Archives of Materials Science and Engineering

Volume 42
Issue 1
March 2010
Pages 53-61

International Scientific Journal published monthly by the World Academy of Materials and Manufacturing Engineering

Influence of thermal boundary condition on casting process of metal matrix composite

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Received 23.01.2010; published in revised form 01.03.2010

ABSTRACT

Purpose: of this paper is to present a computer simulation as a tool for modelling the gravity casting process of metal matrix composite (MMCs) in the sand mould and predicting the arrangement of heterophase reinforcement particles in the composite and impact of the parameter which characterizes the thermal boundary condition on the course of solidification process (speed, direction) and thus, on the arrangement of reinforcement particles.

Design/methodology/approach: Computer simulations have been carried out following the methods and procedures included in the program Fluent. The calculation are based on two-dimensional model in which the Volume of Fluid (VOF), enthalpy method and the Discrete Phase Model (DPM) have been applied to describe two-phase system, solidification and behaviour of reinforcement particles, respectively. The calculations also include the method which allows to model the contact resistance at the interface between mould wall and liquid alloy.

Findings: Obtained results show that the cast solidification as well as final arrangement of heterophase reinforcement particles depend on the assumed thermal boundary conditions. The appearance of the contact resistance lengthens the solidification process and extends the effect of aggregation, sedimentation and particle engulfment or pushing ahead of solidification front.

Research limitations/implications: The created model and procedures can be treated as a basis for more advanced researches.

Practical implications: Presented simulations allows to study phenomena occurring during the casting process and predict the behaviour of the reinforcement particles (distribution of reinforcement) for the different thermal boundary conditions.

Originality/value: The applied simulation methods allows to study the course of the casting process of metal matrix composite and arrangement of the reinforcement particles.

Keywords: Casting; Solidification; Metal matrix composite; Contact resistance; CFD simulations

Reference to this paper should be given in the following way:

R. Zagórski, J. Śleziona, Influence of thermal boundary condition on casting process of metal matrix composite, Archives of Materials Science and Engineering 42/1 (2010) 53-61.

MATERIALS MANUFACTURING AND PROCESSING

1. Introduction

The specific properties of metal matrix composites largely depend on the applied type of material, of which the matrix and reinforcement are made. Recently, a great interest is observed in the composites reinforced with one or more (heterophase) types of ceramic particles e.g. SiC, glass carbon (Cg) [1-6]. This interest is associated with the development of appropriate casting methods to obtain the composites with the requisite internal structure. The structure of this type of composites may result for the impact of the mechanisms responsible for particle redistribution i.e., aggregation, sedimentation and particle engulfment or pushing ahead of solidification front. The occurrence of one or more of these mechanisms is affected by the parameters of the process as well as physical and chemical properties of matrix and reinforcement particles [7,8].

The experimental investigations show that phenomena mentioned above are among others thinks characteristic of gravitational casting. During the casting process of liquid composite the segregation of reinforcement particles can result in the appearance of forces such as: gravity force, buoyancy force, drag force as well as natural convection, difference of density between matrix and reinforcement material, interaction between reinforcement particles [9].

At the present time there are several theoretical methods designed for investigating and describing casting processes. The important element is to describe the solidification rate of the composite, which takes place in the system where the heat exchange appears on the interface between liquid material/mould. It is also essential to take into account the existence of reinforcing phase. Its presence changes the physical properties of some pure matrix and may affect the casting process [10].

On the other hand, the assumed thermal boundary conditions may influence final arrangement of reinforcement. During the simulations of casting process it seems to be indispensable to account the effects due to the existence as well as the lack of contact resistance. The latter can occur between the casting material and the mould as a result of surface tension or mould roughness. Another reason for the contact resistance may be the formation of a gap due to either evaporation of the refractory coating moisture or decomposition of sand binders, or this gap can be filled with gas. The heat transfer at the interface is possible to be controlled by conduction and convection in the gas gap with specific thickness. The elongation of solidification process due to presence of contact resistance may affect the mechanisms responsible for particle redistribution mentioned above [9].

