

Model of heat flow during crystallisation of cast composites

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Analysis and modelling

ABSTRACT

Purpose: The aim of this work was to show possibilities of numerical simulation software, based on heat transfer model, commonly used in foundry industry in cast composite properties engineering.

Design/methodology/approach: The main restriction in most of used software systems is lack of heat transfer, which may occur at composite creation. In this work the reinforcing particle morphology and size were expressed by one quantity – morphological modulus M_m and were examined for influence on heat transfer and conductivity up to the Newton's and Fourier's laws.

Findings: The main restrictions for using Fourier's model based software for composite engineering are shown. The way for crystallization control was presented including influence of morphology, transition zone and thermo-physical properties of components.

Research limitations/implications: Proposed methodology can be used for cast composite properties engineering in cases, where relative motion of components is negligible. In other cases heat transfer coefficient is justified only if the software used is based on Fourier's model and the source code is accessible.

Originality/value: Proposed assumptions create possibility for components selection verification in terms of technological and operating properties of cast composite. An example of such approach was shown in work [1, 23].

Keywords: Casting; Solidification; Composite; Reinforcing particles morphology; Simulation

1. Introduction

The main aim of this work was the optimization of cast composite properties with use of crystallization process control by means of thermo-physical and morphological properties of components used. The main components which may influence heat flow kinetics are metal matrix and reinforcing particles in casting – mould system. From this point of view composite manufacturing and study methodologies are carry some limitations. Identification and analysis of restrictions occurring in solidification process examination is connected with experimental methods and physical models used in numerical simulation software. Proper interpretation of assumptions can enable attaining high properties of cast composites.

2. The components effective properties and technological parameters

The most common state in industrial conditions is when reinforcement temperature is lower than matrix temperature. From proper wettability point of view the opposite case is more beneficial.

2.1. Methodology of components selection

Among reinforcing materials one can distinguish four groups, from thermo-physical point of view:

1. Heat – insulating ceramic materials with very low heat conductivity

2. Ceramic materials with high heat conductivity – based on silicon carbide. Phases with this component show hat conductivity of up to 10 W/mK, while pure SiC reaches 80 W/mK.
3. Carbon materials (without graphite) with conductivity of 4 – 8 W/mK na amorphic quartz materials with heat conductivity of up to 2 W/mK.
4. Materials with high heat conductivity, but out of ceramic range – metallic and graphite reinforcing components. Graphite materials, depending on manufacturing technology can reach heat conductivity of 50 – 200 W/mK.

In majority of crystalline materials additionally the thermal anisotropy can occur, which must be taken into account in some applications, for example gradient composites. Influence of reinforcing material properties anisotropy can reveal by use of physical factors improving composite manufacturing. As an example composite casting n magnetic field can be shown.

Assuming equal temperature of metal matrix and reinforcing particles by composite creation, their heat ratio can be shown as:

$$I_q = \frac{\rho_o [c_o(T_o - T) + L]}{\rho_z c_z (T_z - T)} \quad (1)$$

where: ρ , c , L – are, respectively, mass density, specific heat and crystallization heat, o , z indices refer o matrix and reinforcement.

For Al alloys and popular ceramic materials $I_q \approx 1 \div 2$, where upper value refers to graphite and lower to corundum particles. Three cases can be observed: the ratio value is below 1, equal to 1 and above 1. First case shows, that after temperature equalization, the reinforcement accumulate more heat than the matrix. This is the opposite situation to third case. Case of equal numerator and denominator is hard to obtain, furthermore with including temperature dependent specific heat and density. Nevertheless, such theoretical cases cannot be neglected. Third case, with lower heat capacity of reinforcement than the matrix is a singularity. During solidification can significantly shorten solidification time, causing decrease of main thermal gradient and increase in solidification rate. The initial conditions of such case have to be emphasized: equal temperature of matrix and reinforcement. This is a special case, neglecting measurements precision. Every difference in initial state causes different temperature distribution, thus causing changes in structure.

The particular case is when both components have the same temperature. This state is momentary in technological process. To minimize temperature difference between the components the melt should be intensively stirred. To obtain metal stirring in the mould the force field can be used (electromagnetic etc.).

If the heat conductivity of the reinforcement is lower than the matrix, then even with neglected statistically small heat resistance, form a moment, determined by specific temperature and time, the reinforcing particles create volumes with the highest temperature. In most cases these volumes have smaller heat capacity than the matrix which emits crystallization heat in short time. When the heat conductivity of reinforcement is higher than the matrix the heat can flow from the matrix to the particles (reversed heat transfer) only when the technological process does not enable real temperature equalization. Such case is most desirable for suspensive casting with so-called internal micro-chills. This requires precise calculation of heat diffusion in function of time and in range of matrix solidification.

