temperature at this point is called the *solidus*. The region where the solid fraction is between zero and unity is referred to as the *mushy zone*.

One of two approaches may be used to determine the solid fraction value.

1. *Solid Fraction–Temperature Equilibrium*

With this widely used approach the solid fraction is assumed to be a known function of temperature, essentially a temperature dependent "property" of the metal. There are several ways to describe the solid fraction variation between the liquidus and solidus temperatures. The simplest approach is to assume that the solid fraction varies linearly in the mushy zone. Alternatively, an analytical expression such as the Scheil equation [2] may be used. Perhaps the best approach is to determine the solid fraction–temperature relationship using experimental measurements.

2. *Solidification Kinetics*

The previously described method is simple but only approximate. The reality of the solidification process is that the solid fraction evolves in time in a manner that depends on several parameters. The solidification kinetics approach involves the time integration of a solid fraction evolution equation [3]. This approach permits the accurate prediction of phenomenon such as undercooling. However, the solidification kinetics approach requires detailed metallurgical data which may not be known. Readers interested in the modeling of solidification kinetics can refer to Chapter 5 and Ref. 3.

B. Latent Heat

The release of latent heat during solidification can be accounted for by a heat "generation" term:

$$\dot{Q} = \rho \, \Delta H_f \, \frac{\partial f_s}{\partial t} \tag{10}$$

where ΔH_f represents the latent heat of solidification. The above expression assumes that the latent heat varies in proportion to the solid fraction, which is a reasonable approximation for casting process modeling. There are three common methods of incorporating the latent heat term given by Eq. (10) into the heat conduction equation (2) [4–7].

1. *Latent Heat Source Term*

Here the latent heat release is treated as a source term and is determined from known parameters (not dependent on the unknown temperature). Substituting Eq. (10) into Eq. (2b) yields:

$$\rho c \frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) - \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) - \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z}\right) = \rho \Delta H_f \frac{\partial f_s}{\partial t} \tag{11}$$

This method is commonly used to couple the solidification kinetics approach described in the previous section with a general heat transfer solver.

2. *Apparent Specific Heat*

The latent heat release rate described by Eq. (10) depends on the change in solid fraction which depends on the temperature change. It is therefore necessary to include this temperature dependency on the left-hand side of Eq. (11). The latent heat release rate can be expressed as

$$\rho \Delta H_f \frac{\partial f_s}{\partial t} = \rho \Delta H_f \frac{\partial f_s}{\partial T} \frac{\partial T}{\partial t} \tag{12}$$

The above term can be included in the left-hand side of Eq. (11) by defining an apparent specific heat as

$$c_{\text{app}} = c - \Delta H_f \frac{\partial f_s}{\partial T} \tag{13}$$

For the case where the solid fraction is assumed to vary linearly between liquidus and solidus, the above expression becomes

$$\begin{aligned} c_{\text{app}} &= c + \frac{\Delta H_f}{\Delta T} \qquad && T_s < T < T_l \\ c_{\text{app}} &= c && T \leq T_s \text{ or } T \geq T_l \end{aligned} \tag{14}$$

where ΔT is the difference between the liquidus and solidus temperatures.

The apparent specific heat method is easily implemented as a modification to the temperature dependent specific heat values. Although simple to implement, the method may develop problems when the solidification range ΔT is small. The first problem is one of iterative convergence. A frequently encountered condition is one where some of the temperature values "jump" back and forth (around the mushy zone) and fail to converge to a particular value. The second problem is that it is possible for a temperature value to prematurely jump below the solidus temperature and miss some of the latent heat release. Modifications that improve the performance of the basic method are described in Ref. 4.

3. *Enthalpy Method*

The enthalpy method is currently the most common approach used to model latent heat release during solidification. With this method the latent heat is included in the definition of enthalpy:

$$H(T) = \int_{T_{ref}}^{T} c(T)\,dT + (1 - f_s)\,\Delta H_f \tag{15}$$

and the heat conduction equation is expressed as

$$\rho \frac{\partial H}{\partial t} - \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) - \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) - \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z}\right) = 0 \tag{16}$$

The method involves iteration between temperature and enthalpy values until convergence is achieved. The enthalpy method ensures that all of the latent heat release is accounted for, even when fairly large time steps are used in the calculation.

C. Initial and Boundary Conditions

1. Initial Conditions

The most accurate method of determining the initial conditions is to perform a mold filling simulation (described in Sec. V). The temperature distribution at the end of the mold filling simulation will then serve as the initial temperature distribution for the solidification simulation. However, because of the computational demand, the mold filling simulation is frequently omitted and some reasonable initial temperature values are used. For the cast metal, the initial temperature usually is set somewhere between the liquidus temperature and pouring temperature, depending on the estimated loss of superheat during mold filling. The initial mold temperature depends on the type of casting. For sand castings the initial mold temperature will most likely correspond to the ambient temperature. For investment castings, the mold is preheated to a specified temperature which depends on the metal to be cast. Permanent mold and die castings typically have high production rates and therefore the mold achieves a quasi-steady thermal condition after several castings have been poured. It may be necessary to perform several simulations to accurately determine the thermal condition of the mold. Interested readers can refer to the appropriate chapters of this book.

2. Boundary Conditions

a. Mold Exterior. Although the temperature or heat flux can be prescribed at the mold exterior, the convective condition given by Eq. (3) is most frequently employed. The data shown in Table 1, taken from Ref. 6, should serve as a guide in determining the convection coefficient.

In some casting processes, such as investment casting, heat loss due to radiation is more significant than convection. For these cases, the radiation

Table 1 Convection Heat Transfer Coefficients

Mode	h ($W/m^2\,°C$)	h ($Btu/hr\,ft^2\,°F$)
Free convection, $\Delta T = 30°C$		
Vertical plate 0.3 m (1 ft) high in air	4.5	0.79
Horizontal cylinder, 5 cm diameter, in air	6.5	1.14
Forced convection		
Airflow at 2 m/s over 0.2 m^2 plate	12	2.11
Airflow at 35 m/s over 0.75 m^2 plate	75	13.17
Air at 2 atm flowing in 2.5 cm diameter tube at 10 m/s	65	11.41
Airflow across 5 cm diameter cylinder at 50 m/s	180	31.60

Source: Ref. 6.

condition given by Eq. (8) may be used to replace or perhaps supplement the convection condition.

b. Metal/Mold Interface. The metal and mold are generally not in perfect contact and therefore a temperature discontinuity exists at the metal/mold interface or gap. If the characteristics of the gap such as the thickness variation with time and the properties of the gas within the gap were known, then the heat transfer across the gap could be computed directly. A much simpler and more common approach is to express the interfacial heat flux as

$$q = h_{gap}(T_c - T_m) \tag{17}$$

where T_c and T_m are the temperatures of the casting surface and mold surface, respectively. The gap heat transfer coefficient h_{gap} must be determined empirically. Typical values, taken from Ref. 6, are given in Table 2.

The actual gap heat transfer coefficient depends strongly on the state of the solidifying metal. Although there is generally no gap at temperatures above the liquidus temperature, thermal contact between the casting and the mold is imperfect because of surface tension effects, oxide layers, and mold coatings. The gap coefficient is therefore fairly large, but not infinite. In the mushy region, there is partial contact between the surfaces resulting in a lower gap heat transfer coefficient. Below the solidus temperature, it can be assumed that a gap has formed causing heat loss by convection and radiation. All of this behavior can be modeled using a gap heat transfer coefficient which is dependent on metal surface temperature, as shown in Fig. 1. Such temperature dependent coefficients have been determined using an inverse heat transfer approach [7].

Table 2 Metal/Mold Interface Heat Transfer Coefficients h_{gap}

Casting situation	h_{gap} (W/m^2 °C)	h_{gap} (Btu/hr ft^2 °F)
Ductile iron in cast iron mold coated with amorphous carbon	1709	300
Steel in cast iron mold	1025	180
Aluminum alloy in small copper mold	1709–2563	300–450
Steel chilled by steel mold		
Before gap forms	399–1025	70–180
After gap forms	399	70
Aluminum die castings		
Before gap forms	2506–5012	440–880
After gap forms	399	70

Source: Ref. 6.

c. Cast Metal Surface. At the inflow surface and open risers, the cast metal is exposed to the ambient, typically air. The heat transfer at these surfaces may be considered negligibly small, or can be modeled using a convection boundary condition.