The program Fluent, which belongs to CFD group, can be a useful tool to model the casting process of composite and thus, allows to predict its final internal structure [11]. This program contains several methods based on widely applied theories and techniques which permit to model mass and thermal transfer, multiphase systems and solidification. It also enables to implement the owner's programs written in UDF's code and therefore it is possible to define additional parameters and procedures.

2. Theory

2.1. Simulation model

The carried out computer simulations have been based on the methods and ready procedures included into program Fluent for modelling fluid flow, heat transfer and discrete phase. These methods and procedures implement the general principles of volumetric and surface balancing of the liquid fluid and basic form of the mass, momentum and energy equations.

The 2D simulational domain presented in Fig. 1 has been created in program Gambit by using unstructured rectangular mash. It consists of the following elements: the steel mount on which sand mould is located and fragment of steel pouring vessel. It has been assumed the existence of the two continuous phases: air and liquid matrix with dispersed particles of reinforcement.

2.2. VOF interface tracking method

Volume of Fluid approach has been used to model the two-phase system motioned earlier and within air-matrix free surface and volume fraction of particular continuous phases [12-15]. This approach allows to introduce the surface tension between phases and the wall adhesion of fluid on solid surface. The VOF method enables to assign the interface between immiscible phases on the basis of calculation of continuity equation for volume fraction of one component. The volume fraction of k-phase f_k is a variable which describes the participation in each calculation cell [12]:

$$f_k(\mathbf{r},t) = r\begin{cases} 0 & \text{outside } k_{th} \text{ fluid} \\ 1 & \text{inside } k_{th} \text{ fluid} \\ >0,<1 & \text{at } k_{th} \text{ fluid interface} \end{cases} \tag{1}$$

The appropriate properties and variables change for each control volume within the domain depending on the local value of f_k. For the two-phase system, average values of material property are estimated by following formula:

$$a = a_1 + f_1(a_2 - a_1) \tag{2}$$

where a is a resultant value of parameter (e.g. density ρ, specific heat c_p, viscosity μ, thermal conductivity λ), a_k is a value of parameter for k-th phase, by keeping condition:

$$f_1 + f_2 = 1 \tag{3}$$

The surface tension modelled in Fluent by the continuum surface force scheme (CSF) [13] adds the surface tension to the VOF calculation results in a source term in the momentum equation.

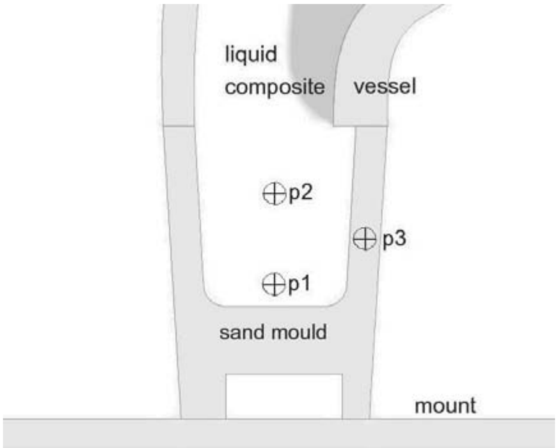

Fig. 1. 2D simulational model

2.3. Solidification model

The enthalpy method has been applied to simulate the solidification of the composite matrix. In this method, the system of differential equations and boundary conditions are counted in the entire computational domain. This method introduces the characteristic parameter called liquid fraction β which characterizes the state of material in specified point of domain and can be calculated by equation [11,16,17]:

$$\beta = \begin{cases} 0 & \text{for} \quad T < T_S \\ \dfrac{T - T_S}{T_L - T_S} & \text{for} \quad T_S < T < T_L \\ 1 & \text{for} \quad T > T_L \end{cases} \tag{4}$$

where T_L and T_S are liquidus and solidus temperature, respectively. The liquid fraction parameter assumes the value from 0 for solid phase to 1 for liquid phase. In the phase transition range ($T_S < T < T_L$) the liquid fraction takes on fractional value.

