Combination of microscopic model and VoF-multiphase approach for numerical simulation of nodular cast iron solidification

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Abstract. The ongoing increase in the size and capacity of state-of-the-art wind power plants is highlighting the need to reduce the weight of critical components, such as hubs, main shaft bearing housings, gear box housings and support bases. These components are manufactured as nodular iron castings (spheroid graphite iron, or SGI). A weight reduction of up to 20% is achievable by optimizing the geometry to minimize volume, thus enabling significant downsizing of wind power plants. One method for enhancing quality control in the production of thick-walled SGI castings, and thus reducing tolerances and, consequently, enabling castings of smaller volume is via a casting simulation of mould filling and solidification based on a combination of microscopic model and VoF-multiphase approach. Coupled fluid flow with heat transport and phase transformation kinetics during solidification is described by partial differential equations and solved using the finite volume method. The flow of multiple phases is described using a volume of fluid approach. Mass conservation equations are solved separately for both liquid and solid phases. At the micro-level, the diffusion-controlled growth model for grey iron eutectic grains by Wetterfall et al. is combined with a growth model for white iron eutectic grains. The micro-solidification model is coupled with macro-transport equations via source terms in the energy and continuity equations. As a first step the methodology was applied to a simple geometry to investigate the impact of mould-filling on the grey-to-white transition prediction in nodular cast iron.

1. Introduction
The development of renewable energies is central to current energy policies worldwide. As an example, building new power supply systems and increasing the share of renewable energy in the total electricity requirement by 2050 by at least 80% is a goal of the Renewable Energy Sources Act of the German Ministry for Economic Affairs and Energy [1]. Such initiatives strongly encourage the wind energy sector to produce even larger wind power plants, alongside upgrading already existing facilities. As key suppliers to wind power plant manufacturers, foundries are also involved in the process: larger windmills demand larger castings. In this situation, both foundries and windmill manufacturers are confronted with a range of restrictions when transporting castings and installing windmills. Consequently, there is a need to reduce the weight of critical parts (hubs, main shaft bearing housings, gear box housings and support bases). These components are manufactured by casting nodular cast iron (spheroidal graphite iron, SGI). Current estimations by foundry experts are that optimization of the geometry aimed at minimizing volume can achieve a weight reduction of up to 20%, enabling significant reduction in the weight of wind power plant.
Over the last couple of decades, casting simulation of mould filling and solidification has been recognized as a powerful tool in ensuring the quality and robustness of casting processes. However, the above-described challenges from industrial practice allow additional improvements to existing software solutions. The solidification process of large castings is characterized by convection-driven phenomena, which could be taken account of through application of the principles of computational fluid dynamics. At the same time, local development of the graphite phase in cast iron needs to be taken into account. A combination of microscopic model and VoF-multiphase approach is proposed here as a method of enhancing quality control during the production of thick-walled SGI castings. Thus, the possibility of reducing tolerances and, consequently, enabling castings of smaller volume is to be expected.

Coupled fluid flow with heat transport and phase transformation kinetics during solidification is described by partial differential equations and solved using the finite volume method. The flow of multiple phases is described using the volume of fluid approach [2, 3]. Mass conservation equations are solved separately for both the liquid and solid phase. At the micro-level the diffusion-controlled growth model for grey iron eutectic grains by Wetterfall et al. [4] is combined with a growth model for white iron eutectic grains by Nastac and Stefanescu [5]. The micro-solidification model is coupled with macro-transport equations via source terms in the energy and continuity equation.

As a first step the methodology was applied to a simple geometry to investigate the impact of variation of the relevant micro-scale parameters on grey-to-white transition prediction in nodular cast iron.

2. Model description

The kinetics of solidification have been modelled by many authors. Within the scope of this work, fundamental microscopic phenomena such as nucleation, undercooling, primary and eutectic solidification are described and incorporated into a macroscopic heat and fluid flow calculation. One option of enhancing the predictive capability of this model with a fully-developed macroscopic model was explored.

