

# Thermophysical Properties Necessary for Advanced Casting Simulations<sup>1</sup>

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Numerical modelling of casting processes has become an up-to-date standard in industry, aiming at a short term design of modern casting with optimized properties. This paper outlines the present modelling approaches and gives an overview on thermophysical properties (parameters) necessary for such simulations. Mould filling and heat transport simulations, stress and strain predictions, Cellular Automaton and phase-field techniques, and recent multiphase volume average approaches are discussed. The number of necessary material properties is shown to be directly correlated to the amount of complexity considered in the corresponding modelling approach.

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**KEY WORDS:** casting; Cellular Automaton technique; heat flow; mould filling; numerical simulation; phase-field technique; solidification; stress and distortion; volume averaging.

## 1. INTRODUCTION

Castings are important in nearly every area of daily life. The essential parts in engines, turbines, and any other machines are castings. Cast parts are used medically, in arts and many everyday objects. However, the production of a casting is quite complicated. Many defects such as cavities, porosity, macrosegregations, cracks or deformations, and distortions may cause the casting to be rejected. Thus, the production of good castings has always needed (and still needs) the expertise of specialists. Since the advance of computer technology, people use numerical models to assist these specialists in designing and producing cast parts with fewer defects.

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<sup>1</sup> Invited paper presented at the Sixth International Workshop on Subsecond Thermophysics, September 26–28, 2001, Leoben, Austria.

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This paper gives an overview on standard and modern simulation techniques for a numerical description of solidification and casting. Mould filling and heat transport simulations, stress and strain predictions, Cellular Automaton and phase-field techniques, and recent multiphase volume average approaches are discussed. Reviews on numerical modelling of solidification and casting processes can be found in Refs. 1–3.

## 2. SIMULATION TECHNIQUES

### 2.1. Heat Flux Simulation with Mould Filling

Nowadays, the simulation of heat flow in the metal and the mould in combination with mould filling can be regarded as a standard for modelling solidification and casting with commercial programs. The basic of every software that is able to simulate casting processes is the solution of the heat flow equation in the metal and the mould. The corresponding equation is given by

$$\frac{\partial}{\partial t} (\rho c_p T) + \vec{\nabla} \cdot (\rho c_p \vec{v} T) = \nabla \cdot (\lambda \nabla T) + \Delta h_f \frac{\partial f_s}{\partial t} \quad (1)$$

Here,  $\rho$  represents the density,  $c_p$  the specific heat capacity,  $\lambda$  the heat conductivity,  $\Delta h_f$  the heat of fusion,  $T$  the temperature,  $\vec{v}$  the velocity of the melt (zero in case of only heat transport), and  $t$  the time. The change of solid fraction with time is commonly replaced by the change of  $f_s$  with temperature via  $\partial f_s / \partial t = (\partial f_s / \partial T)(\partial T / \partial t)$ . Thus,  $f_s(T)$  is an input quantity which should be known from experimental results.

Using this simple differential equation for the solidification process implies that the liquid and the solid are considered as being only one phase with temperature dependent properties. Above the liquidus temperature,  $T_L$ , the corresponding property is given by the property of the liquid, below the solidus,  $T_S$ , by the one of the solid, and between  $T_L$  and  $T_S$  by the property of the solid/liquid mixture. For more complex alloys which solidify with more than one solid phase or which reveal one or more solid state phase transitions, the corresponding property is thought to represent the value of the corresponding phase mixture.

The temperature dependence of the density,  $\rho(T)$ , the specific heat capacity,  $c_p(T)$ , and the heat conductivity,  $\lambda(T)$ , must be known not only for metal and mould but also for all additional components involved in the casting process, such as sand cores, chill plates, etc.

It is well known that surface roughness, surface buckling and/or oxidation will lead to heat resistance at interfaces between different materials. This heat resistance is taken into account by the following empirical relation,

$$q = H \cdot (T_{\text{metal}}^* - T_{\text{mould}}^*). \quad (2)$$

Here,  $q$  represents the heat flow across the interface,  $T_{\text{metal}}^*$  and  $T_{\text{mould}}^*$  are the “macroscopic” temperatures at the interface (here of metal and mould), and  $H$  is the so-called heat transfer coefficient. Although  $H$  is theoretically a function of the interface condition (roughness, gap width, contact pressure, etc.), it is quite often assumed to be a function of  $T_{\text{metal}}^*$  only. Nowadays, more sophisticated models which consider stresses and distortion start to model the heat transfer explicitly by using a functional relation between  $H$  and the gap width and/or the contact pressure [4].