D. Approximate Analysis

With certain assumptions, it is possible to obtain an analytical solution to the heat transfer problem. The results of such analysis may be used to develop quick and approximate methods which are discussed in Chapter 7. These approximate solutions are also sometimes used to avoid the expense of actual

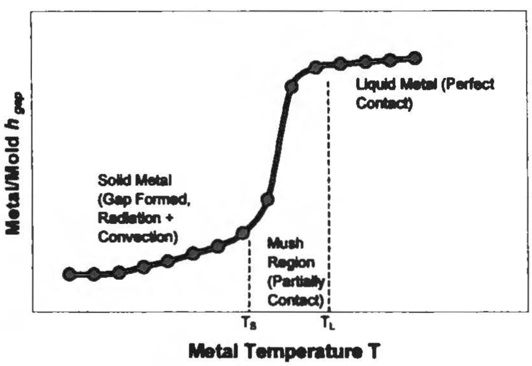

Figure 1 Metal/mold interfacial heat transfer coefficient as a function of temperature.

modeling the mold region. In these cases, only the part region is modeled and the heat flux at the part surface is approximated using analytical expressions. Such methods are most commonly used to approximate solidification in thick molds, which can be approximated as infinitely thick. Assuming constant values for the metal temperature (melting point) and mold thermal properties, analytical solutions can be obtained for castings of simple geometry. For example, the heat flux from a spherical casting surface into a concave, spherical mold wall is given by [8]

$$q = k(T_s - T_i)\left(\frac{1}{R} + \frac{1}{\sqrt{\pi \alpha t}}\right) \tag{18}$$

where T_s is the temperature of the mold surface, T_i is the initial mold temperature, R is the radius of the spherical mold surface, and α is the thermal diffusivity of the mold. Equation (18) can be employed to approximate the heat flux on surfaces of arbitrary geometry by substituting the surface radius of curvature for R in the above expression.

IV. FLUID DYNAMICS

Both the mold filling process and the natural convection that may occur during casting are governed by general fluid dynamics principles [9, 10]. In this section the governing equations of fluid dynamics are presented and several important concepts are discussed.

A. Fluid Dynamics Equations

In general, the equations which describe fluid dynamics are more complicated and require greater computational effort to solve than the heat conduction equation (2). In conservative form, the governing equations can be expressed as [11]

1. Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0 \tag{19}$$

   where $\mathbf{V}$ is the velocity vector. Equation (19) is known as the continuity equation.

2. Conservation of momentum:

$$\frac{\partial}{\partial t}(\rho \mathbf{V}) + \nabla \cdot (\rho \mathbf{V}\mathbf{V} - \mu \nabla \mathbf{V}) + \nabla P = \mathbf{B} + \mathbf{S}_v \tag{20}$$

where P is the pressure, $\mathbf{B}$ is the body force vector, and $\mathbf{S}_v$ consists of viscous terms other than those expressed by $\nabla \cdot (\mu \nabla \mathbf{V})$. The body force vector typically includes the force of gravity $\mathbf{B} = \rho \mathbf{g}$, but may also include other terms such as Coriolis and centrifugal forces in the case of a rotating frame of reference or forces induced by electromagnetic fields. Equation (20) is a vector equation, describing the conservation of momentum in the three coordinate directions. These equations are known as the Navier-Stokes equations.

3. Conservation of energy:

$$\frac{\partial}{\partial t}(\rho H) + \nabla \cdot (\rho \mathbf{V} H - k \nabla T) = S_e \tag{21}$$

where S_e is a source term which may include internal heat generation, viscous dissipation, and other effects.

Equations (20) and (21) may be expressed in the following general form:

$$\frac{\partial}{\partial t}(\rho \phi) + \nabla \cdot \mathbf{J} = S \tag{22}$$

where ϕ is a general dependent variable and $\mathbf{J}$ is a flux vector which consists of convection and diffusion fluxes. The above equations are written in (flux) conservative form. The equations may also be expressed in nonconservative form. For example, using the continuity equation (19), the energy equation (21) may be expressed as

$$\rho \frac{\partial H}{\partial t} + \rho \mathbf{V} \cdot \nabla H - \nabla \cdot (k \nabla T) = S_e \tag{23}$$

Numerical formulations based on finite/control volume concepts (discussed in Sec. VI) are always applied to equations expressed in conservative form. Other numerical methods may be applied to the equations in conservative or nonconservative form.

Appropriate initial and boundary conditions are required to obtain a solution to the fluid dynamics problem. The conditions required to solve the energy equation are the same as described for the heat conduction equation (2). The initial velocity of the fluid is generally taken to be zero. For an internal flow problem, boundary conditions must be prescribed along the walls and at the inflow and outflow regions. For an inviscid fluid, the velocity normal to stationary solid walls must be zero, but the tangential components are not constrained (slip is permitted). For a viscous fluid, all velocity components should be zero (no-slip condition). In practice, however, some type of slip condition is sometimes permitted for high Reynolds number cases. At porous walls, the normal component of velocity is prescribed. At the inflow and outflow boundaries either the velocity or the pressure is required.

B. Types of Fluid Flow

Fluid flow can be described as either compressible or incompressible. The fluids in compressible flows are frequently gases that obey an equation of state which relates the density to the pressure and temperature. For incompressible flows, the fluid density is considered to be independent of pressure. Most liquid flows are considered incompressible because the fluid density is essentially independent of pressure. In casting processes, the metal flow is treated as incompressible, although the density is generally temperature dependent.

Fluids are commonly categorized according to their viscous behavior. A fluid is referred to as a *Newtonian fluid* if the viscous stress varies linearly with the shear rate. Simple fluids such as water, oils, gases, and most liquid cast metals are considered to behave in this manner. Other materials whose viscous stress varies nonlinearly with the shear rate are called *non-Newtonian fluids*. The interested reader may refer to a fluid dynamics text such as Ref. 12 for additional details.

Fluid flow may be classified as either laminar or turbulent. Laminar flow is characterized by smooth and predictable movement of fluid particles. In contrast, turbulent flow is erratic and chaotic with the velocity of the fluid fluctuating in an apparently random manner. The transition from laminar to turbulent flow is associated with some critical value of the Reynolds number. For example, for flow in a pipe, the critical Reynolds number is found to be between 2000 and 13,000, depending upon the smoothness of the entrance conditions and wall roughness [13].

It is generally believed that the governing equations (19) to (21) describe turbulent flows completely. A direct numerical approach is impractical, however, because turbulent motion involves both large and extremely small length and time scales. The current practice is to describe turbulent motion in terms of time-averaged quantities rather than instantaneous ones. The instantaneous quantities are expressed as the sum of the time-averaged value and a fluctuation. Due to the nonlinearity of the governing equations, this process leads to a number of unknown correlations between the fluctuating components of velocity and temperature. Turbulence modeling involves approximating these correlations by expressing them in terms of mean-flow quantities [13].

One of the best known turbulence models is known as the k-ε model [9]. In this model, the turbulence field is characterized in terms of two variables, the turbulent kinetic energy k and the viscous dissipation rate of turbulent kinetic energy ε. A turbulent viscosity μ_t can be directly related to the turbulent quantities k and ε. It is necessary to solve equations for the turbulent quantities in addition to the basic conservation equations. These equations involve a number of turbulence model "constants" which can only be determined empirically. Fortunately, the fluid flow during casting is generally laminar. However, turbulence is experienced in certain cases such as a mold filling simulation for die casting.

V. MOLD FILLING SIMULATION

The simulation of mold filling involves the application of the fluid dynamics principles described in the previous section along with methods to model free surface dynamics and account for factors unique to the casting process.