The requirement to take into consideration additional source terms which are responsible for modification of energy and mass transfer equations during solidification process is described by the change of enthalpy of the material during this phase transition and is counted as the sum of the sensible enthalpy, h, and the latent heat, ΔH [11,16]:

$$H = h(T) + \Delta H \tag{5}$$

where

$$h(T) = \int_{T_{ref}}^{T} c_p dT \tag{6}$$

and T_{ref} is reference temperature, c_p is specific heat at constant pressure. The latent heat content can be written in terms of the latent heat of the material, L:

$$\Delta H = \beta L \tag{7}$$

The latent heat may be estimated between zero (for a solid) and L (for a liquid). The liquid fraction is designed for calculation of continuous thermophysical properties in domain and extinguishing the velocity on a solidified phase border.

2.4. DPM - discrete phase model

An important element included in the calculations has been a combination of the aforementioned theories for modelling the flow of the composite matrix with the method for describing the behaviour of the reinforcement particles. The applied Discrete Phase Model (DPM) assumes that the particles interact with the continuous phase through a set of laws which are connected with the transfer of momentum, heat and mass [11]. In the carried out simulations for gravitational casting of the MMCs the trajectories of individual particles can be treated as the balancing of the forces acting on them:

$$\frac{du_p}{dt} = F_d(u - u_p) + F_g + F_b \tag{8}$$

where u is the fluid phase velocity, up is the particle velocity. F_g is gravitational force equals:

$$F_g = g_x \rho_p V_p \ (9)$$

where : g_x is gravitational acceleration, ρ_p is the density of the particle V_d is volume of particles. F_b is buoyancy force equals:

$$F_b = g_x \rho V_p \tag{10}$$

where ρ is the density of the fluid. $F_d(u - u_p)$ is the drag force equals:

$$F_d = \frac{18\mu}{\rho_p d_p^2} \frac{C_D \, Re}{24} \tag{11}$$

where: d_p is the particle diameter, Re is the relative Reynolds number and C_D is the drag coefficient which is calculated by Morsi & Alexander methods [18]. It has also been assumed that the laminar flow is in the system.

The momentum exchange appears as a momentum sink in the continuous phase momentum balance in any subsequent calculations of the continuous phase flow field. This momentum change is computed as

$$F = \sum \left(\frac{18\mu}{\rho_p d_p^2} \frac{C_D \, Re}{24} (u_p - u) + F_{other} \right) m_p \Delta t \tag{12}$$

where m_p is mass flow rate of the particles, Δt is time step and F_{other} are other interaction forces.

2.5. Physical parameters

The presented model presumes that matrix viscosity, density and thermal conductivity depend on the temperature. In the range between liquidus and solidus temperature values of density and thermal conductivity change linearly, whereas in this range viscosity is defined by special polynomial function. Additionally, the presence of reinforcement particles and their effect on the matrix viscosity have been expressed by equation [19]:

$$\mu_{pop} = \mu\left(1 + 2.5V_f + 7.6V_f^2\right) \tag{13}$$

where V_f is the volume fraction of particles. The change of matrix viscosity during solidification process has been applied indirectly to model the effects of solidification front displacement on the arrangement of reinforcement particles.

2.6. Thermal boundary conditions

The simulational domain contains several types of boundary conditions with an appropriate manner of heat exchange. It has been assumed that for the outside boundary of the system the boundary condition is as follows:

$$T(r,t)\big|_A = T_A\left(r_A, t\right) \tag{14}$$

For the mould wall and inside part of mount wall, which can be treated as a fluid or solid region with two sides (two-sided wall) the heat transfer is calculated directly from the solution in the adjacent cells:

$$q = \alpha\left(T_A - T_l\right) \tag{15}$$

where q is the heat flux, α is the fluid-side local heat transfer coefficient, T_A is the wall surface temperature, T_l is the local fluid temperature.