The amount of heat accumulated in elementary volumes can be controlled by technological treatment, so depending on needs were equal or different. Complications occur when heat transport implicates significant differences in thermal expansion below solidus temperature, which can cause decohesion or rather deadhesion of components and degradation of composite properties. Among these relatively easy one can control the temperature. Other factors, like thermal properties: density and specific heat of components, can be controlled in small range because of negligible variation. Thermal properties regulation by means of chemical composition is often reduced to chemical purity selection. If for proper structure obtainment in casting is necessary to reach assumed cooling rate, then in material with low heat conductivity it is possible only by higher thermal gradient. In other words, forcing assumed cooling rate on thermally different materials interface occurring thermal gradient will be higher when for example reinforcement heat conductivity is much lower than the matrix. Interval of gradient equalization of thermal gradient or its minimization will be greater when reinforcing particle has higher heat capacity. Conditions closer to III boundary conditions cause more stable heat flow. In solidification process regions on matrix/particle interface filled with gas behave as thermal resistance, which can be treated as infinite. In material with lower heat conductivity with assumed cooling rate range of directional structure will be greater than in case of full wetting. It is necessary to control local concentration of elements, transition zone and surface-active additions.

The difference of heat conductivity for reinforcing materials reaches three orders of magnitude ($10^{-1} \div 10^1$ W/mK). Specific heat and mass density differ in range of the same order. Significant difference in heat conductivity restrict in experimental procedure use of statistically symmetrical models of experiment. While the heat capacity b can represent basic thermal properties of reinforcing particles as well as properties of matrix. As a alternative the heat accumulation coefficient can be indicated. The main factor influencing the heat accumulation factor (2) is the crystallization heat:

$$b_o = \sqrt{\lambda_o \rho_o \left(c_{po} + \frac{L_o}{\Delta T} \right)} \quad (2)$$

where: b , λ , ρ , c_p , L , T are, respectively: heat accumulation coefficient, heat conductivity, mass density, specific heat, crystallization heat, temperature, index o refers to the matrix.

In other cases – where is no phase change, heat accumulation factor is described by relation (3):

$$b_z = \sqrt{\lambda_z \rho_z c_{pz}} \quad (3)$$

where: index z refers to reinforcement particles in solid state, without phase changes.

Other physical quantity, which may also describe basic thermal properties is heat diffusivity (4, 5):

$$a_o = \frac{\lambda_o}{\rho_o \left(c_{po} + \frac{L_o}{\Delta T} \right)} \quad (4)$$

$$a_z = \frac{\lambda_z}{\rho_z c_{pz}} \quad (5)$$

where: a is the heat diffusivity.

In table 1 basic thermal properties of components are correlated [2, 3].

Composites manufactured from described components have similar tribological properties, although their solidification conditions were different. Heat conductivity of selected ceramic materials changes approximately with square. Changes comparison is shown in last three columns. The ability to accumulate heat varies proportional. This fact creates possibility of easy to conduct experimental verification for group of wear – resistant composites. AlSi alloys have many practical applications. Presence of some elements, for example magnesium, increases the wetting ability, but also causes occurrence of intermetallic phases such as Mg₂Si by 868 K, Mg₂Si by 828 K, FeSiAl₅ by 848 K, FeMg₃Si₆Al₈ by 840 K, FeSiAl₅ by 885 K [5]. Occurring phases crystallize in temperature near the eutectic point of AlSi – 850 K. Reinforcing particles presence changes the proceeding processes, thus limitation of heat effects connected with additional phases crystallization is necessary. Composite studies results often refer to metal matrix alloy. It is also often unavoidable to employ chemical surface-active agents, which condition composite creation process. They can affect also the matrix structure. Minimization of their content to range of (0,05 – 0,3%) is easy to attain in technological process [6].

2.2. Particularity of solidification process numerical analysis

Numerical analysis is complementary to experimental methods. Its precision depends on engaged physical model for studied phenomena. Correctness of numerical simulation is based mainly on proper modeling of composite solidification conditions. The basic analysis is composite micro-region analysis containing all composite structural components. Primal object is here the analysis of matrix structure near the reinforcing particle. As a result some temperature distribution fields are obtained and respectively – first temperature derivative after time and direction in function of time. The basic case representing composite micro-

region geometry is a particle with statistically representative shape and dimensions surrounded by metal matrix and eventual incomplete wetting regions and transition zone phases. In such case it is needed to match the mesh with reinforcing particles, occurring transition phases and incomplete wetting regions because the size of last two are significantly smaller than reinforcing particle. This mainly applies to ex situ composites, but also in in situ composites transition zone phases can occur. Calculations are mainly based on central located reinforcing particle and assigned to it volume of the matrix. Such approach enables zero heat flux assumption on, for example two heat flow directions. Analyzed is only one main direction of heat flow. Numerical analysis for particle located on heat flow direction is justified. Although such analysis for spherical particle is simple, the experimental validation is not.