A. Free Surface Modeling

Modeling the free surface dynamics during mold filling is one of the most challenging aspects of casting process simulation. Although many methods have been proposed to model free surface flow problems, the volume of fluid (VOF) method developed by Hirt [14] is most commonly used. With this method, a fractional VOF function F is employed, where fluid (liquid metal) regions are assigned values of $F = 1$ and gas (typically air) regions are assigned values of $F = 0$. A region, such as a computational cell, with $0 < F < 1$ is considered to be partially filled with liquid. The VOF equation is obtained by applying the continuity equation (19) to the fluid region:

$$\frac{\partial(\rho_l F)}{\partial t} + \nabla \cdot (\rho_l \mathbf{V} F) = 0 \tag{24}$$

where ρ_l is the density of the liquid (metal). The free surface is tracked by solving Eq. (24) for the VOF function F along with the basic governing equations. Solution of the above equation requires special techniques to ensure that there are no overshoots ($F > 1$) or undershoots ($F < 0$) and that there is little "smearing" in the solution. At the free surface, the VOF function should sharply change from $F = 1$ on the liquid side to $F = 0$ on the gas side. Standard solution methods which avoid overshoots and undershoots typically result in significant "smearing" (spreading of fluid) over several mesh cells. Accurate free surface modeling requires that special methods be employed to eliminate or greatly reduce the level of smearing.

B. Back Pressure Modeling

During mold filling, the gas (typically air) present in the mold escapes through vents and through the mold itself, if porous. In sand and lost foam casting processes the mold is porous and generally does not require venting. Investment, die, and permanent mold castings require vent holes to permit the gas to escape. If not adequately vented, gas pressure will build up, preventing normal mold filling. Furthermore, the entrapped gases result in high levels of porosity. Gas flow through a porous mold can be approximated using D'Arcy's law [15]:

$$V = \frac{p \, \Delta P}{\mu L} \tag{25}$$

where p is the specific permeability of the mold, ΔP is the pressure drop across the thickness of the mold L, and μ is the viscosity of the gas. A similar equation can be used to describe gas escape through vent holes. The gas pressure could be modeled directly using the fluid dynamics equations along with a gas equation of state. Equation (25) would serve as a boundary condition to apply at the part/mold interface. This approach is generally not taken, however, because of the large computational cost involved. Instead, the fluid dynamics equations are typically solved only in the liquid metal region. The gas pressure can be estimated from knowledge of the volume of gas and the change in gas mass as a result of venting.

C. Effect of Solidification on Fluid Flow

The fact that the liquid metal is in the process of solidification must be accounted for in the fluid dynamics computations. This effect may be accounted for by using an apparent viscosity model where the viscosity would increase rapidly as the solid fraction increased, becoming very large at some critical solid fraction value. A more common approach is to use an interdendritic fluid flow model [16]. Here it is assumed that interdendritic flow behaves like flow through a porous material. This assumption results in a friction drag term to be added to $\mathbf{S}_v$ in Eq. (20).

D. Initial and Boundary Conditions

The heat transfer conditions were described in Sec. III.C. The fluid flow and free surface modeling conditions are described below.

1. *Initial Conditions*

Generally the liquid metal is assumed to be initially at rest. The VOF function is initialized depending on the actual conditions. Frequently, a region such as a pouring basin will be assumed to be filled with liquid metal at the start of the simulation.

2. *Boundary Conditions*

a. Inflow. Inflow conditions can involve a known pressure or fluid velocity, which may be determined from the average pouring rate. In some cases, a relationship between the pressure and entrance velocity is determined based on approximate analysis [17].

b. Part/Mold Interface. For the liquid metal, a no-slip condition can be imposed or a partial slip condition may be employed. Gas escape through the mold may be modeled using Eq. (25).

c. Gas Escape Vents. Gas escape through vents may be modeled by using an equation similar to Eq. (25).

d. Liquid Metal Free Surface. The total stress must be continuous across the free surface. This condition establishes a relationship between the liquid viscous stress, liquid pressure, gas pressure, and surface curvature if surface tension is taken into account. The gas pressure may be computed as described in Sec. V.B, or may be assumed equal to the ambient pressure if the mold is well vented.

VI. DISCRETIZATION OF THE GOVERNING EQUATIONS

Discretization involves representing the continuous variables with a number of discrete values associated with the cells (elements) or vertices (nodes) of a computational grid (mesh). Through this process, the differential equations are approximated by a set of algebraic equations, which may be solved for the unknown discrete values.

A. Grid Structure

Computational grids may be classified as structured or unstructured [18]. In structured grids, all the mesh points lie on the intersection of curvilinear coordinate lines. One of two approaches may be used to generate a structured grid for a domain of arbitrary geometry. A two-dimensional example of the first approach is illustrated in Fig. 2. Here a regular grid is overlaid on the problem geometry. Curved boundaries are approximated by a "stair step" type of pattern. This meshing approach is fast and easy to implement, but the representation of the boundary surface is only approximate. With the second approach, a grid is constructed which conforms to the problem geometry. In this case, the boundary representation is very accurate, but the mesh generation procedure is more complex. For most practical problems, it is necessary to divide the domain up into a number of "blocks" and mesh each block separately.

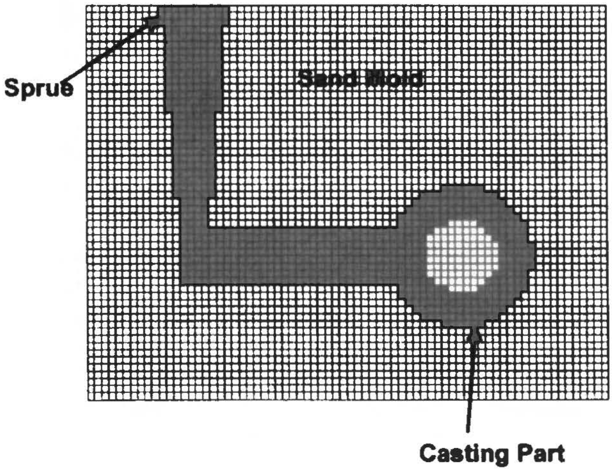

Figure 2 A structured two-dimensional mesh of a cast part and its sand mold.

When applied to three-dimensional problems, this approach can be extremely time consuming.

An unstructured (finite element type) grid for the same geometry is illustrated in Fig. 3. Here the domain may be approximated by triangular and/or quadrilateral cells. A three-dimensional domain may be represented by a combination of hexahedron (brick), triangular prism (wedge), and tetrahedron elements. A typical three-dimensional finite element mesh is shown in Fig. 4. An unstructured mesh permits an accurate representation of geometry, but can be time consuming to generate. In two dimensions, automatic mesh generators generally perform very well for quadrilateral as well as triangular elements. In three dimensions, fully automatic mesh generation is possible only with tetrahedral elements. It should be pointed out that the results obtained from properly constructed quadrilateral (2-D) and brick (3-D) meshes are generally superior to those obtained using triangular and tetrahedral elements, respectively. The superior accuracy stems from both the regularity of the mesh (formal accuracy) and the ability to grade or refine the mesh in regions where the variables are expected to change rapidly.

The vast majority of casting simulation software employ either (1) a regular overlaid structured grid or (2) an unstructured (finite element type) grid. Both approaches have certain advantages and disadvantages. A regular grid is easily generated, but may require an extremely large number of cells to adequately represent castings of complex geometry. A high quality unstructured grid generally requires quite a bit of time to generate, but permits very

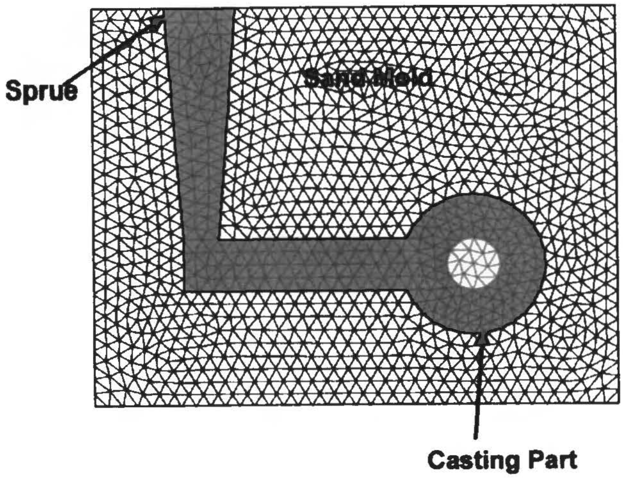

Figure 3 An unstructured two-dimensional mesh of the cast part and mold shown in Fig. 2.