2.1. General multiscale/multiphase modeling frame and VoF model

To model the casting and solidification process for a cast iron alloy precisely, the macroscopic transport phenomena and the microscopic solidification kinetics have to be considered at different scales at the same time. The general multiscale/multiphase modelling framework has been introduced by Beckermann and Viskanta [6] and adopted in the present research. The macroscopic conservation equations for each phase are obtained by averaging the microscopic (exact) equations over the volume $V_0$. Definition of the volume averaging of a quantity $\Psi$ in phase $k$ is given by:

$$\langle \Psi \rangle = \frac{1}{V_0} \int_{V_0} X_k \Psi_k \, dV$$

where $X_k$ is a phase function equal to unity in phase $k$ and zero elsewhere. The volume fraction of phase $k$ is defined as

$$\alpha_k = \frac{1}{V_0} \int_{V_0} X_k \, dV = \frac{V_k}{V_0}$$

The averaged macroscopic conservation equation of mass is given as

$$\frac{\partial}{\partial t} (\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{v}) = \sum_{j,j \neq k} \Gamma_{kj}$$
where $\Gamma_{kj}$ is the interfacial mass transfer due to phase change from phase $j$ to phase $k$. The energy equation is analogous:

$$\frac{\partial}{\partial t} \left( \alpha_k \rho_k (h_k)^k \right) + \nabla \cdot \left( \alpha_k \rho_k (h_k)^k \mathbf{v} \right) = \sum_{j,k} Q_{kj}^\Gamma + Q_{kj}^d \quad (4)$$

where $Q_{kj}^\Gamma$ and $Q_{kj}^d$ are the interfacial energy transfers due to phase change and diffusion respectively. The source terms in equations (3) and (4) represent the connection between the macroscopic transport equations and the microscopic solidification model. These source terms are described in subsection 2.2.

The VoF model description assumes that all immiscible fluid phases contained in a control volume are of the same velocity, pressure and temperature field. Adding the volume-averaged equations, such as (3) and (4) will provide a set of basic governing equations describing momentum, mass and energy transport in a single-phase flow. The equations are solved for an equivalent fluid whose physical properties are calculated as functions of the physical properties of its constituent phases and their volume fractions:

$$\rho = \sum_i \alpha_i \rho_i, \quad \mu = \sum_i \alpha_i \mu_i \quad \text{and} \quad c_p = \sum_i \frac{(c_p)_i}{\rho} \alpha_i$$

The conservation equation of volume fraction $\alpha_i$ is

$$\frac{d}{dt} \int_V \alpha_i \, dV + \int_S \alpha_i \, \mathbf{v} \cdot d\mathbf{a} = \int_V S_{\alpha_i} \, dV \quad (6)$$

where $S_{\alpha_i}$ is the source or sink of the $i$-th phase.

2.2. The eutectic growth model

The first analytical model for describing growth of the graphite/austenite eutectic was proposed by Wetterfall et al. [4], who derived the equation of the advancing velocity of the graphite/austenite interface by taking account of mass conservation at the interface, under the assumption that diffusion in austenite is in a steady state. Stefanescu [7] also derived the austenite shell growth velocity

$$\frac{dR_y}{dt} = D_c \frac{R_G}{(R_G - R)} \frac{C^{G/y} - C^{L/y}}{C^{y/L} - C^{L/y}} \quad (7)$$

where $D_c$ is the diffusivity of carbon in austenite. $C^{G/y}$, $C^{y/L}$ and $C^{L/y}$ are the carbon concentration at the graphite/austenite, austenite/liquid and liquid/austenite interface respectively. They are functions of temperature and can be derived from the Fe–C phase diagram. The local fraction of solid is

$$\alpha_s(\mathbf{x}, t) = N(\mathbf{x}, t) \frac{4}{3} \pi R^3(\mathbf{x}, t) \quad (8)$$

where the volumetric density of nucleation $N(\mathbf{x}, t)$ is a function of time and space. To describe nucleation, many authors use the model from Oldfield [8]:

$$N = \mu N \Delta T^2 \quad (9)$$

In this work, the number of activated nuclei is assumed to be constant from the beginning of the calculation. From equation (8), the volume fraction transfer rate is calculated as

$$\left( \frac{\partial \alpha_s}{\partial t} \right)_{ext} = 4 \pi N R^2 \frac{dR_y}{dt} \quad (10)$$