Solidification process studies refer to phenomena in micro scale: selected morphology of reinforcing particle and in macro scale: in gating system and mould. Application of simulating software enables arbitrary localization of thermo-elements in optional small region. There is also a possibility of temperature observation on crystallization front. The most valuable advantage is the possibility of arbitral association of thermal and geometrical properties for composite systems. Such analyses, connected with numerous calculations are out of reach in experimental studies. Scale of model does not influence calculation method. Simulation software based on Fourier – Kirchhoff's model is widely applied for metals and alloys. In cast composites reinforced with ceramic particles the solidification process differs from solidification of pure matrix.

A proposal for notation of equation describing separately composite components referring to their morphology has been made. One can show that particle shape influences the heat flow in matrix – reinforcement composite system. With assumption of reinforcement elementary volume DV, contact surface DF – with 0 thickness, which is common for matrix and reinforcement and represents complete contact of components and morphological modulus Mm.

Assuming as a initial state case of equal temperature of matrix and reinforcing particle and complete wetting in this system quantity of heat flux referring to elementary surface perpendicular to the interface is a scalar product n versor and thermal gradient:

$$q_n(r, t) = -\lambda n \circ gradT(r, t) \quad (6)$$

Table 1.
Basic thermal properties for deferent components

component	mass density ρ	specific heat c _p	crystallization heat L	heat conductivity λ	thermal diffusivity a	heat accumulation b
	10 ⁶ g/m ³	kJ/kgK	kJ/kg	W/mK	10 ⁻⁶ m ² /s	10 ³ Ws ^{0,5} / (m ² K)
SiO ₂	2,3	1,04	-	1.6	0,67	1,96
Al ₂ O ₃	3,9	1,07	-	3.7	0,89	3,93
SiC	2,9	1,03	-	16.5	5,52	7,02
AlSi11*	2,5	1,19	389	130,0	0,53	178,87

*) data for matrix alloy was determined as an average for solidification range assuming ΔT=4 K [4]

Heat quantity flowing through ΔF surface in Δt time equals to:

$$Q_n(r, t) = -\lambda \bar{n} \circ \text{grad} T \Delta F \Delta t \quad (7)$$

where:

λ – heat conductivity coefficient,

r – generalized space variable, t - time, T - temperature,

F – heat transport surface.

In general, energy equation consistent with I thermodynamic rule for dispersive reinforcing elements can be assumed as:

$$c\rho \frac{\partial T(r, t + \Delta t) - T(r, t)}{\Delta t} \Delta V = \frac{\partial}{\partial r} \left[\lambda \Delta F \frac{\partial T(r, t)}{\partial r} \right] \Delta r \quad (8)$$

for $\Delta t \rightarrow 0$

$$c\rho \frac{\partial T(r, t)}{\partial t} \Delta V = \frac{\partial}{\partial r} \lambda \left[\Delta F \frac{\partial T(r, t)}{\partial r} \right] \Delta r \quad (9)$$

where:

c , ρ , $i V$ – are, respectively: specific heat, mass density and volume accumulating heat.

Taking into account that geometrical and morphological properties of reinforcement are practically temperature independent:

$$c\rho \frac{\partial T(r, t)}{\partial t} = \frac{\Delta F}{\Delta V} \frac{\partial}{\partial r} \left[\lambda \frac{\partial T(r, t)}{\partial r} \right] \Delta r \quad (10)$$

where:

constant – $M_m = \frac{\Delta F}{\Delta V}$ describes morphological influence of reinforcement.

In studied volume of micro-region – in center of composite casting reinforcing particle was placed with shape of regular solids: sphere, cube, tetrahedron and real shape particle (silicon carbide SiC). Heat processes in composite are described with equations of heat conductivity. Transient temperature distribution in two – phase matrix solidifying in temperature range can be described with Fourier – Kirchhoff's equation [7, 8]:

$$c_o(T_o)\rho_o(T_o) \frac{\partial T_o(r, t)}{\partial t} = \text{div} [\lambda_o(T_o) \text{grad} T_o(r, t)] + L_o \rho_{ol} \frac{\partial S_o(r, t)}{\partial t} \quad (11)$$

where:

c_o – specific heat, L_o – crystallization heat, ρ_o – mass density, λ_o – heat conductivity coefficient, S_o – function of solid phase fraction, T_o , r , t are respectively temperature, generalized space co-ordinates and time; indices: o – refers to matrix, l – refers to liquid state.