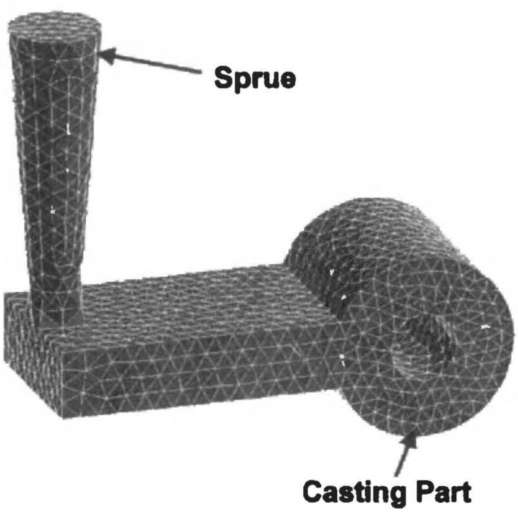

Figure 4 An unstructured three-dimensional mesh of a casting part.

accurate representation of the domain. Unstructured codes require greater memory and CPU time per element (cell) than structured codes, but generally use a mesh of variable density which requires fewer total elements.

B. Spatial Discretization

The three most common numerical methods for fluid flow and heat transfer analysis are the *finite difference method* (*FDM*), *finite (control) volume method* (*FVM*), and *finite element method* (*FEM*) [18]. The various methods will be illustrated using the following one-dimensional model equation:

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \tag{26}$$

The finite difference method uses a structured grid and is perhaps the simplest method to understand and implement on problems of simple geometry. In basic terms, the method consists of replacing the derivatives in the differential equations by finite difference approximations. For example, the second derivative can be approximated using the following central difference formula:

$$\frac{\partial^2 \phi_i}{\partial x^2} \cong \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} \tag{27}$$

where a value of the dependent variable ϕ is associated with each cell or grid point and Δx is the mesh spacing. The formal accuracy of the above expression is said to be of second order. An expression is accurate to order n provided $|\mathrm{TE}| \leq K|\Delta x|^n$ as $\Delta x \to 0$ (sufficiently small Δx) where K is a positive constant, independent of x. The *truncation error* (*TE*) is the difference between the partial derivative and its finite difference representation. Substituting the finite difference expression into Eq. (26) results in an algebraic equation:

$$\dot{\phi}_i - \alpha \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} = 0 \tag{28}$$

where $\dot{\phi}_i$ represents the time derivative at point i. A discretized equation is written for each cell or grid point in the mesh. The resulting set of algebraic equations are then solved for the unknown ϕ_i values.

The finite (or control) volume method is a generalization of the finite difference method that may be used with either structured or unstructured grids. The unknowns are typically associated with the cells and are considered to represent the cell average value rather than the value at a particular point. Integrating Eq. (26) over the control volume,

$$\frac{\Delta x}{\alpha}\dot{\phi}_i = \int_{x-\Delta x/2}^{x+\Delta x/2} \frac{d^2\phi}{dx^2}\,dx = \left.\frac{d\phi}{dx}\right|_{i+1/2} - \left.\frac{d\phi}{dx}\right|_{i-1/2}$$

$$\cong \frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\phi_i - \phi_{i-1}}{\Delta x} \tag{29}$$

$$\dot{\phi}_i - \alpha\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} = 0 \tag{30}$$

Note that for this case the finite volume result, Eq. (30), is identical to the finite difference result, Eq. (28). The key feature of the approach is that the finite volume method is based on flux integration over the control volume surfaces. The method is implemented in a manner that ensures local flux conservation, regardless of the grid structure.

The finite element method is an inherently unstructured method that generally employs some type of weighted integral solution:

$$\int_\Omega W_i\left(\frac{\partial\phi}{\partial t} - \alpha\frac{\partial^2\phi}{\partial x^2}\right) d\Omega = 0 \tag{31}$$

where Ω represents the computational domain and W_i is a weight function. When the weight functions are chosen to be the same as the nodal interpolation functions, the method is referred to as the Galerkin finite element method [18]. Applying this method with linear interpolation between nodes yields the following algebraic equation:

$$\frac{1}{6}\dot{\phi}_{i-1} + \frac{2}{3}\dot{\phi}_i + \frac{1}{6}\dot{\phi}_{i+1} - \alpha\,\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} = 0 \tag{32}$$

Note that the standard finite element method expresses the time derivative term as a kind of weighted average. This is referred to as a "consistent mass" formulation. Frequently a "lumped mass" approximation is used, which for this case produces results identical to the finite difference and finite volume formulations.

When applied to a simple one-dimensional diffusion equation with constant properties on a regular grid, the finite difference, finite volume, and finite element (with mass lumping) methods produce identical discretized equations. However, when applied to multidimensional problems with variable properties and grids, the methods in general result in different algebraic equations.

C. Convection Modeling

In this section the finite difference and finite volume methods are applied to a model convection problem in two dimensions which can be expressed as

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} = 0 \tag{33a}$$

in nonconservative form, and

$$\frac{\partial \phi}{\partial t} + \frac{\partial (u\phi)}{\partial x} + \frac{\partial (v\phi)}{\partial y} = 0 \tag{33b}$$

in conservative form. For this example the velocity is assumed to be a known function of space and time. The numerical methods will be applied using a regular mesh with cells of size $\Delta x \cdot \Delta y$. The index i will be used to number cells in the x direction, and the index j will be used to number cells in the y direction.

Consider the finite difference approximation in nonconservative form using Eq. (33a). Assuming that both components of velocity are positive, an "upwind" difference equation is

$$\frac{\partial \phi_{i,j}}{\partial t} + u_{i,j}\,\frac{\phi_{i,j} - \phi_{i-1,j}}{\Delta x} + v_{i,j}\,\frac{\phi_{i,j} - \phi_{i,j-1}}{\Delta y} = 0 \tag{34}$$

The one-sided differencing of the first derivatives is referred to as "upwinding." In this case, "full upwinding" is used, which means that downstream values of ϕ (such as $\phi_{i+1,j+1}$) are not permitted to have any influence on the solution for $\phi_{i,j}$. This treatment of the convective terms results in a monotone (oscillation free) solution, but is formally only first-order accurate.

A finite volume expression analogous to Eq. (34) is obtained by considering the integral form of Eq. (33b):

$$\int_\Omega \frac{\partial \phi}{\partial t} + \int_\Gamma \phi_{uw} \mathbf{V} \cdot d\Gamma = 0 \tag{35}$$

where Ω represents the finite volume and Γ represents the surface of the volume. The expression ϕ_{uw} indicates that an upwind value of the dependent variable is to be used. Application of Eq. (35) yields:

$$\begin{aligned} \Delta x\,\Delta y \frac{\partial \phi_{i,j}}{\alpha t} + \Delta y\, u_{i+1/2,j}\phi_{i,j} + \Delta x\, v_{i,j+1/2}\phi_{i,j} - \Delta y\, u_{i-1/2,j}\phi_{i-1,j} \\ - \Delta x\, v_{i,j-1/2}\phi_{i,j-1} = 0 \end{aligned} \tag{36}$$

Upon dividing by the volume $\Delta x\,\Delta y$, we obtain

$$\frac{\partial \phi_{i,j}}{\partial t} + \frac{u_{i+1/2,j}\phi_{i,j} - u_{i-1/2,j}\phi_{i-1,j}}{\Delta x} + \frac{y_{i,j+1/2}\phi_{i,j} - v_{i,j-1/2}\phi_{i,j-1}}{\Delta y} = 0 \tag{37}$$

Several mold-filling codes have been developed based on the SOLA-VOF approach [13], which uses finite difference expressions very similar to Eq. (34). More recently developed codes are based on conservative finite volume equations similar to Eq. (37). Note that when applied to a regular grid under conditions of constant velocity, the two methods produce identical results.

The above expressions for the convective terms are only of first-order accuracy, which has the effect of adding "false viscosity" to the equations. To correct this deficiency, upwinding schemes of second-order accuracy [19] may be found in general computational fluid dynamics (CFD) codes. To the authors' knowledge, such schemes have not been used in commercial casting simulation software.

