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Thermal verification procedure for dispersive composite solidification process

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Methodology of research

ABSTRACT

Purpose: The aim of this work was optimization of composite matrix solidifcation process with use of thermal properties of components and geometrical characteristics of transition zone related with reinforcing particles morphology.

Design/methodology/approach: The method was based on quantitive image analysis. The reinforcing particles morphology was described by morphological modulus. With use of numerical simulation the changes in temperature and its derivatives after time and direction in studied composite micro – region appeared.

Findings: As a result of this studies the forecast procedure for composite structure evaluation was obtained and for which optional solidification theory can be used. Analysis of particles morphology influence on matrix solidification process is a proposed novelty.

Research limitations/implications: The work enables in enginereeng practice verification of components from technological point of view by thermal and geometrical properties selection and thus by introducing changes to the particle – matrix (casting) – mould – surrounding system. In this stage the procedure does not include the diffusion between matrix and reinforcement related to its relative motion. Evaluation of incomplete wetting and transition zone phases occurance does not permit tribological or fatique properties forecasting.

Originality/value: The proposed procedure is useful for composite properties forecasting based on components thermal and geometrical characteristics.

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

1. Introduction

For composite materials it is necessary to utilize characteristic properties of matrix, reinforcement as well as all other phases caused by technological process. The stress state predicted for casting component made from composite material and manufacturing conditions are the main premises for components selection. Material optimization is now based mainly on component and transition phases type selection. These phases are surrounded by the matrix. As a consequence, accurate composite properties optimization requires control of matrix microstructure in the reinforcing particle neighborhood.

Cast composite manufacturing process, connected with multiphase liquid – solid dispersive system solidification, starts in temperature higher than liquidus temperature of the matrix. In compare to standard casting alloys, solidification of composites is characterized by much larger contact surface between liquid alloy and reinforcing particles. Chemical and physical phenomena in macroscale system: “casting–mould–surroundings” require introduction of elements typical for microscale system: “reinforcement–transition phases–matrix between particles–mould–surroundings”. Connection of both systems creates classical solidifying composite system. Thus it is justified to study all factors influencing the composite solidification process. Structural components of the composite create system in respect of thermal properties and geometry characteristics [1÷5]:

1. thermal conductivity,
2. specific heat,

Table 1.
Morphological modulus values for particles with regular solid shapes in respect of particles size, μm^{-1}

Morphological modulus 1/μm		Screen mesh size 71 μm	56	40	32	20	16	10
Particle shape	SPHERE	0,085	0,107	0,150	0,188	0,300	0,375	0,600
	CYLINDER	0,120	0,152	0,212	0,265	0,424	0,530	0,849
	CUBE	0,147	0,186	0,260	0,325	0,520	0,650	1,039
	TETRAHEDRON	0,761	0,964	1,35	1,688	2,700	3,375	5,400

3. heat accumulation coefficient,
4. heat exchange coefficient,
5. initial temperature,
6. heat abstraction rate related to entire casting or its part, connected with composite technology (mould material etc.),
7. thermal capacity of the mould related to heat capacity of the casting,
8. volumetric content of the components,
9. contact surface morphology identified with reinforcement properties under assumption of full wetting between reinforcement and matrix,
10. casting development of external surface or its part related to its volume which is represented by solidification modulus.

Composite structure is physically formed by reinforcing particles and its distribution, but also by typical for matrix quantities, such as: dendrite size, dendrite arm spacing, eutectic lamellar spacing, defects quantity, size and shape (for example shrinkage and gas porosity). In matrix following quantities can be controlled, which determine the casting properties: solidification rate, solidification time, thermal gradient, etc [6].

It is assumed, that fine equiaxed structure is the most desirable – and safe in regard of operating loads. Use of composite materials for casting allows to assign specific load states for every element. Although the transition zone has a local character, its mechanical properties describe total composite quality. In dispersive *ex situ* composites, but also *in situ* particles introduced have got random orientation and only some of their surfaces could create coherent interfaces – under condition of proper reinforcement and/or transition phases selection. From the composite manufacturing point of view the significance of primal structure is obvious. Fine structure is desirable in first row in particle neighborhood then in the rest of space between the particles. Works [7÷13] indicate reinforcement quantity of 2,5÷3%, with size of 0,01÷0,1 μm and average distance between particles of 0,1 μm. Minimization of reinforcement size cause decrease in particles distance. Then the matrix plastic zone is extended on entire structure. Significant differences in components properties force use of more accurate structure shaping in transition zones [14÷16]. Studied were two types of factors: components thermophysical properties and reinforcing particles geometrical characteristics, which in significant way influence the heat flow kinetics.