In addition to heat transport, many software packages are able to describe the filling of the mould with the liquid metal [5]. In order to simulate this filling procedure, the Navier–Stokes equation together with the mass conservation equation has to be solved:

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \vec{\nabla} \cdot (\rho \vec{v} \otimes \vec{v}) = -\vec{\nabla} p + \vec{\nabla} \bar{\tau} + \rho \vec{g} \quad \text{with} \quad \bar{\tau} = \rho \mu \{ \vec{\nabla}(\vec{v}) + [\vec{\nabla}(\vec{v})]'\} \quad (3)$$

$$\frac{\partial}{\partial t} \rho + \vec{\nabla} \cdot (\rho \vec{v}) = 0. \quad (4)$$

Here,  $\vec{v}$  represents the velocity of the melt,  $p$  the pressure,  $\bar{\tau}$  the stress tensor,  $\vec{g}$  the gravity vector, and  $\mu(T)$  the kinetic viscosity.  $\otimes$  is the dyadic product. Above  $T_L$ ,  $\mu(T)$  represents the viscosity of the liquid alloy. Below  $T_S$ , the rigid solid reveals a viscosity more than ten orders of magnitude larger than the melt. Between  $T_L$  and  $T_S$ ,  $\mu(T)$  represents the viscosity of the solid/liquid mixture. Depending on the nature of the solidification process, the solid/liquid mixture still may be mobile within the mushy regions. This is taken into account by introducing a coherency temperature somewhere between  $T_L$  and  $T_S$ . Above this coherency temperature, the viscosity of the mixture is just that of the liquid, and below, it is already six to eight orders of magnitude larger. This approach is somehow arbitrary. Nevertheless, apart from special situations in which the gating system is accidentally frozen up during filling, the result of the filling simulation is generally not much influenced by the choice of the coherency temperature and the chosen viscosity enlargement at this temperature.

In order to simplify the simulation of the filling procedure, the flow of the air in the cavity (or other gases) is often neglected. However, the use of

**Table I.** Material Properties Necessary for a Simulation of Heat Flow with Mould Filling (Properties Marked with \* Are Necessary for Both Metal and Mould)

Symbol	Property	Unit
$\Delta h_f$	Latent heat of fusion	$\text{J} \cdot \text{kg}^{-1}$
$T_L, T_S$	Liquidus and solidus temperature	K
$\rho(T)$	Density*	$\text{kg} \cdot \text{m}^{-3}$
$c_p(T)$	Specific heat capacity*	$\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$
$\lambda(T)$	Thermal conductivity*	$\text{J} \cdot \text{s}^{-1} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$
$f_s(T)$	Fraction solid	—
$\mu(T)$	Kinetic viscosity	$\text{m}^2 \cdot \text{s}^{-1}$

simple analytical expressions for the pressure release at venting holes allows the evaluation of the overall pressure within the cavity. The air/melt interface tension as well as oxidation skins at the air/melt interfaces are generally ignored.

In Table I the material properties necessary for a simulation of casting processes considering only heat flow with mould filling are listed.

## 2.2. Simulation of Stresses and Distortion

The prediction of deformations and distortion is quite important for the production of castings with a well defined shape fitting into given limits of tolerance. It is obvious that the thermal contraction of metal and mould, the volume change due to solidification and the nonuniform cooling of the metal and the nonuniform heating of the mould lead to geometrical changes of the cast part. The simulation of stresses and distortion is generally closely related to the temperature history of metal and mould. The basis for such simulations [6–9] is the constitutive equation for the elastic case which relates the elastic strain vector  $\vec{\varepsilon}^{\text{el}} = \{\varepsilon_{xx}^{\text{el}}, \varepsilon_{yy}^{\text{el}}, \varepsilon_{zz}^{\text{el}}, \varepsilon_{xy}^{\text{el}}, \varepsilon_{xz}^{\text{el}}, \varepsilon_{yz}^{\text{el}}\}^T$  to the stress vector  $\vec{\sigma} = \{\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz}\}^T$  via

$$\vec{\sigma} = \bar{\bar{D}}^{\text{el}} \cdot \vec{\varepsilon}^{\text{el}} \quad (5)$$

The elasticity matrix  $\bar{\bar{D}}^{\text{el}}$  is given by

$$\bar{\bar{D}}^{\text{el}} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \vdots & 1-\nu & \nu & 0 & 0 & 0 \\ \vdots & \vdots & 1-\nu & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \frac{1-2\nu}{2} & 0 & 0 \\ \vdots & \text{symmetrical} & \vdots & \vdots & \frac{1-2\nu}{2} & 0 \\ \dots & \dots & \dots & \dots & \dots & \frac{1-2\nu}{2} \end{bmatrix}, \quad (6)$$

where  $E(T)$  stands for the Youngs Modulus and  $\nu(T)$  for the Poisson ratio. Visco-plasticity occurs if the comparison stress reaches the yield stress of the considered material,  $\sigma_y(T)$ . If the van Mises comparison stress,  $\bar{\sigma}$ , is chosen for analysis, the following flow condition counts (van Mises flow condition) [6]

$$\begin{cases} \bar{\sigma} - \sigma_y < 0 & \text{elastic} \\ \bar{\sigma} - \sigma_y = 0 & \text{elastic-plastic} \end{cases} \quad (7)$$

with

$$\bar{\sigma} = \left[ \frac{1}{2} (\sigma_{xx} - \sigma_{yy})^2 + \frac{1}{2} (\sigma_{yy} - \sigma_{zz})^2 + \frac{1}{2} (\sigma_{zz} - \sigma_{xx})^2 + 3(\sigma_{xy}^2 + \sigma_{xz}^2 + \sigma_{yz}^2) \right]^{1/2} \quad (8)$$