For reinforcement:

$$c_z(T_z)\rho_z(T_z) \frac{\partial T_z(r, t)}{\partial t} = M_m \Delta s \cdot \text{div} [\lambda_z(T_z) \text{grad} T_z(r, t)] + L_z \rho_{zl} \frac{\partial S_z(r, t)}{\partial t} \quad (12)$$

where:

c_z , ρ_z , λ_z , L_z – thermo-physical properties of the reinforcement, S_z - function of solid phase fraction in solidifying reinforcement; T_z , r , Δs , t – are respectively temperature, generalized space co-ordinates, reinforcement thickness increment and time; indices, z – refers to reinforcement,

and assuming:

$$L_z \rho_{zl} \frac{\partial S_z(r, t)}{\partial t} = 0 \quad (13)$$

for $T_{sol z} \geq T_{zal o}$ and dispersive reinforcement without phase changes – when particles do not melt, after components temperature equalization:

$$c_z(T_z)\rho_z(T_z) \frac{\partial T_z(r, t)}{\partial t} = M_m \Delta s \cdot \text{div} [\lambda_z(T_z) \text{grad} T_z(r, t)] \quad (14)$$

Converted Fourier's equation, showing connection of heat flow kinetics in matrix – reinforcement system, gives in its general form image of changes proceeding in solidifying composite. Its conversion in proposed form shows on proportional relation between the size, surface and volume of particles enclosed in morphological modulus M_m [9].

Relative movement between the components intensifies the heat transport. Verification of interactions between the components must be conducted with use of Newton – Fourier model (6). The state previous to solidification is characterized by unstable liquid flow round the particle. Heat flux density taken by the liquid from solid surface in Newton's model is described by (5):

$$q = \alpha(T_s - T_p) \quad (15)$$

where: heat convection coefficient, $W/(m^2K)$; T_s – solid surface temperature, T_p – liquid matrix temperature.

Heat flux density in direction perpendicular to solid surface (reinforcement) also can be described by Fourier's law. Connecting both models, the thermal gradient in reinforcement near the surface can be shown with relation (6):

$$\left(\frac{\partial T}{\partial n} \right)_z = -\frac{\alpha}{\lambda_z} (T_z - T_o) \quad (16)$$

Decrease of temperature and relative velocity connected with growing viscosity and order of ions before solidification causes decay of movement. For matrix this can be described by (7):

$$\left(\frac{\partial T}{\partial n}\right)_o = -\frac{\alpha}{\lambda_o}(T_o - T_z) \quad (17)$$

Heat flux taken through contact surface of matrix and reinforcement is equal to liquid metal enthalpy decrease with mass flux m' :

$$m' = dm/dt \quad (18)$$

where mass flux density is:

$$\mu = dm'/dA \quad (19)$$

$$\alpha(T_z - T_o)dA = -m'c_p d(T_z - T_o) \quad (20)$$

$$\int \alpha dA = A \bar{\alpha} \quad (21)$$

$$A \bar{\alpha} = -m'c_p \ln \frac{(T_z - T_o)_2}{(T_z - T_o)_1}$$

where: $\bar{\alpha}$ – average coefficient on exchange surface, $(T_z - T_o)_1$ and $(T_z - T_o)_2$ – temperature differences between components, $T_{z,o}$ – temperature of reinforcement and matrix, dA – elementary surface of components contact, A – sum of elementary contact surfaces – heat transfer surface, c_p – specific heat for liquid matrix, which in narrow range of solidification is constant, m' – mass flux.

Mass flux connected to heat transfer between matrix and reinforcing particle flows to the particle through intersection equal to particle projection on plan perpendicular to mass flux direction. In case of convex particle projection section will be equal to maximum intersection of the particle. The quantity of mass flowing through depends on size of the section and its shape. Hard to determine value of this quantity one can calculate with use of equation (12):

$$m' = m \cdot v \cdot \frac{F}{O} \quad (22)$$

where: m – portion of liquid metal flowing round the particle until the relative movement decays, v – relative velocity, F – surface area of particle projection, O – perimeter of particle projection.