Single dispersive particle which can be ceramic or other reinforcing phase is shown in Fig. 1. Particle in short solidification process can work as a heat micro-sink or micro-emitter. It can also work as a neutral element, in special cases. Forecasting of particle behavior enables control and optimization of composite structure and properties [17÷21].

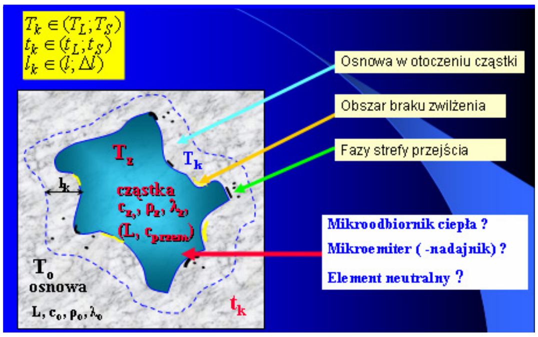


Fig. 1. Physical characteristics of composite microregion

2. Procedure concept

Joint influence of particles morphology and components thermophysical properties requires studies of particle geometrical form. In this work particles were studied with use of computer quantitative analysis before introducing them to liquid alloy matrix.

Heat flow simulation was based on comparison between solidification kinetics of microregion containing real–shape particles and particles with ideal geometry with solidification kinetics of microregion with no particle. Typical components were studied: eutectic Al-Si alloy as a matrix and corundum and carborundum reinforcement. To facilitate evaluation of relations between particle shape and its surface development a morphological modulus was introduced - M_m [22].

$$M_m = \frac{F}{V} = \frac{O}{S}\,[\mathrm{m}^{-1}] \tag{1}$$

where:
F, V, O, S- respectively: external area and volume of particle, perimeter and area of particle projection.

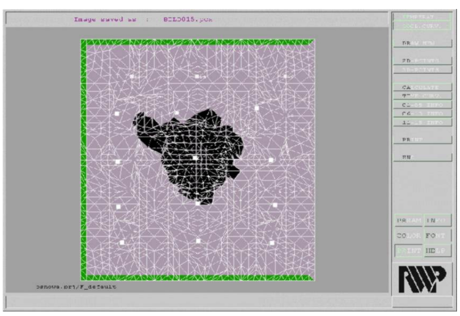
In table 1 example values of morphological modulus are shown for particles of regular solid shapes in range of sizes typical for *ex situ* composite manufacturing.

Table 2.
Geometrical relations for model ceramic particles

	Quartz		Carborundum		Corundum	
	average	standard deviation	average	standard deviation	average	standard deviation
Area μm^2	31102	13401	20743	4788	16564	5959
Length µm	236	74	221	40	203	50
Width	185	52	146	23	127	33
Perimeter µm	656	255	586	77	546	116
Number of objects	49 in 12 fields		56 in 8 fields		50 in 7 fields	
Length/Width ratio	1,28		1,51		1,59	
M_m 1/µm	0,021		0,028		0,033	

It results in different accuracy of determined quantities. For thermal derivative meshing accuracy resulting from definition is out of reach. Approximation with assumed error is a necessary compromise. In all simulations similar surface meshing and number of elements were preserved. In all cases heat flow kinetics was studied with little interest in quantitative evaluation of studied phenomena. Reinforcement temperature was set to 573 K, lower than matrix and isolation which was 993 K. Thermophysical properties were taken from the software database and are shown in table 3.

a)



b)