Depending on the visco-plastic flow model used, different yield laws can be found in the literature [8, 9]. One often used is given by [6]

$$d\vec{\varepsilon}^{\text{visco-plast}} = \frac{\left\{ \frac{\partial F}{\partial \bar{\sigma}} \right\}^T d\bar{\sigma} \frac{\partial F}{\partial \bar{\sigma}}}{n} \quad \text{with} \quad F = \bar{\sigma} - \sigma_y \quad (9)$$

Here,  $n(T)$  is the hardening coefficient.

During solidification and subsequent cooling of the casting, large temperature changes occur. Theoretically, this can be taken into account by considering the increments of stress and strain. For the total strain increment the following decomposition is valid

$$d\vec{\varepsilon}^{\text{Total}} = d\vec{\varepsilon}^{\text{el}} + d\vec{\varepsilon}^{\text{visco-plast}} + d\vec{\varepsilon}^{\text{therm. expan.}} + d\vec{\varepsilon}^{E(T), \nu(T)}. \quad (10)$$

The last contribution is caused by the temperature dependence of the Young Modulus and the Poisson ratio via  $d\vec{\varepsilon}^{E(T), \nu(T)} = \bar{D}^{\text{elast}} \cdot d\bar{D}^{\text{elast}} \cdot \vec{\varepsilon}^{\text{elast}}$ . The strain increment caused by thermal expansion is given by [6]

$$d\vec{\varepsilon}^{\text{therm. expan.}} = (\alpha dT + \frac{1}{3} \Delta\alpha df_s) \{ 1, 1, 1, 0, 0, 0 \}^T, \quad (11)$$

with  $\alpha(T)$  being the thermal expansion coefficient and  $\Delta\alpha$  the relative volume change on solidification. In most cases  $\alpha(T)$  is artificially modified to include  $\Delta\alpha$ .

With the incremental version of the constitutive equation, Eq. (5), and the expressions for the different strain increments, Eqs. (9)–(11), the following generalized constitutive equation can be derived [6, 9]

$$d\vec{\sigma} = (\bar{D}^{\text{elast}} - \bar{D}^{\text{plast}}) \cdot (d\vec{\varepsilon}^{\text{Total}} - d\vec{\varepsilon}^{\text{therm.expan.}} - d\vec{\varepsilon}^{E(T), \nu(T)}) - d\vec{\sigma}_0 \quad (12)$$

$$\text{with} \quad d\vec{\sigma}_0 = \begin{cases} 0 & \text{elastic} \\ \frac{\bar{D}^{\text{elast}} \frac{\partial F}{\partial \bar{\sigma}} \frac{\partial \sigma_y}{\partial T} \Delta T}{n + \left\{ \frac{\partial F}{\partial \bar{\sigma}} \right\}^T \cdot \bar{D}^{\text{elast}} \frac{\partial F}{\partial \bar{\sigma}}} & \text{elastic-plastic} \end{cases} \quad (13)$$

$d\vec{\sigma}_0$  is a fictive stress which accounts for the temperature dependence of the yield stress. The plasticity matrix is defined as [6, 9]

$$\bar{D}^{\text{plast}} = \frac{9\left[\frac{E}{2(1+\gamma)}\right]^2}{(n+3\left[\frac{E}{2(1+\gamma)}\right]) \cdot \bar{\sigma}^2} \begin{bmatrix} \sigma_1'^2 & \sigma_1'\sigma_2' & \sigma_1'\sigma_3' & \sigma_1'\sigma_4' & \sigma_1'\sigma_5' & \sigma_1'\sigma_6' \\ \vdots & \sigma_2'^2 & \sigma_2'\sigma_3' & \sigma_2'\sigma_4' & \sigma_2'\sigma_5' & \sigma_2'\sigma_6' \\ \vdots & & \sigma_3'^2 & \sigma_3'\sigma_2' & \sigma_3'\sigma_2' & \sigma_3'\sigma_6' \\ \vdots & & & \sigma_4'^2 & \sigma_4'\sigma_2' & \sigma_4'\sigma_6' \\ \vdots & & & & \sigma_5'^2 & \sigma_5'\sigma_6' \\ \dots & \dots & \dots & \dots & \dots & \sigma_6'^2 \end{bmatrix} \quad (14)$$

$$\sigma_1' = \sigma_1 - (\sigma_1 + \sigma_2 + \sigma_3)/3$$

$$\text{with } \sigma_2' = \sigma_2 - (\sigma_1 + \sigma_2 + \sigma_3)/3. \quad (15)$$

$$\sigma_3' = \sigma_3 - (\sigma_1 + \sigma_2 + \sigma_3)/3$$

$G = \left[\frac{E}{2(1+\gamma)}\right]$  is known as the shear modulus. The solution of the generalized constitutive equation, Eq. (12), can be achieved by using the results of the heat flow simulation as input for the stress calculation without any backflow from the stress calculation. In more sophisticated models, as in Ref. 5, possible gaps between different materials are calculated which then influence the change of heat flow across the corresponding interface. An increasing heat transfer caused by a rising contact pressure can also be taken into account by these models.