The fluid-side heat transfer coefficient is computed on the grounds of the local flow-field conditions. For this case it has been assumed to exist two types of heat transfer on the interface between separated regions. The first corresponds to the ideal contact condition as follows:

$$n\lambda\nabla T\big|_A = n\lambda\nabla T\big|_l \tag{16}$$

where λ is the thermal conductivity of the solid, n is a normal to the wall. Obviously, it is the big simplification. Modelling casting system it is important to take into account the presence of thermal resistance between walls and solidified material. Thus, the second type included in the calculations has been performed by using additional element of the applied solidification model. This element introduces the heat transfer resistance between walls and cells with liquid fraction less than 1 by the contact resistance which alters the thermal conductivity of the fluid near the wall [11,20]:

$$R = \Delta x/\lambda_m \tag{17}$$

where Δx is the wall thickness, λ_m is the thermal conductivity of the wall material.

3. Results and discussion

3.1. Simulational parameters

The simulations for aluminium matrix composite reinforced with Cg/SiC have been carried out for two values contact resistance of the mould wall with the wall thickness (Table 1) and without thermal resistance (R0 system). Table 1 contains also the value of other relevant simulational parameters whereas Table 2 shows the physical parameters of the alloy, sand mould, steel mount and reinforcement particles.

It has been established that all calculations have started from the initial state, prepared during time-independent steady simulation. The energy equation has been solved only for the system with two phases: air and liquid composite in the selected location. The main time-dependent calculations have included additionally the counting of the flow and volume fraction equations. Several numerical calculations led to establishment of optimal solver settings (Table 3).

Table 1.
Simulational parameters

Parameter	Value
contact resistance	0.001 (R1 system), 0,00826 m^2K/W (R2 system)
wall thickness	0.0002 m
pouring temperature of liquid composite	725ºC (998 K)
outside wall temperature	25ºC (298 K)
initial temperature of the system	25ºC (298 K)
total mass of casting alloy	0.167 kg
volume fraction and diameter of reinforcement:	
SiC	10%, 25μm
Cg	10%, 100 μm

Table 2.
Physical properties of material: alloy (cast) and steel (mould, mount). Data are based on Fluent database [11] and J. Sobczak. [19]

Material parameters	Aluminium alloy (AK356)	Sand mould	Steel mount	SiC	Cg
density (liquid and solid) ρ	2380 – 2700 kg/m^3	1580 kg/m^3	8030 kg/m^3	3230 kg/m^3	1400 kg/m^3
heat capacity cp	870 – 1180 J/kg·K	1045 J/kg·K	502.48 J/kg·K	630 J/kg·K	1680 J/kg·K
thermal conductivity λ	73 – 151 W/m·K	152 W/m·K	16.27 W/m·K	0,32 W/m·K	10 W/m·K
viscosity of liquid matrix μ	1.5×10^{-3} Pa·s				
solidus temperature $T_{solidus}$	559ºC				
liquidus temperature $T_{liquidus}$	572ºC				
latent heat L	339 kJ/kg				
tension air-alloy interface	0.9 N/m^2				
contact angle	120°				

Table 3.
Solver parameters (constant for all simulations)

Parameter	Value
Solver type	two-dimensional, pressure-based, segregated, unsteady
Discretization	PRESTO! for pressure, Geo-Reconstruct for volume fraction, first order upwind for others
Pressure-velocity coupling	SIMPLE

3.2. Course of temperature changes

The interesting aspect of the described investigations on solidification is studying the changes of the temperature in the system during the casting process. The Fig. 2 presents the change of maximum temperature in the whole simulational domain for the considered systems: R0 (solid line), R1 (dotted line) and R2 (dashed line). It has been observed the characteristic course (plateau) of temperature change in the modelling system for all the cases. It arises from phase transition heat. If in any part of casting material the temperature is in the range from $T_{liquidus}$ to $T_{solidus}$, the additional source of the energy appears and the phase transition takes place.