D. Time Integration

The equations which describe the casting process are partial differential equations of the following form:

$$\frac{\partial \phi}{\partial t} = f\left(\phi, \frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}, \frac{\partial^2 \phi}{\partial x^2}, \ldots\right) \tag{38}$$

The above expression states that the time rate of change of the variable is some function f of the variable itself and the spatial derivatives of the variable. Discretization of the spatial derivatives by finite difference, finite volume, and finite element methods were described in the previous sections. We now consider the treatment of the transient aspect of the equations. The time derivative can be approximated as

$$\frac{\partial \phi}{\partial t} \cong \frac{\phi^{n+1} - \phi^n}{\Delta t} \tag{39}$$

where the superscript n refers to the time level and the time step $\Delta t = t^{n+1} - t^n$. The function f in Eq. (38) can be evaluated using either *explicit* or *implicit* time integration.

When explicit time integration is used, the function f is evaluated at time level n:

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = f^n \tag{40}$$

Explicit time integration permits the direct advancement of the solution using only values at time level n. A disadvantage of this approach is that the time step must be limited in order to obtain stable results. For example, consider the limits for (1) convection and (2) conduction in one dimension. For convection (with full upwinding), the following condition must be satisfied:

$$\frac{u\,\Delta t}{\Delta x} < 1 \tag{41}$$

which is known as the CFL condition (named after Courant, Friedrichs, and Lewy) [20]. For conduction, the time step restriction is given by

$$\frac{\alpha\,\Delta t}{\Delta x^2} < \frac{1}{2} \tag{42}$$

where α is the thermal diffusivity $\alpha = k/\rho c$.

With implicit time integration, the function f is generally evaluated using a weighted average of the values at time level n and $n+1$:

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \theta f^{n+1} + (1-\theta) f^n \tag{43}$$

Selecting the implicit factor θ to be unity results in a "fully implicit" scheme, whereas selecting θ to be zero reduces to the explicit scheme. The scheme is unconditionally stable for $\frac{1}{2} \leq \theta \leq 1$, although accuracy considerations may place limits on the permissible time step size. The time integration is first-order accurate for all values of θ except $\theta = \frac{1}{2}$, which is second-order accurate. Although formally less accurate, values of θ greater than $\frac{1}{2}$ are often used to reduce or eliminate numerical oscillation in the initial transient solution. The cost to be paid for the unconditional stability of the implicit approach is the requirement to solve a system of simultaneous equations for the unknown ϕ^{n+1} quantities at each time step.

Mold filling is generally characterized by convection dominated free surface flow. For this type of simulation, explicit time integration may be used to accurately model the free surface movement and correctly predict the liquid metal temperature distribution. For conduction-dominated solidification, implicit time integration is often used in order to permit time steps much larger than the explicit limit.

VII. SOLUTION OF SIMULTANEOUS EQUATIONS

The numerical formulations presented in the previous sections result in large sets of simultaneous equations that must be solved at least once and possibly several times during each time step of the simulation. It is therefore essential to employ solution methods which minimize computing time and memory requirements. The methods used to solve the discretized equations depend on the characteristics of the matrix equation. All of the numerical methods which have been discussed in this chapter (FDM, FVM, and FEM) result in a large, sparse matrix equation. In other words, only a relatively small number of the matrix elements are nonzero. The precise pattern of sparsity depends on the grid structure and the method of discretization. Some standard sparse matrix solution methods will be mentioned briefly. Recently, very efficient solution methods, particularly multigrid methods, have been employed in general purpose commercial software.

A. Methods for Structured Grids

With structured grids, the simultaneous algebraic equations may be solved efficiently with minimum memory requirements by taking advantage of the inherent order of the grid. For a one-dimensional problem, an implicit algorithm results in a tridiagonal system of equations. A tridiagonal matrix is easy to solve because nonzero elements are found only on the diagonal and one element on each side of the diagonal. For multidimensional problems, alternating direction implicit (ADI) or fractional step methods [20] are generally employed which involve splitting the problem into separate steps for each dimension of the problem. Each step involves implicit operations in only one coordinate direction. As a result of this "splitting," only tridiagonal systems of equations need to be solved.

B. Methods for Unstructured Grids

A finite element type of grid has no inherent structure and therefore the previously described methods cannot be employed. For unstructured grid methods, it is usually more economical to compute and store the matrix elements rather than compute them "on the fly" each time they are needed. Currently a common approach is to use an iterative method such as the conjugate gradient method [20] for symmetric matrices or a generalization of the method for nonsymmetric matrices. With a symmetric matrix, the lower triangular half of the matrix is a mirror image of the upper half. This means that only the diagonal and either the lower or upper triangular half of the matrix need be stored. In either case, special sparse matrix storage schemes are used because the matrix is extremely sparse with no particular sparsity pattern.

VIII. TYPES OF MODELING SOFTWARE

Many casting process modeling software packages are commercially available. Although all of this software have been developed for the purpose of providing assistance in optimizing the casting process, selecting the right package to satisfy a particular foundry's specific needs can be a difficult task. Perhaps the most obvious difference between the various software packages is the structure of the grid used in the computations. As described in Sec. VI.A, computational grids may be classified as either structured or unstructured. Essentially all of the simulation software is based on either (1) a regular, structured grid using finite difference and/or finite volume numerical methods or (2) an unstructured grid using finite element methods. In addition, many software packages offer some type of quick (and approximate) analysis capability. The choice of modeling software depends on the expertise, preferences, and computational resources of the user as well as the process modeling requirements. The characteristics of each type of software is summarized in the following paragraphs.

A. Structured Grid Software

The first commercially available casting modeling software used a structured grid approach. The original codes used FDM; more recently developed codes may employ FVM. The most important advantage of structured grid software is that it is fairly easy to use. Because the mesh consists of simple rectangular cells, the meshing process is a straightforward task. However, the resulting "zigzag" mesh does not represent the geometry very accurately, especially for complex thin walled castings. Generally, a uniform cell size is used which can result in a large number of cells if the casting has both thin and thick sections. FDM/FVM software has been successfully used to model the heat transfer, fluid flow, and solidification during casting. At present, this type of software cannot calculate casting stress distribution directly. In order to calculate thermal stress, a separate FEM stress analysis is needed. If stress analysis is desired, the computed temperature history must be written out and mapped onto an FEM mesh of the same geometry. The thermal stress analysis is then performed by the FEM software using the temperature data obtained from the previous FDM/FVM analysis.

B. Finite Element Software

This type of software uses a completely unstructured FEM type of mesh which represents the model geometry very accurately. However, finite element meshing can be a complicated task. Automatic tetrahedral meshing is commonly employed to reduce the time demand on the user. This type of software generally requires greater memory and CPU time per element (cell), but may use elements of variable size to reduce the required number of elements. The most important advantage of this type of software is that it can perform heat transfer, fluid flow, and stress analysis with a single model. The stress analysis can be performed separately or simultaneously with the heat transfer calculations. Because stress analysis is a time consuming task, a separate calculation (only one stress analysis is performed after several heat transfer calculation steps) is most widely used.

C. Quick Analysis

This type of software typically uses a modulus (surface to volume ratio) approach to calculate the casting solidification sequence and identify hot spots (the last places to solidify) which tend to form macroshrinkage type defects. This type of approach usually does not properly account for the geometry of the different solid materials (insulation, chills, etc.) in the model. Recently, however, methods have been developed to better account for the geometry of the various materials and also generate the thermal history (temperature distribution as a function of time) [21]. Quick and approximate methods have also been developed to model the mold filling sequence. The most important advantage of quick analysis software is that the computation may be performed in minutes instead of hours required by traditional numerical methods. The disadvantage of this type of method is that the results are generally less accurate than traditional computations and may be unsuitable for prediction of microstructure evolution and defect formation (e.g., amount of porosity) during casting.

IX. GENERAL PROCEDURES OF CASTING MODELING

The previous sections laid out the fundamentals of fluid flow and heat transfer phenomena involved in modeling casting processes. These fundamentals not only serve as the basis for casting software development, but are also helpful to a software user in building casting models and running simulations. A software user, such as a process engineer in a foundry plant, might not have to understand the details of how the software is written, but needs to know how to efficiently employ the software to conduct computer modeling for his own casting process. This section will discuss the general procedures of casting process modeling using simulation software, either in-house developed software or a commercial casting simulation package.