In Table II the material properties necessary for the simulation of stresses and distortion are listed. Although a rigid dendrite network may be able to pick up small stresses, very often  $E(T)$ ,  $\nu(T)$ ,  $\sigma_y(T)$ , and  $n(T)^{-1}$  have nonzero values only below  $T_S$ . As mentioned above,  $\alpha(T)$  sometimes includes the volume change on solidification. Then,  $\alpha(T)$  has a artificial curve form between  $T_L$  and  $T_S$ .

**Table II.** Material Properties Necessary for a Simulation of Stresses and Distortion (Properties Marked with \* Are Necessary for Both Metal and Mould.)

Symbol	Property	Unit
$E(T)$	Young's Modulus*	MPa
$\nu(T)$	Poisson's ratio*	-
$\sigma_y(T)$	Yield stress*	MPa
$n(T)$	Hardening coefficient*	-
$\alpha(T)$	Thermal expansion*	K <sup>-1</sup>
$\Delta\alpha$	Relative volume change on solidification	-

### 2.3. Cellular Automaton Technique

Cellular Automata (CA) for the prediction of the evolution of dendritic grains during solidification have achieved quite promising results [10–14]. These kinds of simulations are based on two different interacting modelling strategies. On the one hand, the temperature distribution is calculated by solving the heat flow equation, Eq. (1), on a relatively coarse FD or FE grid. On the other hand, the actual Cellular Automaton acts on a much finer regular grid. The volume elements of this CA grid should be smaller than the grains to be modelled. In sophisticated programs the Cellular Automaton estimates the amount of latent heat to be released (via nucleation and growth of grains). This amount of latent heat is then taken into account by the heat flow simulation. From the heat flow simulation the CA obtains the actual temperature at each CA volume element by interpolation. Therefore, in these programs the heat flow simulation and CA are strongly coupled [12–14].

Generally, a Cellular Automaton is characterized by (i) the geometry of the cells (volume elements of the CA grid), (ii) the state of a cell, (iii) the relation to its neighbors, and (iv) a rule for the change of the cell state [10]. In order to describe a solidification process the cell state may be defined as “liquid,” “mushy,” or “boundary.” A “liquid” state means that the metal in the cell is totally liquid, a “mushy” state means that it is totally mushy (partly liquid and partly solid), and the “boundary” state denotes that an envelope of a dendritic grain is located within this cell. The rule for a change of a cell state (i) physically describes the nucleation and the grain growth and (ii) the actual state of the corresponding cell and its neighbors. This paper does not give detailed descriptions of the numerical procedure of a Cellular Automaton. However, as new material parameters are introduced, the corresponding model considerations to describe nucleation and growth are briefly described.

Nucleation is thought to be a stochastic process which is modelled on probability. In order to distinguish heterogeneous nucleation at the metal/mould interface and heterogeneous nucleation in the bulk melt, two distributions of nucleation sites,  $dn/d(\Delta T)$ , are considered. Such distributions describe the grain density increase,  $dn$ , which is induced by an increase in the undercooling  $d(\Delta T)$ . In Refs. 10–14 a Gaussian distribution according to

$$\frac{dn}{d(\Delta T)} = \frac{n_{\max}}{\sqrt{2\pi} \Delta T_{\sigma}} e^{-\frac{1}{2} \left( \frac{\Delta T - \Delta T_N}{\Delta T_{\sigma}} \right)^2} \quad (16)$$

is used. Here,  $n_{\max}$  represents the maximal possible grain density,  $\Delta T_N$  the undercooling at which a maximum nucleation rate is obtained, and  $\Delta T_{\sigma}$  the

Gaussian distribution width. The total density of grains,  $n(\Delta T)$ , at a given undercooling,  $\Delta T$ , is given by

$$n(\Delta T) = \int_0^{\Delta T} \left( \frac{dn}{d(\Delta T')} \right) [1 - f_s(T')] d(\Delta T'). \quad (17)$$

where the extinction of nucleation sites by the growing grains is also taken into account. For the presented nucleation model  $n_{\max}$ ,  $\Delta T_N$ , and  $\Delta T_\sigma$  should be known from experimental results. They are generally considered not to be temperature-dependent.