To account for grain impingement, the Johnson-Mehl approximation is used. The volume transfer rate in equation (10) is called extended volume fraction transfer rate, which is obtained under the
assumption that there is still sufficient liquid melt present to allow the grains to grow freely without impingement. Only its fraction is real; if we assume that nucleation occurs randomly, this fraction is approximated as volume fraction of melt, and thus the real volume fraction transfer rate of grey eutectic is calculated as

$$\frac{\partial \alpha_s}{\partial t} = 4 \pi N_{ge} R^2 \frac{dR_n}{dt} \alpha_t$$ \hspace{1cm} (11)

To cover the complete physical model during a eutectic reaction, it is also necessary to model the stable-to-metastable transition. Growth of white eutectic can be modelled based on a nucleation model and velocity at which the solid/liquid interface advances. However, there is some difficulty in handling microscopic morphology since white eutectics have lamellar and rod shapes [5]. In the present work, the emphasis is on implementation of growth competition between grey and white eutectics. A kinetic model that assumes spherical grain growth from Nastac and Stefanescu [5] is adopted.

$$\frac{\partial \alpha_s}{\partial t} = 4 \pi N_{we} R^2 \mu_{we} \Delta T^2 \alpha_t$$ \hspace{1cm} (5)

where $N_{we}$ is the grain density (m$^{-3}$) and $\mu_{we}$ is the growth coefficient of white eutectic. Many authors have proposed a value of $\mu_{we}$ in the range $6.0 \times 10^{-7}$ to $2.4 \times 10^{-6}$ m$^{-1}$. K$^{-2}$.

3. Model parameter study

3.1. Simulation settings, case description

The gray and white eutectic solidification kinetics model has been implemented in STAR-CCM+. The newly introduced parameters are tested and their impacts on phase transition kinetics observed. When applying this model, special attention must be paid to very sensitive parameters. Some parameters may be very difficult to obtain. If it can be shown that a parameter is not sensitive, the use of an approximated value is acceptable. In test cases material parameters used by Wu and Ludwig [9] are shown in Table 1.

| Material parameters used in test case (from Wu and Ludwig [9]). |
| --- | --- | --- | --- | --- | --- |
| Density | $\rho = \rho^{ge} = \rho^{we} = 7027.25$ kg · m$^{-3}$ |
| Heat | $c_p = c_p^{ge} = c_p^{we} = 808.25$ J · kg$^{-1}$ · K$^{-1}$ |
| Thermal conductivity | $K = K^{ge} = K^{we} = 33.94$ W · m$^{-1}$ · K$^{-1}$ |
| Mass latent heat of phase change | $\Delta h = 256476$ J · kg$^{-1}$ |

Table 2. Values of microscopic solidification parameters to be tested.

| Value | Lowest | Lower | Default | Higher | Highest |
| --- | --- | --- | --- | --- | --- |
| $D_C^A$ (m$^2$ · s$^{-1}$) | – | 9.0e–11 | 4.0e–10 | 1.0e–9 | – |
| $R_A^0$ (m) | – | 1.0e–9 | 1.0e–8 | 1.0e–7 | 1.7e–6 |
| $\mu_{we}$ (m$^2$ · s$^{-1}$ · K$^{-2}$) | – | 0.8e–6 | 2.4e–6 | 7.2e–6 | – |
| $N_{ge}$ (m$^{-3}$) | – | 5.0e+9 | 5.0e+10 | 1.0e+12 | 5.0e+12 |
| $N_{we}$ (m$^{-3}$) | – | 5.0e+8 | 1.1e+9 | 2.2e+9 | – |
| $\Delta T_E$ (°C) | – | 10 | 30 | 60 | – |
| $dt/dT$ (K · s$^{-1}$) | – | 0.02 | 0.2 | 2.0 | – |

In equation (7) the diffusion coefficient of carbon in austenite $D_C^A$ was reported by Liu and Elliott [10] to have a value in the range of $9 \times 10^{-7} \sim 1.0 \times 10^{-5}$ cm$^2$ · s$^{-1}$. The initial radius of the austenite shell $R_A^0$ is also required, although this parameter is difficult to measure and is not found in the literature. To estimate an approximately reasonable range, the critical nucleus radius for homogeneous nucleation of copper $1.28 \times 10^{-9}$ m proposed by Kurz and Fisher [11] is taken as the lower limit of
the initial radius of the austenite shell. The upper limit is approximated to be 1% of the final grain radius.