Casting computer modeling usually consists of three stages: (1) preprocessing, (2) running the simulation, and (3) postprocessing. Preprocessing is most critical to the success of the modeling effort since this is the stage where the user actually builds the computer model for his particular casting process. The preprocessing stage consists of several steps: building geometry, meshing, assigning material properties, specifying initial and boundary conditions, selecting simulation control parameters, etc. Running the simulation involves performing the primary calculations and monitoring the results. Postprocessing is the stage to retrieve, process, and most importantly, make sense out of the simulation results. Postprocessing can be the most exciting when a nice, smooth, converged solution is obtained from the simulation, but can also be the most disappointing when meaningless temperature contours appear on the computer screen.

A. Building Geometry and Meshing

1. Building Geometry

The geometry for the casting process model includes part geometry itself and process-related geometry such as runners, gates, and risers. There are two options to build the geometry of the part. The first option is to create the geometry from the *blueprints* of the part. Some of the commercial casting simulation packages have a built-in capability to allow the user to create a geometry model consisting of complex shapes and dimensions. It is convenient to use this built-in capability if the geometry of the part is simple. The second option is to use an *electronic data interface*. At the part development and design stage, an electronic data file of a solid model of the part is created by a design engineer with CAD (computer aided design) or CAM (computer aided manufacturing) software. When casting process modeling is needed, the electronic data file can be retrieved and translated with electronic interface software to a format that can be read by the casting simulation package. All of the commercial casting simulation packages have the capability to directly read some type of electronic files created by CAD/CAM packages. The interested user can refer to Chapter 8 for details of the electronic data interface process. The most convenient way to build the complete model geometry is to import cast part geometry data file and then use the built-in geometry creation capability to add runners, gates, risers, etc.

2. Meshing

The part to be cast is usually of complex geometry. Meshing such a part is not a trivial exercise. It takes quite a bit practice for a user to develop the skilled experience necessary to generate a high quality mesh. The quality of the mesh affects not only the accuracy of the results, but also the stability and convergence of the solution. In addition, mesh density directly determines the computational efficiency, i.e., the computer CPU time and memory as well as the hard storage space required to run the simulation. In general, the higher the mesh density (meaning more elements and nodes in a specified volume), the higher the simulation accuracy. However, higher mesh density also significantly increases the computer CPU time, memory, and storage space. Thus, it is important to establish minimum mesh density required to ensure a reliable and stable numerical solution. For example, generally a minimum three elements is required to obtain a reliable solution for fluid flow calculation. Most commercial casting simulation packages have internal meshing capability regardless of whether the package uses a structured or an unstructured mesh. Some of the packages also allow the user to import mesh files generated from other software.

B. Assigning Material Properties

Material properties can be assigned to individual cells (or elements) based on the material type occupying the cells (or elements). The material properties related to fluid flow and heat transfer include thermophysical properties, such as density, specific heat, thermal conductivity, radiative emissivity, viscosity, thermal expansion coefficient, surface tension coefficient, solidus and liquidus temperatures, and latent heat of fusion. These properties are usually temperature and composition dependent. Most of the casting simulation packages have *built-in material databases* that can be retrieved through the pre-processor. The databases store the thermophysical properties for the materials that are most commonly used in casting processes, such as cast irons, ductile irons, carbon and stainless steels, aluminum and its alloys, copper and its alloys, superalloys, titanium alloys, various sands, and some ceramics. Once a particular material is assigned to a certain region of the computational domain, the property values will be retrieved from the database and assigned to the computational cells in the region. The user can modify and edit the property data through the pre-processor to meet his particular needs.

C. Specifying Initial Conditions

The user is generally required to provide initial conditions, such as initial metal positions and initial temperature distributions. Sections III.C and V.D briefly described basic concepts of initial conditions for heat transfer and mold filling.

1. Heat Transfer

When only heat transfer is calculated, the mold cavity is assumed to be initially filled with metal. In this situation, the initial temperature has to be provided or specified. Most of the commercial casting simulation packages allow the user, through the pre-processor, to specify *constant temperatures* for metal and mold, respectively. The metal can be given a constant value of temperature, such as the pouring temperature, and the mold can be given another one, such as the mold preheated temperature. This is suitable for situations involving quick filling of a thick wall casting. If the mold filling takes place slowly or the mold is preheated nonuniformly, an initial *temperature distribution* must be provided. This can be implemented through a user subroutine similar to the one described in the previous section. The temperature distribution can be specified manually based on the user's knowledge, or obtained through a mold filling simulation.

2. *Mold Filling*

When mold filling is involved, an additional initial condition must be provided for the metal position. This can easily be implemented through the pre-processor of the casting simulation package.

D. Specifying Boundary Conditions

The boundary conditions are usually much more complicated than the initial conditions described in the previous section. Generally there are four types of boundaries that are referred to here: mold exterior walls, metal flow ingates, metal/mold interface, and metal free surfaces. The latter two types are sometimes called "interior boundaries" since they are not usually located at the outside boundaries of the computational domain. Sections III.C and V.D included a short discussion on the boundary conditions for different types of boundaries.

1. *Mold Exterior Walls*

The mold exterior walls can be given one or more of the following conditions: a constant temperature, a constant heat flux, a convection condition that could be natural or forced convection, and a radiation condition. All these conditions are available in most of the commercial casting simulation packages and can be specified during pre-processing. Which type of condition(s) should be applied really depends on the process that is modeled. For example, generally a constant temperature or convection condition should be applied to sand casting mold exterior walls and a radiation condition should be employed to investment casting exterior ceramic shell surfaces. The reader should refer to Secs. III.C and V.D as well as Chapter 11 in the latter part of this book for the details.

2. *Metal Flow Ingates*

The conditions at the metal flow ingates, sometimes called inflow conditions, must be specified when fluid flow (mold filling) is involved. This is fairly easy to implement, as described in Sec. V.D. For example, constant temperature and velocity may be specified at the ingates. This can be implemented through the pre-processor of any simulation package. Some packages allow the user to specify time-dependent ingate conditions.

3. Metal/Mold Interface and Metal Free Surfaces

The conditions at the boundaries, such as metal/mold interface and metal free surfaces, are discussed in Secs. III.C and V.D. These conditions can be specified through the preprocessor. Most of the simulation packages also set some default conditions, such as a perfect contact and no-slip condition at the metal/mold interface and a zero-heat-flux and zero-stress condition at the metal free surfaces.

4. Other

Some processes may have particular boundaries, either exterior or interior. For example, a permanent mold or die casting is usually equipped with gas escape vents. Special models might be needed to specify conditions for these particular boundaries. In this situation, the user should check the manual.

It should be pointed out that the above discussion on boundary conditions is quite general. These conditions change from case to case for the different casting processes. The reader can refer to a corresponding chapter of this book when dealing with a particular process.

E. Selecting Simulation Control Parameters

Simulation control parameters include total simulation time (the operation time in the casting process, not the computer CPU time), time step size control variables, convergence criteria, computational relaxation factors, and frequency of result output, etc. Although from a theoretical point of view these parameters look trivial, in practice they significantly affect the solution accuracy, stability, convergence, and computational efficiency. One of the most frustrating experiences in casting modeling is to find that a long battle for a good simulation was a result of a bad choice of simulation control parameters. Although some tips, given in the following paragraphs, can be used to select a workable combination of these parameters, there are unfortunately no general rules that guarantee an accurate, smooth, and converged solution. It may take several trial-and-error simulations for the user to obtain a good feeling about what will work and what will not. The user is recommended to read the manual provided by the simulation package that he/she chooses and consult experienced modeling personnel instead of sitting in front of a computer and wasting a huge amount of time on trial and error.

1. Total Simulation Time

Total simulation time should be determined by the process to be simulated. This time in turn directly determines the computer CPU time. It is suggested that the total simulation time for the first trials be set to such a number that fewer time steps are needed. This will significantly shorten the trial-and-error time, especially for a simulation that is expected to take more than several hours of CPU time to complete. After smooth and converged solutions are obtained for the first several time steps, a complete job covering the entire process can be submitted. In practice, two methods are commonly used to decide the total simulation time. One method is to stop the simulation when the highest temperature in the casting reaches a specified value, usually several degrees lower than the metal solidus temperature. The other method is to stop the simulation when the total simulation time reaches a specified value, based on an estimation how long the casting will take to completely solidify.