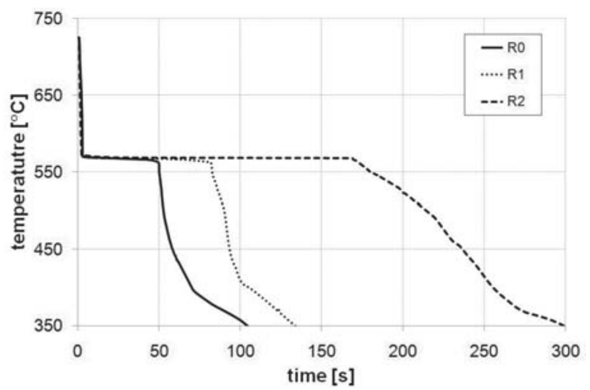

Fig. 2. Maximum temperature vs. time for systems: R0 (solid line), R1 (dotted line) and R2 (dashed line)

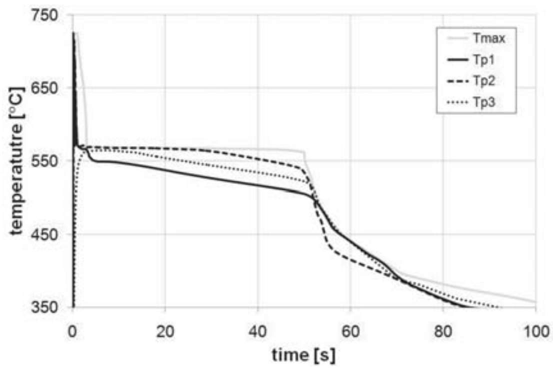

Fig. 3. Local temperatures vs. time for systems R0 (black colour) at the points p1 (solid line), p2 (dashed line), p3 (dotted line) and maximum temperature (grey solid line)

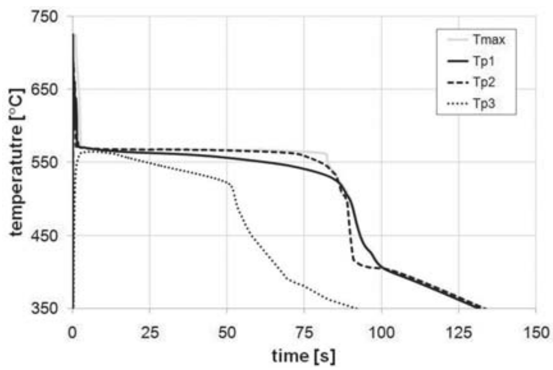

Fig. 4. As in Fig. 4 but for the R1 system

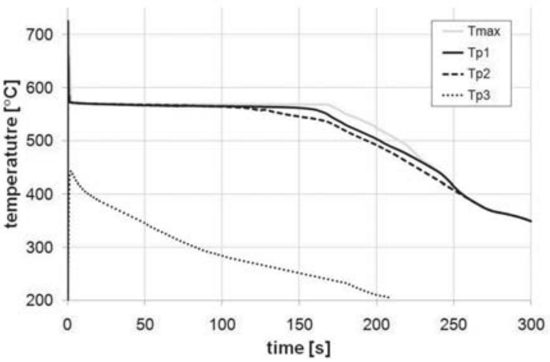

Fig. 5. As in Fig. 4 but for the R2 system

It is also worth studying the changes of local temperature. Figs. 3, 4 and 5 present the course of local temperature changes in selected points p1 and p2 which are located in the inside part of the mould and p3 on the mould itself. For the R0 system (Fig. 3) the local temperature at the point p1 is practically lower in comparison with temperature at the point p2. At the bottom part of the cast the local temperature decreases faster than at the upper one. It is connected with the efficient heat exchange on the interface between the mould wall and cast phase. The same situation is observed for the R1 system (Fig. 4) but the difference is less significant. The local temperature for the R2 system changes similarly (Fig. 5). The contact resistance limits the heat exchange on the mould wall and the upper part of the cast cools quickly.

The differences between temperature courses for the considered systems are due to the impact of thermal resistance or its lack. As a confirmation of this impact it can be the course of the local temperature change on the mould located at the point p3 - the dotted line on the Figs. 3, 4 and 5. As the Fig. show the temperature on the mould depends largely on the assumed thermal boundary conditions.

3.3. Solidification process of the cast

The Figs. 6, 7 and 8 present the solid fraction β_s of the casting composite matrix at the time sequences for which the value of solid fraction equals adequately (a) 0.3, (b) 0.5 and (c) 0.8. This parameter is defined as follows:

$$\beta_s = (1-\beta) \tag{18}$$

Additionally, these Fig. also include the distribution of the reinforcement particles.

