Capturing the Complexities of Ductile Iron Solidification Through Simulation

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ABSTRACT

As the metal casting marketplace continues to expand, and as the migration of raw material drives baseline costs higher, the stability of ductile iron makes it the workhorse alloy for high strength applications. In addition, the unique expansion behavior of ductile iron during solidification allows for high yields compared to other materials, making it an economical choice. However, understanding the complex interconnections of alloy composition, process definitions and cooling rates is quite difficult when attempting to determine if the casting is adequately risered, if the inoculants will be effective or if the myriad of other concerns that affect the overall expansion and porosity are adequate to produce a good casting.

This paper will examine how computer simulation of the ductile iron casting process can accurately predict the material behavior through intricate microstructure calculations and include magnesium fading effects, inoculant effects and other factors which will determine the expansion / shrinkage of the alloy.

INTRODUCTION

Ductile or nodular cast iron components are quite popular for a host of applications as they combine high toughness, increased ductility, high strength, fatigue and wear resistance. Nodular cast iron is created through an alloying process (usually with Mg) where nucleation favors the formation of graphite nodules instead of flakes of grey iron, thereby giving the material increased ductility and superior elongation properties. Some typical automotive ductile iron parts include steering knuckles, exhaust manifolds, brake calipers, camshafts, clutch drums, brake cylinders, connecting rods, etc.

MICROSTRUCTURE MODELING

Cast iron is unique in that carbon is added in excess of its solubility in iron at room temperature. During solidification, as the molten metal cools and the solubility limit of the carbon in the iron decreases, excess carbon usually precipitate under the form of graphite lamella. Graphite lamella can be present in cast iron alloys in different shapes. All these different forms can be achieved from the same melt by varying the chemical composition or by changing the cooling rate. Spheroidal Graphite cast Iron (also called ductile or nodular cast iron) is a specific cast iron material in which the graphite is present as nodules (Figure 1 right). Because of additional elements, i.e. magnesium or cerium, introduced in the molten iron before casting, the graphite nucleates as spheres (nodules), rather than as lamella of any of the forms characteristic of grey iron. The formation of these graphite nodules leads to a volume expansion during solidification that must be correctly modeled in casting simulation for good correlation with real production parts.

Microstructure formation during the solidification of the alloy is a very important factor for the control of the properties and the quality of casting products. There are different types of microstructures for different alloys. The types of phases present, the volume fraction of the phases, the grain size, and grain shape determine these final casting properties. To obtain microstructure predictions, simulation software couples thermodynamic calculations with microstructure models and the macro-scale thermal and fluid flow calculations. Depending upon the chemical composition,
the microstructure module automatically detects the phases which will appear and the type of microstructure which should be computed (dendritic, eutectic, nodular, etc.).

For instance, if nodular cast iron is defined, automatically the nodule counts, austenite radius, pearlite and ferrite fractions will be computed, together with the corresponding mechanical properties (such as elongation, hardness, yield and tensile strength). The eutectic transformation process in ductile iron is a divorced growth of austenite and graphite, which do not grow concomitantly. Because of the density variation resulting from this phenomenon, the expansion/contraction of the grain is taken into account by allowing the final grain size to vary. Therefore, during ductile solidification, the densities of the different phases are computed according to the composition of the phase at that particular temperature (Figure 2). In the calculation, the graphite expansion is also included.

**Fig. 2. Example of microstructure and its corresponding local density in cast iron observed in a simple test**

In region 1, due to the high cooling at the corner of the casting, the microstructure is mainly constituted of metastable phase (Ledeburite). In this region, a local density with no expansion is taken into account. In region 2, where the cooling is slower, a local material expansion is taken into account due to the nodule formation generated in that region.