Recently, an alternative nucleation model for the prediction of grain size in inoculated castings has been suggested [15]. The model assumes that each refiner particle of diameter  $d$  is immediately covered with solid. Nevertheless, the solid can only grow if its curvature (which is now inversely proportional to  $d$ ) falls below the critical nucleation curvature. This leads to the following condition for the necessary undercooling for further growth,

$$\Delta T_{\text{fg}} = \frac{4\sigma}{\Delta s_f d}. \quad (18)$$

Here,  $\sigma$  represents the solid/liquid interface tension, and  $\Delta s_f$  the entropy of fusion. As refiners do reveal a size distribution, Eq. (18) turns this distribution into an undercooling distribution which defines the amount of nucleation events occurring at different undercoolings. For this nucleation model  $\sigma$ ,  $\Delta s_f$ , and the size distribution of the refiner particle must be known. Again, these input parameters are assumed not to be temperature-dependent.

Cells which are thought to have nucleated change their state from "liquid" to "boundary." In the middle of such a cell, a dendritic grain is considered to grow according to the following growth law,

$$v(\Delta T) = a_2 \Delta T^2 + a_3 \Delta T^3. \quad (19)$$

Here,  $a_2$  and  $a_3$  are empirical constants which depend on the material under consideration. Dendritic growth theory is able to relate these constants to the redistribution coefficient,  $k$ , the liquidus slope,  $m$ , the solid/liquid interface tension,  $\sigma$ , the entropy of fusion,  $\Delta s_f$ , and the diffusion coefficient  $D$ . Therefore, either  $a_2$  and  $a_3$  should be known from experimental results or  $k$ ,  $m$ ,  $\sigma$ ,  $\Delta s_f$ , and  $D$  must be known if the dendritic growth theory is applied. As usually during the growth of grains the temperatures do not change drastically, the above quantities can be considered not to be temperature-dependent.



**Table III.** Material Properties (Parameters) Necessary for a Cellular Automaton Simulation (In Addition to These Quantities, the Properties Listed in Table I Are also Needed. Quantities Marked With <sup>+</sup> May Replace the Growth Parameters  $a_2$  and  $a_3$ . Following a New Nucleation Law [15], the Nucleation Parameters Can Be Replaced by Corresponding Parameters for the Description of the Size Distribution of Refiner Particles)

Symbol	Property	Unit
$n_{\max}, \Delta T_\sigma, \Delta T_N$	Nucleation parameter (see Eq. (16))	$\text{m}^{-3}, \text{K}, \text{K}$
$a_2, a_3$	Growth parameter (see Eq. (19))	$\text{m} \cdot \text{s}^{-1} \cdot \text{K}^{-2}, \text{m} \cdot \text{s}^{-1} \cdot \text{K}^{-3}$
$D_l(T)$	Diffusion coefficient in the liquid <sup>+</sup>	$\text{m}^2 \cdot \text{s}^{-1}$
$m(T)$	Liquidus slope <sup>+</sup>	$\text{K}/\text{wt.}\%$
$k(T)$	Redistribution coefficient <sup>+</sup>	–
$\sigma(T)$	Solid/liquid interface tension <sup>+</sup>	$\text{J} \cdot \text{m}^{-2}$
$\Delta s_f$	Entropy of fusion <sup>+</sup>	$\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$

Tracking the actual size of the grain shows whether or not the growing grain hits a neighboring cell and “infects” it with solidification. As the grains are considered to have a cubic envelope, preservation of the grain orientation has to be handled with special care. Otherwise, the orientation of a growing grain switches to the main direction of the underlying CA grid.

Table III shows material properties (parameters) necessary for a Cellular Automaton calculation.

## 2.4. Phase-Field Method

In recent years the number of papers on phase-field simulations has rapidly increased [16–28]. Early simulations only considered dendritic growth of pure materials into undercooled melts. In the next step, solutal dendrites were modelled. Nowadays, multiphase approaches for eutectic, peritectic, and monotectic solidification processes as well as phase-field models for solidification with convection are available.

The basis for such simulations is the introduction of a quantity called phase-field  $\phi(r, t)$ . This quantity is defined to be 1 in the solid and 0 in the liquid. At the solid/liquid interface its value changes continuously from 1 to 0. In the case of a multiphase approach a phase-field variable is introduced for each of the  $n$  phases present in the system.  $\phi_1 + \dots + \phi_n = 1$  is always valid. For the phase-field  $\phi(r, t)$  a differential equation is derived which allows the estimation of the time-dependent spatial distribution. The following differential equation is often used:

$$\frac{1}{M_\phi} \frac{\partial \phi}{\partial t} = \varepsilon^2 \nabla^2 \phi - \frac{\partial f(\phi, c, T, W)}{\partial \phi}. \quad (20)$$

Here,  $f(\phi, c, T, W)$  represents the Gibb's free energy density taken from thermodynamic considerations.  $W$  is a constant which is proportional to the energy barrier between solid and liquid (height of the double-well potential).  $\varepsilon$  is a quantity representing the effect of the solid/liquid interface tension mathematically, and  $M_\phi$  describes how quickly the system tends to equilibrium.