The time and course of solidification are different for considered systems. For the system without thermal resistance (R0 system) the solidification practically starts just at the moment of pouring the mould (Fig. 6). The proper solidification begins at the bottom part of the mould next, moves up and finishes at the upper part of it after about 50 s. A similar casting process is observed for the R1 system (Fig. 7). But the appearance of the contact resistance extends the time of solidification. The solidification occurs from the bottom to the upper part of the modul and achieves the end after about 83 s.

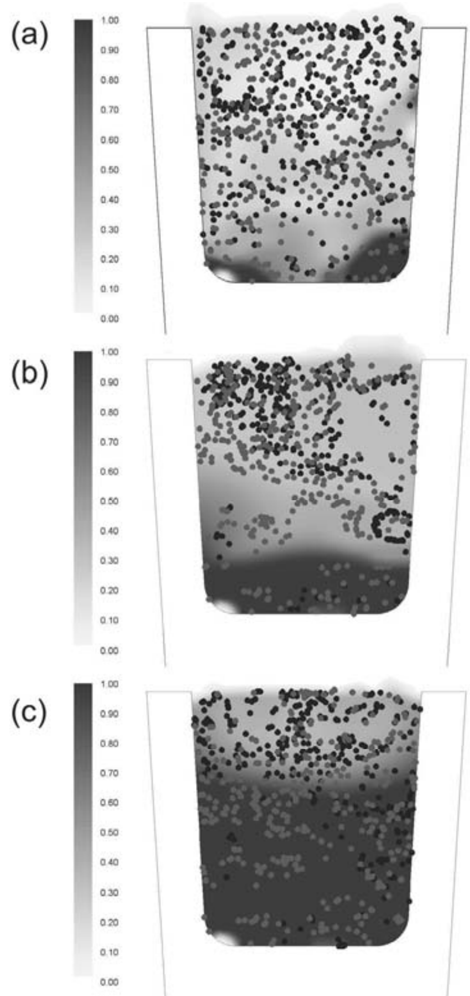

Fig. 6. Solid fraction of the casting material for R0 system and time sequences for which value of solid fraction equals: (a) 0.3 (2 s), (b) 0.5 (7 s) and (c) 0.8 (31 s) and redistribution of reinforcement particles: SiC (grey points), Cg (black points)

A quite different course of the solidification process of the casting material is observed for the R3 system (Fig. 8). The existence of the strong contact resistance both significantly lengthens the solidification and changes course and direction of this process. In the initial part of the casting process the solidification proceeds in the entire mould but near the mould wall it happens more intensively. The proper solidification begins at the upper part of the mould, moves down and finishes below the middle part of the cast after about 114 s.

The Fig. 9 shows the increment of the solid fraction of the casting composite during solidification process for the systems: R0 (solid line), R1 (dotted line) and R2 (dashed line). The presence of contact resistance affects distinctly the course and duration of the solidification process. The increase in value of cast solid fraction is continuous and also confirms the elongation of the solidification time for a bigger contact resistance.

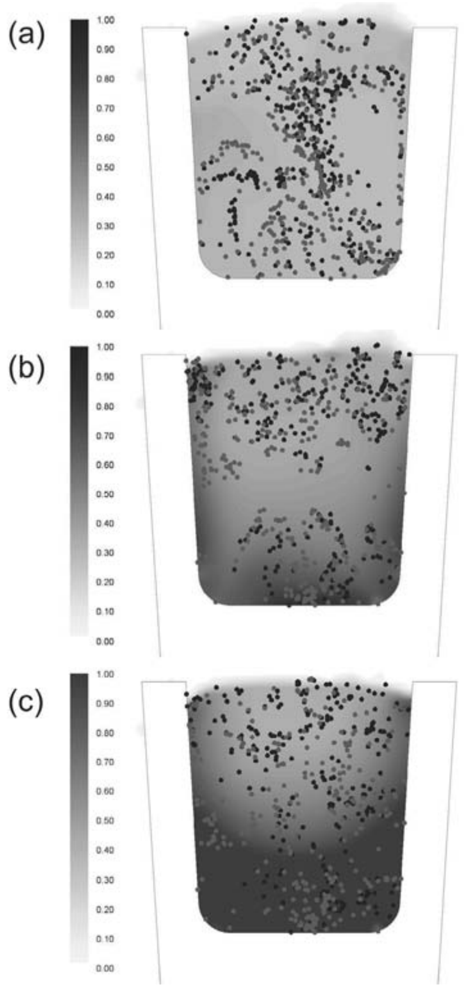

Fig. 7. As in Fig. 6 but for the R1 system time sequences for which value of solid fraction equals: (a) 0.3 (6 s), (b) 0.5 (18 s) and (c) 0.8 (55 s)