Velocity value can be evaluated basing on difference of mass density of components. At forced convection the force fields influence must be taken into account. From technological point of view it is necessary to create in liquid metal shear stresses by intensive stirring. It improves the wetting. As an example the use of inductive furnace for heating and stirring of components and creating relative velocity between them. When components in composite creation phase are subjected to force fields action resulting difference in relative velocity can be evaluated base on specific permeance. Value of m coefficient can be calculated

using reinforcement content in the composite. Projection surface F and its perimeter O are easily evaluated from quantitative analysis of reinforcing material. Quotient F/O is equal to M_m^{-1} . Then average value of exchange coefficient will be:

$$\bar{\alpha} = -\frac{m'c_p}{A} \ln \frac{(T_z - T_o)_1}{(T_z - T_o)_2} \quad (23)$$

$$\bar{\alpha} = -\frac{m \cdot v \cdot c_p}{M_m A} \ln \frac{(T_z - T_o)_1}{(T_z - T_o)_2} \quad (24)$$

where: M_m – is a morphological modulus.

Connecting Newton's and Fourier's laws there is possibility to evaluate thermal gradient in matrix and reinforcement. On heat transfer coefficient significant influence has the unstable metal movement. Heat transport has dynamic character. Metal movement is decelerated and this deceleration is hard to evaluate. By intensive stirring cavitation may occur. Solidification of matrix causes significant change in its heat transfer coefficient [10]. Order of magnitude for heat transfer coefficient of liquid metal is $10^2 - 10^4$ W/(m²K) [11]. By phase change from gas to liquid it can exceed 10^5 . Such state not always is connected with significant relative velocity of components. For many solutions free convection may be sufficient.

By dispersive composite creation there are three characteristic states (from heat exchange point of view):

1. State of different initial components temperature, accompanied by relative movement of components. Simultaneously there is heat give up to the mould and surroundings. Initial temperature state can be defined on two manners: $\Delta T_{comp} > 0$; $\Delta T_{comp} < 0$;
2. Instantaneous state of equal temperature in components $\Delta T_{comp} = 0$, by which heat exchange does not exists;
3. State, in which with temperature decrease and growing viscosity movement decays and heat transfer coefficient decreases to 0.

Mentioned states can be described by relation:

$$\alpha(T_z - T_o)dA = -m'c_p d(T_z - T_o) \quad (25)$$

Assuming small change in heat exchange surface in range of solidification, we get:

$$\alpha = -\frac{m'}{A} c_p \ln \frac{(T_z - T_o)_1}{(T_z - T_o)_2} \quad (26)$$

In analyzed state 1 $\Delta T_{kompon.} = |(T_z - T_o)|$ also reaches maximum, which leads to maximum value of heat transfer coefficient. Momentary state 2, which duration is inversely proportional to difference in thermal conductivity of components and direct proportional to reinforcement content and takes value in range 1 – 0. For simplification the relative velocity change can be taken as a linear and, as a consequence also for the m' value with maximum value in state 1 going to 0 in state 3. The last state

duration depends on heat give up from the whole system to the surroundings. In practice there is significant difference between permanent mould and ceramic mould casting. Mainly by higher cooling rates is a possibility for reversed heat flow – to reinforcing particle from the matrix – by low thermal conductivity of reinforcement and its high heat accumulation.

Broadly discussed problem is the evaluation of simulation results reliability based on thermal gradient determination precision [12–14]. One can gain impression that micro scale tasks such as composite solidification analysis can be realized by preliminary validation of simulation results and subsequent further numerical analysis. Modeling of casting solidification of classic alloys is a complex problem: deterministic models are considered taking into account mass and energy transport conditions or micro models with defined isothermal crystallization. Crystallization analysis is based on stochastic models describing phase morphology with Monte Carlo method or cellular automaton [15]. Size and shape of crystallizing dendrites is considered in function of thermal gradient and fractal dimensions [16].

3. Conclusions

According to [13] with use of empirical postprocessing algorithms some structural parameters and mechanical properties can be determined. In many publications [17–20] describe micro and macroscopic modeling of crystalline structure. Microscopic simulation is based on nucleation, crystal growth and crystallization heat give up. Connecting validation experiments and numerical simulation of heat flow in macro scale with micro simulations enables structure determination in every point of casting. Some publications, describing directional crystallization, show that kinetics of thermal and chemical diffusion is infinitely rapid and can be neglected [21, 22] what can be a subject of another discussion. Apart from metal structure forecasting techniques improvement, application of macro models for micro scale phenomena studies is justified as long as justified are laws describing substance properties. On base of physical factors influence importance one can assume simplified methodology for their studies. It can be based on physical model of heat flow connected with conductivity, thus on solidification simulation with relative movement of components neglected. Such simulation has no relevance to classic micro model. Proposed micro-region refers to real – sized system of single particle.

Microstructure and diffusion are not modeled. Proposed assumptions are indispensable for recognition of basic physical factors influencing heat flow kinetics.

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