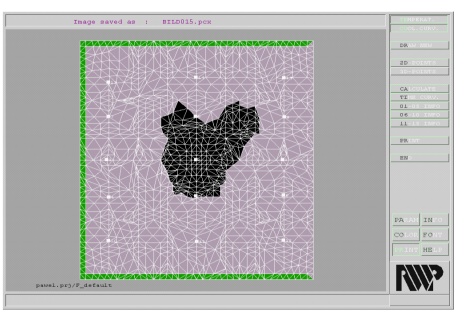


Fig. 2. Examples of micro - regions geometry containing single partilce - created for simulation reasons. In figures geometry for real particles is shown: a) SiC, b) Al_2O_3

Table 3
Thermophysical properties taken for simulation

Material	value	unit
matrix specific heat c_{po}	$2{,}633 \cdot 10^6$	$J/(m^3 \cdot K)$
matrix thermal conductivity coefficient λ_o	112	$W/(m \cdot K)$
matrix crystallization heat L	$1{,}080 \cdot 10^9$	J/m^3
Al_2O_3 specific heat c_{Al2O3}	$4{,}983 \cdot 10^6$	$J/(m^3 \cdot K)$
SiC specific heat c_{SiC}	$3{,}022 \cdot 10^6$	$J/(m^3 \cdot K)$
Al_2O_3 thermal conductivity coefficient λ_{Al2O3}	8,72	$W/(m \cdot K)$
SiC thermal conductivity coefficient λ_{SiC}	16,50	$W/(m \cdot K)$

In Fig. 2 real-shape particles are shown for a) corundum and b) carborundum, for which proper thermophysical properties were assigned.

For regular solid particles simulations were made for corundum and carborundum properties. A particular and characteristic example of temperature distribution is registered after relative equalization of components temperature, shown in Fig. 3(b).

After the particle reaches the equal temperature the matrix, which has higher thermal conductivity gives the heat away quicker. Thermal inertia of the particle is grater.

There can be found regions and intervals when heat flow direction is reversed. An example of this phenomenon is shown in Fig. 3 c) showing temperature range 577÷600 ^oC. Similar states can be observed in all simulated cases – regardless to particle shape and it type. Temperature changes in simulated region are shown in figure 3 for hexagonal Al_2O_3 particle. Fig. a) shows particle heating, Fig. b) shows relative temperature equalization, Fig. c) shows state in which heat flow direction is temporary reversed (to reinforcing particle) – similar states are shown in Fig. b and d), but in smaller scale. Next, system returns to typical heat flow direction. Fig. 3 e) and f) show state, in which particle is a local heat storage.

In 6^{th} row of table 4, thermal conductivity coefficient ratio for corundum and carborundum is shown. Following the Fourier law, thermal gradient is inversely proportional to thermal conductivity, what regardless of simulation inaccuracy is clearly shown here.