For the growth kinetic of white eutectic, the key parameter is the growth coefficient \( \mu_{we} \). In this study, \( 2.4 \times 10^{-6} \) m \( \cdot \) s\(^{-1} \) \( \cdot \) K\(^{-2} \) by Nastac and Stefanescu [5] it is applied as default value. The volumetric nucleus density for grey and white eutectics, \( N_{ge} \) and \( N_{we} \), used in equations (11) and (12) are estimated according to the values given by Liu and Elliott [10] and Pedersen and Tiedje [12]. The metastable eutectic temperature should be dependent on local composition. The microsegregation model of the third element is not currently included in this implementation; according to Nastac and Stefanescu [5], it is reason to estimate the range to be 10~60 K lower than stable eutectic temperature.

3.2. Discussion of results

The impact of microscopic solidification parameters on the solidification results (temperature \( T \), growth velocity of grey and white eutectic grains \( V \), fraction of solid \( f_s \), fractions of grey and white eutectic \( f_{ge} \) and \( f_{we} \), grey-to-white transition \( G/W \), radius of grey and white eutectic grains \( R \) and mass transfer rate for grey and white eutectic \( M_{ls} \) ) are summarized in Table 3.

| Parameter | \( T \) | \( V \) | \( f_s \) | \( f_{ge} \) | \( f_{we} \) | \( G/W \) | \( R \) | \( M_{ls} \) |
|-----------|--------|--------|---------|---------|---------|--------|-------|--------|
| \( D_C^A \) | 0 | + | 0 | + | + | + | + | 0 |
| \( R_A^0 \) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| \( \mu_{we} \) | + | + | 0 | + | 0 | 0 | 0 | 0 |
| \( N_{ge} \) | + | + | 0 | + | + | 0 | 0 | 0 |
| \( N_{we} \) | + | + | 0 | 0 | 0 | 0 | 0 | 0 |
| \( \Delta T_E \) | − | 0 | − | 0 | + | + | 0 | 0 |
| \( dT/\text{dt} \) | − | + | − | − | + | + | − | + |

The diffusion coefficient of carbon in austenite \( D_C^A \) will not impact the cooling curve much, since the latent heat values of both grey and white eutectic are assumed to be the same. The volume fraction and total mass transfer rate is also not greatly impacted. The grain growth velocity of grey eutectic is proportional to \( D_C^A \), so that the volume fraction of grey eutectic also increases significantly. At the same time, the amount of white eutectic is impacted by the increased amount of grey eutectic. The final ratio of grey and white eutectic phases is significantly impacted by the \( R_A^0 \). The initial radius of the austenite shell \( R_A^0 \) has no impact on predicted solidification results. The growth coefficient of white eutectic \( \mu_{we} \) was shown to have significant impact on cooling curve and grain growth velocity, but no impact on fractions of grey and white eutectic, grain eutectic radius and mass transfer rate. The volumetric nucleus density of grey eutectic \( N_{ge} \) (Figure 1) strongly impacts the predicted fractions of grey and white eutectic and shows a significant impact on cooling curve and solidification velocity. The volumetric nucleus density of white eutectic \( N_{we} \) has almost no impact on the predicted solidification results. The difference between stable and metastable eutectic temperature \( \Delta T_E \) showed a weak impact on solidification velocity, eutectic grain radius and mass transfer rate, as well as significant impact on cooling curve and fractions of grey and white eutectic. The cooling rate applied \( dT/\text{dt} \) is a very important parameter, since its impact on solidification results is very marked.