In the phase-field technique it is essential that the solid/liquid interface ( $\phi = 1 \rightarrow \phi = 0$ ) extends over a certain distance  $\Delta_\phi$ . To simulate the evolution of the solidification microstructure on a microscopic scale of a few microns,  $\Delta_\phi$  must be chosen to be much larger than the true solid/liquid interface width of only a few nanometers. Theoretically, the phase-field equation, Eq. (20), can be evaluated for the case that  $\Delta_\phi$  tends towards the true solid/liquid interface width  $\delta$ . This so-called sharp interface asymptotic is used to relate  $W$ ,  $\varepsilon$ , and  $M_\phi$  to the material properties solid/liquid interface width,  $\delta$ , solid/liquid interface tension,  $\sigma$ , and kinetic coefficient,  $\mu_k$ . The following proportionalities were found [16–18],

$$\delta \approx \varepsilon / \sqrt{W}, \quad (21)$$

$$\sigma \approx \varepsilon \sqrt{W}, \quad \text{and} \quad (22)$$

$$\mu_k \approx M_\phi \varepsilon / \sqrt{W}. \quad (23)$$

$\mu_k$  is defined via  $V = \mu_k(T_L - T)$ , with growth velocity,  $V$ , and undercooling,  $(T_L - T)$ . The anisotropic nature of the solid/liquid interface tension  $\sigma(\theta)$  and that of the kinetic coefficient  $\mu_k(\theta)$  (mostly equivalent and a four-fold symmetry for cubic materials and a six-fold symmetry for hexagonal materials at the basal plane) gives an anisotropy of  $\varepsilon(\theta)$  and  $M_\phi(\theta)$ .

As in the phase-field technique the solid/liquid interface is not sharp and the difference in the solubility of liquid and solid cannot be taken into account simply by a boundary condition at the interface. Therefore, the thermodynamic background of the difference in the solubility is considered. This then leads to a somewhat different diffusion equation compared to the usual one

$$\frac{\partial c}{\partial t} = \nabla \cdot \left[ M_c c(1-c) \nabla \left( \frac{\partial f(\phi, c, T, W)}{\partial c} \right) \right]. \quad (24)$$

Here,  $M_c$  represents how quickly the system tends to chemical equilibrium. For  $M_c$  the following relation can be derived

$$M_c = \frac{v_m}{RT} (D_L \phi + D_S(1-\phi)). \quad (25)$$

$v_m$  represents the molar volume,  $R$  the gas constant, and  $D_L$  and  $D_S$  the diffusion coefficient in the liquid and the solid. For a simulation of an alloy solidification the phase-field equation, Eq. (20), and the modified diffusion equation, Eq. (24), have to be solved simultaneously.

Table IV shows the material properties necessary for a phase-field simulation. In the case of multiphase simulations it is necessary to know the values for  $\delta$ ,  $\sigma$ , and  $\mu_k$  for each pair of phases. In addition, the Gibb's free energy density must be known as a function of all phase variable,  $f(\phi_1, \dots, \phi_n, c, T, W)$ . In most cases the temperature dependence of the material properties are neglected because the calculation domain does not involve large temperature changes.

## 2.5. Multiphase Volume Averaging

The multiphase volume averaging technique allows the prediction of macrosegregations (macroscopic concentration inhomogeneities) in columnar solidifying castings (without moving solid) [29–35] or in equiaxed solidifying castings (with moving solid) [36–40].

In the multiphase volume averaging technique applied to solidification, both liquid and solid are treated as interpenetrating and interacting “fluids.” The volume fractions are assumed to be continuous functions of space and time and their sum is equal to one:

$$f_l + f_s = 1 \quad (26)$$

Conservation equations for each phase are derived. These equations include different interaction terms through which the microscopic solidification phenomena are incorporated into the conservation equations. For the

**Table IV.** Material Properties (Parameters) Necessary for a Phase-Field Simulation  
(In Addition to these Quantities, the Properties Listed in Table I Are also Needed.  
 $\sigma$  and  $\mu_k$  Depend on the Crystal Orientation  $\theta$ )

Symbol	Property	Unit
$\sigma(\theta)$	Solid/liquid interface tension	$\text{J} \cdot \text{m}^{-2}$
$\mu_k(\theta)$	Kinetic coefficient	$\text{m} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$
$\delta$	Thickness of the solid/liquid interface	$\text{m}$
$D_l(T, c)$	Diffusion coefficient in the liquid	$\text{m}^2 \cdot \text{s}^{-1}$
$D_s(T, c)$	Diffusion coefficient in the solid	$\text{m}^2 \cdot \text{s}^{-1}$
$\gamma_m$	Molar volume	$\text{m}^3$
$f(\phi, T, c, W)$	Gibb's free energy density	$\text{J} \cdot \text{m}^{-3}$

phase  $i$  (solid:  $s$ , liquid:  $l$ ) the conservation equations of mass, momentum, species, and enthalpy are given as