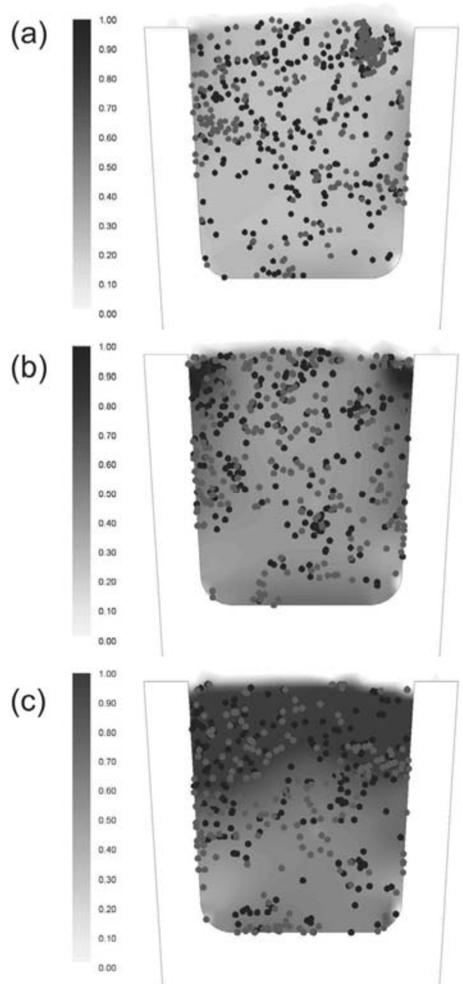

Fig. 8. As in Fig. 6 but for the R2 system time sequences for which value of solid fraction equals: (a) 0.3 (22 s), (b) 0.5 (57 s) and (c) 0.8 (114 s)

3.4. Arrangement of reinforcement particles

The Fig. 6, 7 and 8 as mentioned above show the redistribution of the reinforcement particles as well as present the variation of the position of these particles during casting process. Moreover, the Fig. 10 includes the final arrangement of reinforcement particles for the systems: (a) R0, (b) R1 and (c) R2 and the horizontally averaged fraction of reinforcement from bottom to the top of the cast: Cg (black line) and SiC (grey line).

Because of the rapid solidification of the liquid composite matrix and the change of its viscosity at the bottom part for the R0 system (Fig. 6), the homogenous arrangement of reinforcement particles SiC as well as Cg has been observed. In the upper part of the cast the solidification proceeds slower, so the separation of the reinforcement appears. The SiC particles (larger density vs. matrix density) move down under the influence of the gravitational force

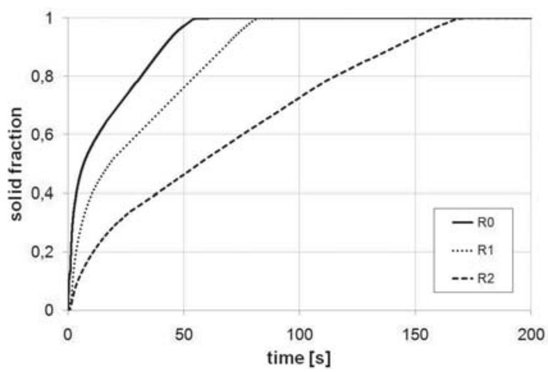

Fig. 9. Solid fraction vs. time for systems: R0 (solid line), R1 (dotted line) and R2 (dashed line)