2. *Time Step Size*

Most commercial casting simulation packages have an option of automatic adjustment of time step sizes (or time increments). If the solution converges at the current time step and the temperature change falls in a predetermined value, the package will enlarge the time step size for the next time step. When using this option, the user is required to provide an allowed minimum and maximum time step size. Some packages stop the simulation if the allowed minimum time step size is reached. The maximum time step size should be selected based on two criteria: stability requirement and time truncation error tolerance. For a solution method using explicit time integration, the CFL criterion, Eq. (41), must be satisfied to assure the solution stability. This will usually result in a satisfactory time truncation error. For a solution using implicit time integration which is unconditionally stable, a relatively large time step size can be selected as long as the time truncation error is kept below a tolerable level. However, there are no measures to directly calculate the time truncation error. It can only be estimated by examining the results or comparing them with experimental data. Frequently, the maximum time truncation error is specified in terms of CFL number.

3. *Convergence Criteria*

Convergence criteria are used only in the solution schemes with an implicit time integration where an iteration sequence is needed to solve a nonlinear system of equations. There are typically two types of convergence criteria: the residual of the discretized equation and the deviation error of the variable between two consecutive iterations. It is best if both criteria are satisfied. For example, the residual of the discretized energy equation at the current iteration falls to a level 2 orders of magnitude smaller than that at the first iteration. At the same time, the temperature difference between the current and last iteration becomes less than 1°C. Appropriate values should be selected for the convergence criteria. Too large a value will result in inaccurate solutions and too small a value will consume unnecessarily a large amount of computer CPU time. Most of the simulation packages have default values set for the convergence criteria. The user is recommended to use these default values.

4. Computational Relaxation Factors

Computational relaxation factors usually refer to the under-relaxation factors used in nonlinear iteration sequences. Similar to the convergence criteria discussed above, the computation relaxation factors are only applied in the solution schemes using implicit time integration. The simulation packages that use the implicit solution schemes may require the user to specify the underrelaxation factors through the preprocessor. The values of the underrelaxation factors can be different for each variable, such as temperature, solid (or liquid) fraction, pressure, and velocity components. Again, appropriate values must be selected for the underrelaxation factors. Too large values may cause convergence problems and too small values will unnecessarily slow down the simulation significantly.

5. Data Output Frequency

A complete simulation of a casting process may need several hundred or thousand time steps. Because of the restriction of computer hard storage space, it is impossible and unnecessary to store the results at every time step. Most of the casting simulation packages allow the user to specify an output frequency for writing out the simulation results. Some packages even allow the user to use a variable output frequency. This gives the user the flexibility to limit computer storage space and still be able to catch the most important characteristics of the results in the time sequence.

F. Selecting a Computational Model

Most of the casting simulation packages include several computational models. The user can select a specific model or a combination of some models to meet his own simulation needs.

1. Quick Analysis Model

Some casting simulation packages provide the quick analysis model for heat transfer known as "modulus model," such as the one described in Chapter 7. The model does not solve the partial differential equations but calculates heat balance based on an integrated effect of boundaries. This simple analysis model has its unique advantage: superior computational efficiency. The model takes little CPU time to complete a simulation (less than an hour for a mesh with a million nodes). The disadvantage of the model is its accuracy. It may be used as a tool for rough estimates or prestudy. It can also be used to conduct parametric studies if the model can be validated through comparisons with experiments or with a more accurate model, such as the mold filling and heat transfer model described in Sec. V.

2. Heat Conduction Model

The heat conduction model is a good choice if the mold filling takes place quickly and its effect on metal and mold temperatures is small. This model needs more CPU time (maybe a few to several hours) than the quick analysis model but is still much faster than a coupled mold filling and heat transfer model.

3. Mold Filling and Heat Transfer Model

This is the most accurate but least computationally efficient model. It may take several days to complete a simulation. The model is used only when it is necessary, for example, when mold filling is very slow, or an incomplete filling due to solidification is suspected, or a high degree of accuracy is desired.

4. Thermal Stress Model

When stress-related defects are of concern, thermal stress calculation can provide some insight to better understand the problem. Stress-related defects include hot tearing, cold cracking, dimensional distortion, and recrystallized grains in single crystal and directionally solidified turbine airfoils.

G. Running the Simulation

After the simulation job is submitted to the computer, it should be monitored as frequently as possible. This will help the user save modeling cycle time which refers to the time needed from building the geometry to the point when a good solution is achieved. The user should use the postprocessor to exam the results that are written out for the existing output time steps. If serious problems are found in the results, he should stop the simulation and go back to tune the model. If the problem is minor, he might restart the simulation and save the results for future reference. At the same time, he may start another simulation with better tuned model parameters.

H. Postprocessing

The postprocessing includes two aspects: visualization of the simulation results and analysis of these results to provide a better understanding of the casting process. The simulation results include direct output quantities of the FDM/FEM analyses and indirect output quantities which are calculated from those direct output quantities. The direct output quantities are raw data and provide only limited information regarding the details of the casting process. To have a better understanding of the casting process details and to find a solution for eliminating potential casting defects, indirect output quantities are more useful. Most of the casting simulation packages have a built-in visualization software which can be used to visualize simulation results. Some of the visualization software allow the user to animate the results such as the mold filling and solidification sequence.

The direct output quantities of the FDM/FEM analyses are:

Heat transfer analysis: Temperature distribution at various time steps
Fluid flow analysis: Free surface locations, velocity vectors, and pressure distribution at various time steps
Stress analysis: Stress and strain distribution at various time steps

Although direct output quantities provide some understanding of the casting process, other indirect quantities would be more useful to predicting defect formation and microstructure evolution during casting. Some of the most commonly used indirect output quantities and their physical meanings are briefly described in the following part of this section. The reader should refer to Chapters 4 and 5 for details on how to use these quantities to predict defect formation and microstructure evolution.

1. *Mold Filling*

Metal fluid flow velocities, pressure, and free surface location can be plotted in a time sequence to visualize mold-filling process. This mold-filling sequence will reveal how the metal flows from the pouring sprue to the end of casting, and consequently reveals potential problems associated with the mold filling. These problems include the potential danger of no filling, formation and locations of weld lines, and residual gas bubbles.

2. *Isotherms*

Temperature spatial distributions can be plotted out as isotherms at different times. A series of isotherms can be generated to visualize a whole picture of thermal evolution process during mold filling and cooling. These isotherms can show solidification sequences and hot spots, which in turn indicate the location and size of potential macroshrinkage.

3. *Isochrons*

Another more effective way to show hot spots and predict potential macroshrinkage is through the use of isochrons. An isochron plot shows the time to reach a specific temperature, such as liquidus or solidus temperature. One isochron plot is equivalent to a series of isotherm plots in terms of the information concerning hot spots and macroshrinkage locations.

4. *Cooling Curves*

Temperature history at each nodal point can be plotted out as cooling curves. These cooling curves can be used for model validation purposes by comparing them with experimental thermocouple (TC) measurements. Figure 5 shows cooling curves at four spatial locations in the metal and mold during a permanent mold casting of Al 6010 alloy. Thermocouple (TC) data was used to verify the accuracy of the model results.

5. *Cooling Rate*

Cooling rate has the unit of °C/s. There are two types of cooling rates which can usually be calculated and used for defect and microstructure prediction.

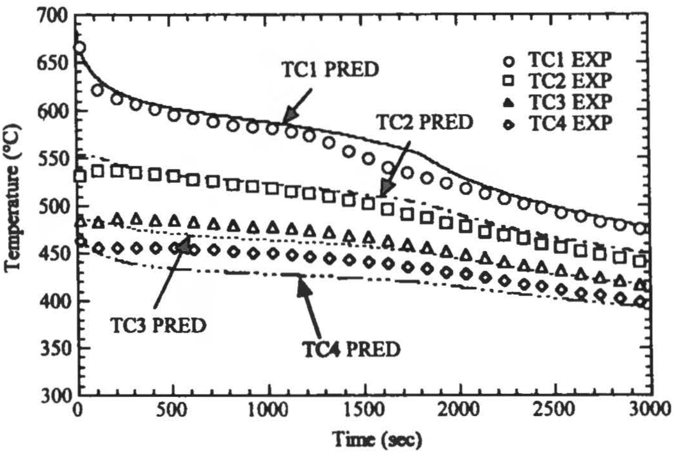

Figure 5 Cooling curves at four spatial locations in metal and mold during a permanent mold casting of Al 6010 alloy. Also shown are thermocouple data represented by symbols.