$$\frac{\partial}{\partial t} (f_i \rho_i) + \nabla \cdot (f_i \rho_i \vec{v}_i) = M_i, \quad (27)$$

$$\frac{\partial}{\partial t} (f_i \rho_i \vec{v}_i) + \nabla \cdot (f_i \rho_i \vec{v}_i \otimes \vec{v}_i) = -f_i \nabla p + \nabla \cdot \bar{\tau}_i + f_i \rho_i \vec{g} + \vec{U}_i$$

with  $\bar{\tau}_i = \rho_i \mu_i f_i (\nabla \cdot \vec{v}_i + (\nabla \cdot \vec{v}_i)^T),$  (28)

$$\frac{\partial}{\partial t} (f_i \rho_i c_i) + \nabla \cdot (f_i \rho_i \vec{v}_i c_i) = \nabla \cdot (f_i \rho_i D_i \nabla c_i) + C_i, \quad (29)$$

$$\frac{\partial}{\partial t} (f_i \rho_i h_i) + \nabla \cdot (f_i \rho_i \vec{v}_i h_i) = \nabla \cdot (\lambda_i \nabla \cdot T_i) + Q_i$$

with  $h_i = \int_{T_i^{\text{ref}}}^{T_i} c_{p,i} dT + h_i^{\text{ref}}.$  (30)

Here,  $\rho_i(T)$  represents the density,  $\mu_i(T)$  the viscosity,  $D_i(T)$  the diffusion coefficient,  $\lambda_i(T)$  the thermal conductivity, and  $c_{p,i}(T)$  the specific heat capacity of phase  $i$ .  $T_i^{\text{ref}}$  is the reference temperature and  $h_i^{\text{ref}}$  the corresponding reference enthalpy of phase  $i$ . The quantities velocity,  $\vec{u}$ , concentration,  $c$ , enthalpy,  $h$ , and temperature,  $T$ , do have a phase index, because they are separately defined for solid and liquid. However, because of the ideal heat transfer between the solid grains and the surrounding melt, the temperature of solid and liquid is assumed to be equal. The mass transfer rate from (or to) the phase  $i$  is described by  $M_i$ , the momentum transfer rate by  $U_i$ , the species transfer rate by  $C_i$ , and the enthalpy transfer rate by  $Q_i$ . The essential modelling considerations in the multiphase volume averaging techniques are within the definition of this exchange term. However, this paper only briefly reviews selected details of the exchange terms.

The choice of an adequate model for the mechanical momentum exchange between moving dendritic grains and the flowing melt is the subject of ongoing scientific discussions. Commonly, this exchange term is described by  $\vec{U}_{sl}^d = K_{sl}(\vec{u}_s - \vec{u}_l)$ .  $K_{sl}$  ( $= K_{ls}$ ) is called the interphase momentum exchange coefficient. The most general expression for  $K_{sl}$ , valid for a solid fraction from zero up to 0.7, is the classical model of Kozeny–Carman [31]. For a solid which is resting and behaves like a porous medium, the most general model for  $K_{sl}$  is that of Blake–Kozeny [31]. These two models can be combined if a critical solid volume fraction above

which equiaxial crystal merge to form a rigid solid structure,  $f_s^{\text{crit}}$ , is introduced:

$$\begin{aligned} K_{sl} &= -18f_l^2 \frac{\mu_l f_s C_e}{d^2} & \text{for } f_s \leq f_s^{\text{crit}} & \quad \text{with } C_e = 10 \frac{f_s}{f_l^3} \\ &= -f_l^2 \frac{\mu_l}{K} & \text{for } f_s > f_s^{\text{crit}} & \quad \text{with } K = K_0 \frac{f_l^3}{f_s^2}. \end{aligned} \quad (31)$$

Here, empirical expressions for the settling ratio,  $C_e$ , and the overall permeability,  $K$ , are also given.  $d$  represents the average grain diameter and  $K_0$  an empirical constant. In columnar dendritic solidification the permeability of the mushy zone is known to be anisotropic; it differs normal and parallel to the dendrite trunks.  $d$  is evaluated from a conservation equation for the grain density which includes nucleation (and disappearance of grains). Thus, a nucleation law has to be considered, and needs parameters such as  $n_{\text{max}}$ ,  $\Delta T_N$ , and  $\Delta T_\sigma$  (see Section 2.3).