**COUPLING MICROSTRUCTURE WITH POROSITY**

Shrinkage porosity, as shown in Figure 3, can be characterized by the following:

a) Pipe shrinkage, including surface sinks which occurs early during solidification when the liquid metal on the surface of the casting, exposed to the atmosphere, is under a depression due to the contraction of the solidifying metal on the inside. The metal is then pushed downwards (or inwards) by atmospheric pressure forming a pipe, or sink, which is visible on the surface of the casting.

b) Macro shrinkage occurs when the liquid is surrounded by enough solid material which is strong enough to resist the depression of the contracting liquid. Usually the size of the pores is greater than 3mm. These defects are internal and can generally be prevented by optimal pouring temperature, riser positioning and size. During solidification the expansion of the metal due to graphite expansion can cause liquid to be pushed back into the gating system resulting in problems with porosity during subsequent solidification.
c) Micro shrinkage occurs late during solidification and is formed between the solidifying dendrites. Usually the amount of micro shrinkage is influenced by the cooling rate, pressure and alloy freezing range. In nodular iron casting, due to the formation of the graphite nodules during solidification, a total net volume expansion can result, as shown in Figure 4. However, contrary to what might be expected, micro-porosity may still form. The expansion of the solid skeleton during solidification should be taken into account to explain this phenomenon. Like a sponge which expands in water, we can consider a similar phenomenon during solidification where suction of the liquid occurs similar to that inside the interstices of the sponge. This leads to a pressure drop which during solidification is responsible for micro-shrinkage. Good gating design can help to take advantage of this phenomenon.

Predicting the behavior of the metal during solidification is not trivial as one needs to consider the different modes of shrinkage as well as trace the evolution of the liquid metal free surface. One has to distinguish between how much of the volume change results in macro shrinkage and how much results in micro shrinkage.

The amount of shrinkage will depend on the following factors during solidification:

- Filling behavior
- Pouring temperature
- Casting material properties
- Thermal cooling conditions
- Inoculation
- Amount of graphite expansion occurring during solidification
- Mold/Core material properties
- Mold/Core rigidity which will influence the pressure in the liquid

**INVESTIGATING THESE UNIQUE SOLIDIFICATION FACTORS**

On the surface of this investigation, it is clear that the basic casting process will affect the development and thus solidification behavior of the casting. The filling pattern sets up the temperature gradient in the casting from which the solidification will continue. In that respect, the duration that the gate contact remains liquid will influence the compensation of the rigging system during the liquid shrinkage of the casting. A quickly solidifying gating system with no additional
risering requires the microstructure to generate additional expansion to make up for the volume lost during the density change as the alloy temperature nears liquidus. Optimally, the majority of the casting will also be near liquidus when the gate freezes. The selected pouring temperature also dictates the amount of volume change in the liquid. A pouring temperature near the liquidus minimizes this shrinkage; however, may result in a non-fill scenario. Conversely, a high pouring temperature may result in a high volume of liquid shrinkage. Thus a judicious selection of pouring temperature is required to maximize the expansion effect during solidification.

This net amount of volume change is tracked by the software, and the liquid pool takes the proper free surface level to accommodate the proper amount of metal mass in the casting. As regions solidify, such as the gate, and once the fraction solid of the alloy reaches a critical fraction solid at which feeding ceases, isolated liquid pools are formed, and are independently tracked by the software. Further “un-fed” shrinkage may result in a loss of mass, allowing voids to develop.

In the cast of these irons that expand during solidification, it is quite possible that voids do not develop. As previously described, spherical graphite nodules may form and may expand to a sufficient size to close potential voids. This nodule development is directly related to the casting properties (i.e., composition) as well as the cooling conditions and inoculation of the alloy. As mentioned, the composition determines the potential for spherical nodules formation and the cooling conditions determine the phase transformation. These items are locally tracked in the casting region with a coupled interaction with the empirical phase information. The inoculation aids in providing a specific amount of nucleation sites for the graphite formation. The nucleation itself is interactively defined following Oldfield’s nucleation model, which determines the nucleation as a function of the undercooling. However, that count may be influenced by the fading effect, which affects the inoculation particle size. The longer the time between inoculation and the actual casting of the metal, the larger the particle size, which decreases the number of particles per volume, leading to less nodules. The fading effect on particle size is given by the relation (Equation 1):

\[ d = \left( d_o^3 + kt \right)^{1/3} \]  

where, \( d \) is the final particle diameter, \( d_o \) is the initial particle diameter, \( k \) is a kinetic constant, and \( t \) is time.