Instantaneous cooling rate is calculated at a specified temperature and *average cooling rate* is calculated over a temperature interval such as the interval between solidus and liquidus temperatures. These cooling rates can be used to develop empirical relations to predict dendrite arm spacing (DAS) and grain sizes.

6. Local Solidification Time (LST)

Local solidification time (LST) is the time needed for a specific spatial location to cool down from liquidus temperature to a eutectic or solidus temperature. LST can be calculated based on the temperature history and is often used in the prediction of DAS.

7. Temperature Gradient G

Temperature gradient G is defined as the rate of change in temperature over the spatial coordinates. It has the unit of °C/m and is actually a vector which can be decomposed to three components, e.g., G_x, G_y, and G_z in a Cartesian coordinate system. These components can easily be calculated from the simulation results and the vector sum can then be deduced.

8. Solidification Rate R

Solidification rate R is defined as the moving speed of solidification front over the spatial coordinates. It has the same unit as velocity, i.e., m/s. It can be calculated at a specific time and a specific spatial location.

9. Combination of G and R

A combination of solidification rate R with temperature gradient G can be very useful in prediction of solidification structure, feeding capability, and microporosity formation tendency. For instance, G/R is usually used to predict solidification structure. As shown in Fig. 6, the values of G/R determine whether a particular region of the casting part will have an equiaxed dendritic structure, or columnar dendritic structure, or plane front structure. Another use of the combination of G and R is the prediction of the microporosity formation tendency of the casting part, such as Niyama criterion for microporosity formation in steels and LCC criterion in aluminum alloys.

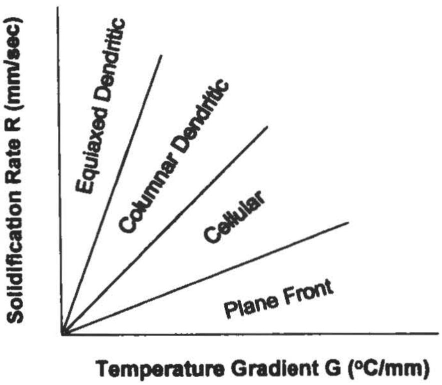

Figure 6 Effect of cooling rate and solidification rate on solidification structure.

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3
Stress Analysis

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I. INTRODUCTION

This chapter deals with the development of stresses and distortions in shaped castings and their prediction using numerical methods, specifically the finite element method. It also discusses the topics of hot tears, hot cracks, and patternmakers' allowance which are related to the more general subject of stresses and distortions.

Casting of a part involves a complex interaction between several metallurgical and mechanical phenomena, e.g., solidification and subsequent cooling of the molten material; grain nucleation and growth; transfer of heat from the melt to the mold and, finally, to the environment; development of stresses and distortions; and so forth. In order to make the task of computer simulation manageable, Chandra has proposed a scheme shown in Fig. 1 [1]. According to this scheme, after a finite element or finite difference mesh of the cavity, mold, and the feeding system is prepared, three separate simulations can be performed in sequence. The first of these, that is, the mold-fill simulation, is based on the mathematics of fluid mechanics and convective heat transfer. It is carried out until the mold is completely filled and the convective effects have become negligible. Such simulation is capable of predicting loss of superheat, turbulence levels, mold erosion, and misrun (nonfill) and cold shut type defects. The output of this simulation in terms of temperatures at various locations or nodes at the end of mold filling is passed on to the next step, that is, the solidification simulation, to serve as the initial conditions.

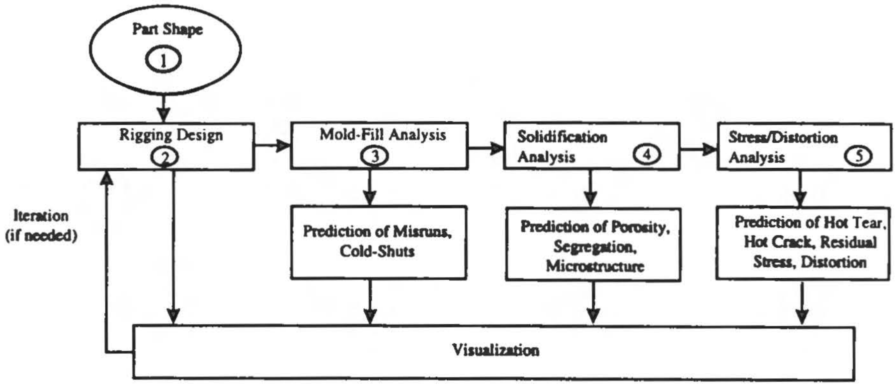

Figure 1 Schematic of the casting process simulation procedure.

The solidification simulation is based on the mathematics of conduction heat transfer in the melt and the mold, kinetics of solidification, and a convective or radiative heat loss from the mold surface. Convection within the melt may be neglected during this period. This simulation step assists in predicting porosity, macroshrinkage, and segregation type defects, cast microstructure and, at least conceptually, the mechanical properties of the cast part. The output of this simulation in terms of temperatures and grain density and size at various locations in the assembly of the cast part, mold, and feeding system can be passed on to the last step, that is, the stress/displacement analysis, which could predict hot tears, hot cracks, residual stresses, and distortions in the cast part, mold cracks, and shrinkage allowance for pattern making.

The scheme shown in Fig. I, involving three consecutive simulations, was appropriate a few years ago when the primary interest in casting process simulation lied in the prediction of porosity. At that time, the efforts in the areas of mold-fill simulation and microstructure prediction were in their early stages, and the subject of coupled thermal-mechanical analysis was not yet fully developed. Due to recent advances in all of these fields, it is now possible to reduce the simulation steps from three to two. The first step is again of mold-fill simulation based on the mathematics of fluid mechanics and convective heat transfer. Thermal output of the first step is fed to the second step which now combines solidification, subsequent cooling, and stress/displacement analyses together. Simulation in this step may also include the mathematics for microstructure and/or hot tear prediction. The original scheme of three-step simulation (Fig. I) is the basis of a sequential thermomechanical analysis, whereas the two-step simulation scheme forms the basis of a coupled thermomechanical analysis.

In this chapter, it is assumed that a mold-fill simulation has already been performed up to a point that the mold is completely filled, and the convective effects have become negligible (also see Chapter 2). The temperatures at the end of mold-filling are available at the various locations or nodes in the assembly of the cast part, mold, and feeding system which serve as the initial condition for a subsequent coupled thermomechanical analysis.

In the discussion so far, the casting was assumed to be confined within its mold. But, the stresses and distortions in a finished cast part are also influenced by subsequent operations in its processing history, e.g., mold removal, finish machining, heat treatment and/or straightening. Therefore, in order to accurately predict stresses and distortions in a casting, these operations should also be analyzed. In this chapter, the stresses and distortions due to solidification, cooling, mold removal, and finish machining will be discussed, but the subjects of heat treatment and straightening will not be considered.

In Sec. II, some basic concepts related to stress/displacement analysis of casting processes are reviewed. Then, in Sec. III, a brief review of the transient, nonlinear thermomechanical analysis is presented; both sequential and coupled forms are discussed. In Secs. IV through IX, the treatment of several special topics such as the release of latent heat and formation of hot tears in the mushy region, thermal and mechanical interaction between the mold and the metal, and others, is discussed. It is the treatment of these topics which separates the simulation of the casting processes from a conventional thermomechanical analysis employed in product evaluation. However, a detailed discussion of these topics would require an entire book and is beyond the scope of this chapter. Finally, in Sec. X, some results of thermomechanical analyses of simple test castings are presented to highlight the formation of gap and contact at the mold-metal interface, prediction of hot tears, residual stresses, and distortions.

II. BASIC CONCEPTS

Before going further, it is instructive to clarify certain definitions and concepts related to hot tears, hot cracks, distortions, and transient as well as residual stresses in shaped castings. A clear understanding of these will help the reader appreciate the full extent of the task at hand. This discussion is divided into two parts: before mold removal and after mold removal.

A. Before Mold Removal

Consider a simple *I*-section casting shown in Fig. 2a. The cooling curve of an arbitrary point within this casting is shown in Fig. 2b. Temperatures T_P, T_L,