As an example, results from the parameter test for the volumetric nucleus density of grey eutectic \( N_{ge} \) are given here. The impact of \( N_{ge} \) on the predicted cooling curve, growth velocity of grey and white eutectic grains, fractions of grey and white eutectic, radius of grey and white eutectic, latent heat release rate and mass transfer rate for grey and white eutectic is shown in Figure 1.
Figure 1. Parameter test shows the impact of the volumetric nucleus density of grey eutectic $N_{ge}$ on the solidification results: predicted cooling curve (top left), growth velocity of grey and white eutectic grains (top right), fractions of grey and white eutectic (middle left), radius of grey and white eutectic grains (middle right), latent heat release rate (bottom left) and mass transfer rate for grey and white eutectic (bottom right). The various $N_{ge}$ ($m^{-3}$) values are shown in colour: 5.0e+9 (lower), 5.0e+10 (default), 1.0e+12 (higher) and 5.0e+12 (highest); the line style represents different phases: melt, grey eutectic and white eutectic.
4. Casting trial simulation
The enmeshment of the simulated casting trial geometry is shown in Figure 2. Alongside cast blocks, the gating system and the sand mould, the flasks are also modelled. Results of the solidification simulation are shown in Figure 3: the temperature distribution and fraction of liquid, grey eutectic and white eutectic in a vertical cross-section of a 500 mm thick block. For cast alloy, a ferritic SGI grade EN-GJS-400-18-LT is used and the mould is made of furan resin sand. The initial melt temperature is 1305°C.

Figure 2. Geometry enmeshment of five blocks, gating system, sand mould and flasks; polyhedral mesh with prism layers in 3D-view (top) and vertical section (bottom)

Figure 3. Temperature distribution (middle left) and fractions of liquid (middle right), grey eutectic (bottom left) and white eutectic (bottom right) in cross-section of a 500 mm thick block (top) at approx. 7 h solidification time

A first comparison between measured and simulated temperature curves in a 500 mm thick block is given in Figure 4. The difference in predicted solidification time (approx. 10%) indicates a necessity for further optimization of the heat transfer conditions on the metal/mould interface.

5. Conclusion, Outlook
This paper describes coupling the general multiscale/multiphase modelling framework with the VoF model. An overview of the parameters used in the microscopic model is given, followed by the test case description. Finally, the simulation results of the parameter test are presented. As example, the impact of volumetric nucleus density of grey eutectic on the solidification simulation results (cooling curve, solidification velocity, fractions of grey and white eutectic, eutectic grain radius and mass transfer rate) is given. In the parameter study presented it is shown that variation of the initial radius of the austenite shell \( R_A^0 \) has no impact on the afore-mentioned solidification results. At the same time, the importance of selecting a correct value for cooling rate, volumetric nucleus density of grey eutectic and the difference between stable and metastable eutectic temperature is highlighted. Ongoing
research covers the eutectoid reaction, phase transformations in the solid state and prediction of local mechanical properties.

**Figure 4.** Comparison of measured and calculated temperature curves in a 500 mm thick block

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**References**

[1] The Federal Ministry for Economic Affairs and Energy, Germany 2014 Renewable Energy Sources Act §1 6

[2] Jakumeit J, Subasic E and Bünck M 2014 Shape Casting: 5th International Symposium, ISBN: 978-1-118-88818-6

[3] Jakumeit J, Laqua R, Peric M and Schreck E 2006 Proceedings of Modeling of Casting, Welding and Advanced Solidification Processes XI 63

[4] Wetterfall S-E, Fredriksson H and Hillert M 1972 Solidification process of nodular cast iron *J. Iron Steel Inst.* 210 323–33

[5] Nastac L and Stefanescu D M 1997 Modeling of the stable-to-metastable structural transition in cast iron *Adv. Mat. Research* 4-5 469–78

[6] Beckermann C and Viskanta R 1993 Mathematical modelling of transport phenomena during alloy solidification *Appl. Mech. Rev.* 46 1–27

[7] Stefanescu D M 2007 Modelling of cast iron solidification – The defining moments *Met. Mat. Trans.* A 38 1433–47

[8] Oldfield W 1966 A quantitative approach to casting solidification: freezing of cast iron *Trans. ASM* 59 945–61

[9] Wu M and Ludwig A 2006 A three-phase model for mixed columnar-equiaxed solidification *Met. Mat. Trans.* A 37 1613–31

[10] Liu J and Elliott R 1998 Numerical modelling of the solidification of ductile iron *J. Cryst. Growth* 191 261–7

[11] Kurz W and Fisher D J 1986 *Fundamentals of solidification* Trans Tech Publications Ltd 244

[12] Pedersen K M and Tiedje N S 2008 Graphite nodule count and size distribution in thin-walled ductile cast iron *Mat. Characterization* 59 1111–21