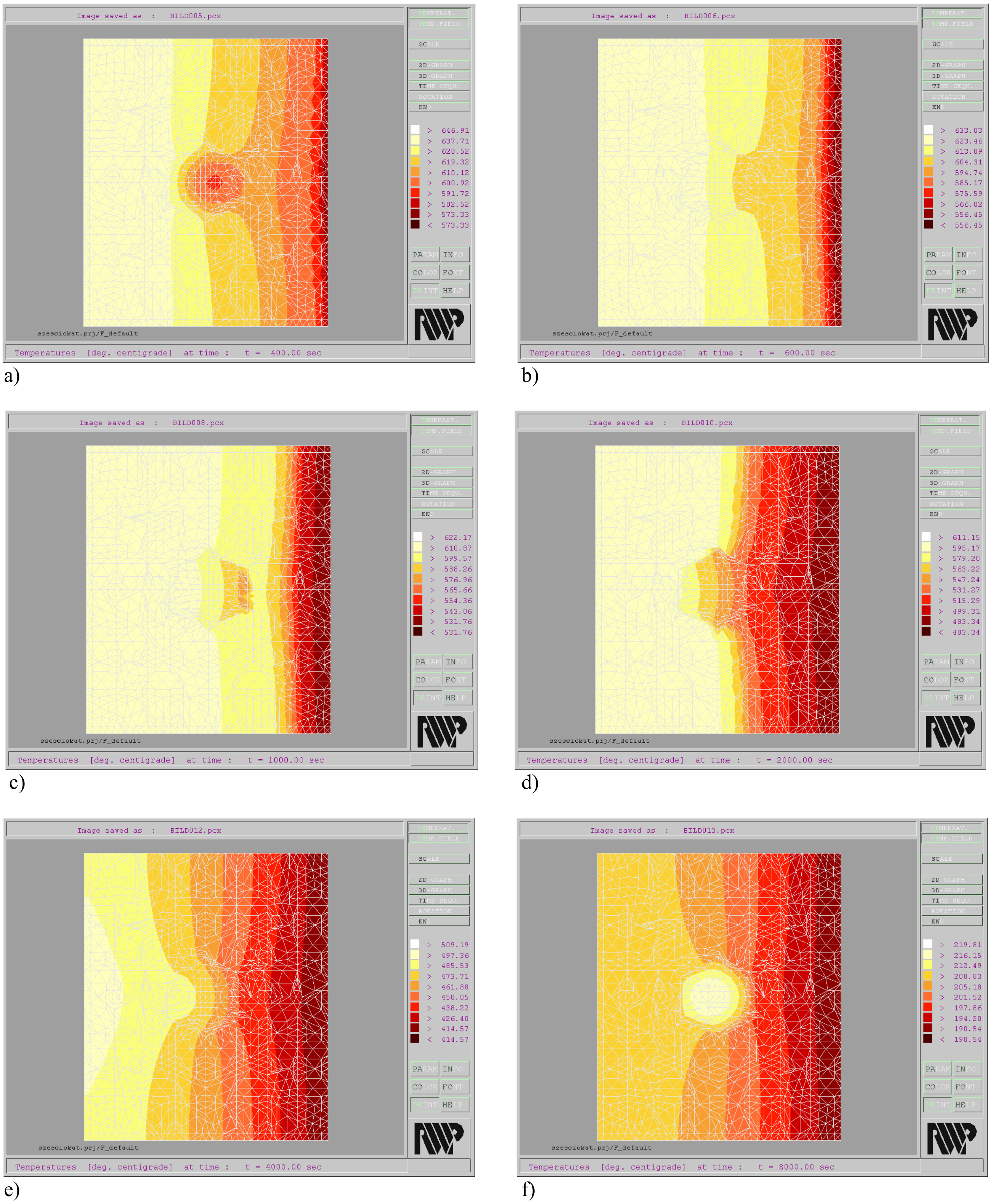


Fig. 3. Selected temperature distributions in composite region with hypothetical Al_2O_3 particle with hexagon geometry: a), b) equal temperature state; c), d) examples of temperature distribution in solidification range; e), f) examples of shifted cooling of particle in relation to the matrix; c) and f) fragments of regions with reversed heat flow direction

Table 4
Maximum thermal gradient in simulated regions with different particles

quantity	Reinforcing particle shape					average value
	triangle	square	hexagon	circle	real – shape particle	
max. G Al_2O_3 [K/cm]	58	50	31	38	29	41,2
max. G SiC [K/cm]	17	33	18	31	18	23,4
max. G Matrix [K/cm]	17					9
$\frac{G_{Al2O3}}{G_{SiC}}$ [1/1]	3,4	1,5	1,7	1,2	1,6	1,88 (1,76)*
$\frac{\lambda_{SiC}}{\lambda_{Al2O3}}$ [1/1]	-					1,89

First average value is taken from particles neighborhood region and shows *ratio average value*, value with (*) shows average value ratio in the same system.

3. Simulation results discussion

1. Around the reinforcing particles thermal gradient shows extreme values, especially at temperature and time just before solidification.
2. Maximum gradient site occurrence depends on particle shape and its orientation related to heat flow direction.
3. Perpendicular interfaces generate the biggest surface areas under thermal gradient curves.
4. The highest amplitudes occur in regions with significant difference in thermal conductivity coefficient.
5. Maximum values of generated gradient ratio are comparable with reversed thermal conductivity ratio, what is in agreement with Fourier's law.
6. Intensive heat movement in particle close neighborhood is favorable for fine matrix structure.
7. Physical interaction of the reinforcement can intensify heterogeneous nucleation of the composite matrix.