The calculation continues by determining the amount of graphite expansion through solidification. This is governed by determining the phase transformations that evolve. Again, the phases are determined by the coupling with the empirical alloy database. Knowing the phases involved activates certain equations which govern the phase situation and may include a graphite / austenite transformation, metastable eutectic (Ledeburite) and eutectoid transformation. Due to thermodynamic equilibrium, each grain must adhere to conservation of mass and solute (Equations 2 and 3).

\[ \rho_G \frac{4}{3} \pi R_G^3 + \rho_r \frac{4}{3} \pi (R_r^3 - R_G^3) + \rho_l \frac{4}{3} \pi (R_l^3 - R_r^3) = m_{av} \]  

\[ \rho_G \cdot \frac{4}{3} \pi R_G^3 + \int_0^R \rho_c c(r,t) 4 \pi r^2 dr + \rho_l c_l \frac{4}{3} \pi (R_l^3 - R_r^3) = c_{av} \]  

By combining these conservation equations, which involve phase densities (\( \rho \)), phase radii (\( R \), which are allowed to vary) and phase concentrations (\( c \)), with Fick’s Law of diffusion, equations for graphite and austenite growth rates may be derived. Therefore, the amounts of graphite and austenite are calculated, and by applying the proper densities to each phase, it is known whether expansion or contraction occur and to what extent.

Finally, it is not only important to know how the casting alloy will behave, it is also important to include the role of the molding media in the case of expanding irons. At minimum, the thermophysical properties of the mold components will help control the cooling rate and solidification pattern. The mechanical properties of these components also play significant roles in the effectiveness of the expansion in reducing or eliminating porosity. If the mold is firmly compacted or a hard molding material is used, the mold will be quite rigid against any pressures imparted by the expanding casting. Thus, in the case of a casting where the gate has solidified and there are no open risers or other exposed volumes, expansion is directed inward, minimizing shrink. However, if the mold is soft, the walls of the mold will move, creating a larger volume for the still low-solids alloy to occupy. Therefore, the casting will still be vulnerable to porosity.

In casting analysis, the mold rigidity may be approximated by a simple “rigidity factor” which is applied to the overall expansion of the alloy. A more accurate method for examining the influence of mold rigidity is to couple a mechanical (stress) analysis of the casting and mold during solidification. This allows a more correct calculation of mold movement.
during expansion, although the method requires significantly additional solution time. Additionally, the influence of expansion further packing the sand and thus making it more rigid has not been explored. In general, true mechanical properties of sand has not been well examined in the industry and remains not fully understood.

EXAMPLE I

In order to model the phenomenon realistically, the same parameters as in the actual production must be considered in simulation. As explained above, during casting, nodular cast iron does not simply contract when it solidifies; rather, it expands due to graphite expansion. If the outer surface of the casting is constrained from expanding, then an increasing pressure inside the casting can help to compensate the formation of micro and macro shrinkage porosity. This physical phenomena is not trivial to understand and subsequently not straightforward to model. Microstructure, process conditions, material properties and mechanical properties of the mold need to be accurately considered to accurately predict porosity in cast iron. Today, by coupling a thermodynamic database with a micro- and macro-porosity model, it is possible to predict porosity by taking into account alloy expansion.

![Graphite expansion not considered](image1)

**Figure 5: Graphite expansion not considered**

![Graphite expansion with low level of inoculation (left) and a high level of inoculation (right)](image2)

*Fig.6. Graphite expansion with low level of inoculation (left) and a high level of inoculation (right).*

Figure 5 shows the porosity plot when graphite expansion is not considered. This will result in an over-design of the feeding system and hence results in low yield. The unique properties specific to and advantageous of ductile cast iron are not being considered; thus, the simulation results will not realistically model what happens on the shop floor. Figure 6 shows the porosity plot with varying levels of inoculation. This will differ from foundry to foundry depending on their respective foundry practices.

EXAMPLE II

The example shown in Figures 8 of a casting without riser sleeves also illustrates the influence of graphite expansion on the porosity results. The porosity results are shown in Figures 7 and 8. This contour plot of the cross section shows porosity, where red indicates macro porosity and yellow indicates a 100% vacant region or “hole”. When taking graphite expansion into account, as shown in Figure 8, the porosity is considerably lower than when not considering expansion.
CONCLUSION

The current model available within the software for simulating ductile iron castings helps understand the solidification behavior and determine the effect of graphite expansion on porosity. Optimal gating design can then be determined to help take advantage of this expansion effect in ductile iron castings. This effect allows experienced foundry engineers make use of riserless methods, thus maximizing process efficiency and casting yield.

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