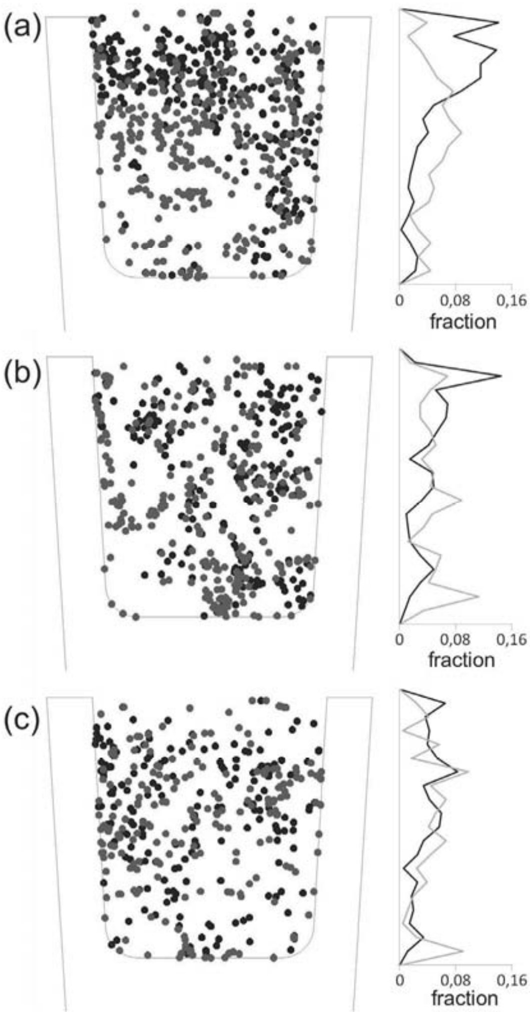

Fig. 10. Final arrangement of reinforcement particles: SiC (grey points), Cg (black points) for systems: (a) R0, (b) R1 and (c) R2. Right part shows the horizontally averaged fraction form bottom to top of the cast for reinforcement particles: Cg (black line) and SiC (grey line)

force and form the distinct layer. The Cg particles shift towards the upper part of the cast. The created layers of the reinforcement are not uniform. It can result from additional convection motions, which appear during the heat flow of the cooling cast - Fig. 10 (a).

The similar rate of the solidification process for the R1 system gives the same effects on the distribution of the reinforcement particles as for the R0 system (Fig. 7). The elongation of the casting process as well as the increase of the impact on the effects connected with convection motions and displacement of the solidification front modelled by the change of composite matrix viscosity cause the broadening of the layer. But most of SiC particles settle at the bottom part of the cast and Cg at the upper one - Fig. 10 (b).

In the case of R2 system the problem is more complicated (Fig. 8). The elongation of the solidification process and its course as well as the slower increase of matrix composite viscosity facilitate the movement of reinforcement particles and its aggregation. The fluid flow as a result of natural convection and solidification front additionally move these particles. The separation of the reinforcement particles is observable. The SiC particles form two distinct layers: in the bottom and above of the middle part of the cast. Whereas most of Cg particles are located in upper part of the cast - Fig. 10 (c).

4. Conclusions

The determination of the final arrangement of the heterophase reinforcement particles, as the simulations show, is closely connected with the phenomena observed during the gravitational casting process of the composite. The thermal boundary conditions especially the contact resistance between the liquid phase of the composite and mould wall as well as the physical properties of used materials significantly affect this arrangement. The presence of thermal resistance and its increase reduces the heat exchange at the interface these phases. The result of this is the elongation of the solidification process of the composite material. The longer time of the solidification and the slower increase of matrix viscosity allow the fluid flow which can be connected with natural convection.

Program Fluent proposes the procedures and techniques which can be useful to predict the distribution of the heterophase reinforcement particles during the casting process. Nevertheless, it is essential to extend the capabilities of these procedures for more exact exploration of the behaviour of the casting material, especially reinforcement particles. As an example, it is important to take into consideration the influence of the displacement of solidification front or effects connected with interaction between reinforcement particles. Hence, the described simulations can be used as a basis for next advanced investigations.

Acknowledgements

The present work is supported by the Ministry of Science and Higher Education grant PBU 77/RM4/2009.

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