As mentioned above, the solid phase is treated as pseudo fluid; hence, the solution to its momentum conservation equation requires the solid phase to have ‘‘viscosity.’’ This effective solid viscosity is thought to be caused by collisions between individual rigid grains. For equiaxial crystals, the effective solid viscosity increases with increasing solid volume fraction and crystal size because of stronger crystal interactions. For  $f_s > 0.2$ , the solid/liquid mixture can be viewed as a nonNewtonian slurry, with the viscosity depending on crystal size and shape, the solid fraction, and the shear rate [31]. The exact nature of the corresponding relation for the effective solid viscosity is still not known. As Ishii and Zuber [41] found for the viscosity of a solid/liquid mixture

$$\mu_{\text{mix}} = \mu_l (1 - f_s / f_s^{\text{crit}})^{-2.5 \cdot f_s^{\text{crit}}} \quad (32)$$

and because of  $\mu_{\text{mix}} = f_l \mu_l + f_s \mu_s$  it is proposed [31] that

$$\mu_s = \frac{\mu_l}{f_s} \left( (1 - f_s / f_s^{\text{crit}})^{-2.5 \cdot f_s^{\text{crit}}} - (1 - f_s) \right). \quad (33)$$

For  $f_s > f_s^{\text{crit}}$ , as well as for columnar growth at any solid fraction (no solid movement),  $\mu_s$  is infinitely large.

In Ref. 32 the effect of back-diffusion (diffusion from the solid/liquid interface towards the inside of a dendritic grain) on the appearance of macrosegregation is modelled by introducing two new quantities: the ratio between the solid/liquid interface area and the volume of a dendritic grain,

$S_s$ , and an effective diffusion length in the solid grain,  $l_s$ . With these two quantities the species transfer rate is given by

$$C_l = kc_l \left( M_l + S_s \frac{\rho_s D_s}{l_s} \right). \quad (34)$$

The first term in the bracket of Eq. (34) describes the solute redistribution caused by a mass transfer  $M_l$  (solidification and/or remelting) and the second the contribution from back-diffusion.

Table V shows the material properties necessary for a multiphase volume averaging simulation applied to solidification. According to the complexity of the model used additional quantities may be necessary.  $K_0$ ,  $S_s$ , and  $l_s$  are quantities which are rarely known. Here, the dependence on the dendrite arm spacing,  $\lambda_2$ , seems to be much more important than temperature dependence.

### 3. CONCLUSIONS

From the description of the different simulation techniques, the following conclusions can be drawn:

- Physical models for a process description, such as solidification and casting, need material property data as input.

**Table V.** Material Properties (Parameters) Necessary for a Volume Averaging Simulation With and Without Moving Solid Phase ( $K_0$ ,  $S_s$ ,  $l_s$  May Depend on Microstructure Quantities such as the Dendrite Arm Spacing,  $\lambda_2$ . According to the Complexity of the Model Used, Additional Quantities May Be Necessary)

Symbol	Property	Unit
$T_L, T_S$	Liquidus and solidus temperature	K, K
$h_l(T), h_s(T)$	Enthalpy of $l$ and $s$	$\text{J} \cdot \text{kg}^{-1}$
$\rho_l(T, c), \rho_s(T, c)$	Density of $l$ and $s$	$\text{kg} \cdot \text{m}^{-3}$
$c_{p,l}(T), c_{p,s}(T)$	Specific heat capacity of $l$ and $s$	$\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$
$\lambda_l(T), \lambda_s(T)$	Thermal conductivity of $l$ and $s$	$\text{J} \cdot \text{s}^{-1} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$
$\mu_l(T), \mu_{\text{mix}}(T)$	Kinetic viscosity of $l$ and the $s/l$ mixture	$\text{m}^2 \cdot \text{s}^{-1}$
$D_l(T, c), D_s(T, c)$	Diffusion coefficient in $l$ and $s$	$\text{m}^2 \cdot \text{s}^{-1}$
$k(T)$	Redistribution coefficient	–
$m(T)$	Liquidus slope	$\text{K}/\text{wt.}\%$
$K_0$	Permeability constant (see Eq. (31))	$\text{m}^2$
$f_s^{\text{crit}}$	Limit for solid mobility	–
$n_{\text{max}}, \Delta T_\sigma, \Delta T_N$	Nucleation parameter (see Eq. (16))	$\text{m}^{-3}, \text{K}, \text{K}$
$S_s$	Solid/liquid interface area per volume	$\text{m}^{-1}$
$l_s$	Average diffusion length in dendr. grain	$\text{m}$

- The more sophisticated the model, the more material properties (parameters) are involved.
- However, reasonable data for material properties necessary for standard simulation models are often quite difficult to find. Even worse is the situation for properties needed in more sophisticated numerical models such as Cellular Automaton and phase-field techniques or multiphase volume averaging methods. They are only known in very few cases.
- In conclusion, we predict that the absence of reasonable material property data will act as a brake on the use of sophisticated models in industrial daily routines. Thus, we believe that global economic growth is hindered by the lack of material data.

## ACKNOWLEDGMENTS

The author would like to acknowledge the members of the subgroup “Thermophysical Data” of the EU-network MEBSP “Microstructural Engineering by Solidification Processing” for many important discussions during several subgroup meetings, especially P. Quested from NPL, Teddington (UK). In addition, the author expresses his gratitude to P. R. Sahm, Director of the Foundry Institute of the Technical University Aachen, for his strong personal support over the last decade.

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