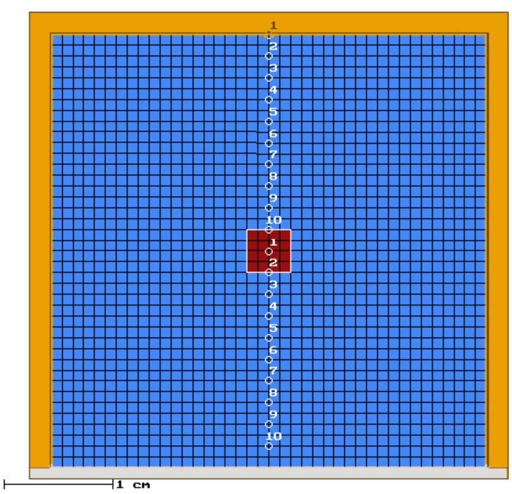


Fig. 4. 2D region geometry with theoretical square particle

Lack of difference in thermal gradient was the reason for another simulation of matrix – reinforcement system. Its experimental geometry is shown in Fig. 4. Simulated region is shown in Fig. 5. For simulation the ColdCAST software was used. It is based on finite difference method [24].

For matrix the aluminum with high thermal conductivity was selected – typical for cast composites. Reinforcing particle was made form corundum – quartz material. This material is close to aluminosilicate microsphere.

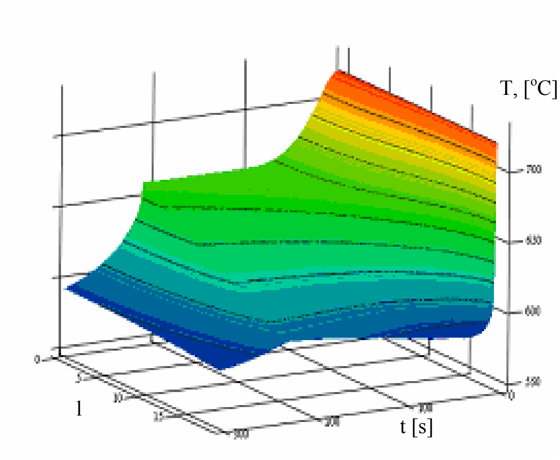
Investigated region is limited in three directions with thermo-isolated boundaries. Fourth direction is selected as a permanent mould wall with thermophysical properties close to those of composite region and initial temperature of 573 K.

In the evaluation influence of other particles surrounding investigated single-particle region was also taken into account. Average thermal parameters for temperature range are shown in table 5. More specific description of these studies contain works [25÷27].

Table 5.
Thermophysical properties taken for simulation

Material	value	unit
matrix specific heat c_{po}	$2,803\cdot10^6$	$J/(m^3\cdot K)$
matrix thermal conductivity coefficient λ_o	144	$W/(m\cdot K)$
matrix crystallization heat L	$0,980\cdot10^9$	J/m^3
specific heat Al_2O_3/SiO_2 c_{pz}	$4,983\cdot10^6$	$J/(m^3\cdot K)$
reinforcement thermal conductivity coefficient Al_2O_3 λ_z	0,12	$W/(m\cdot K)$

In Fig 5. (a, c, e) diagrams are shown for temperature, thermal gradient and temperature derivative after time for region analogical to composite region, without reinforcing particle. For all the cases values, which represent surface integral show degree of thermal mismatch of the components or their diversification in solidification process. In similar way this analysis can be made for other temperature ranges. Temperature difference variation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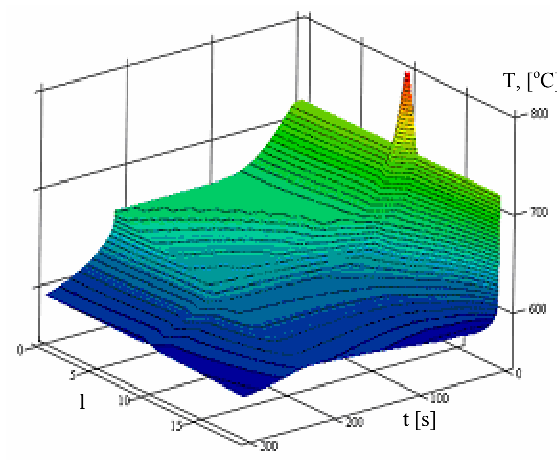
a)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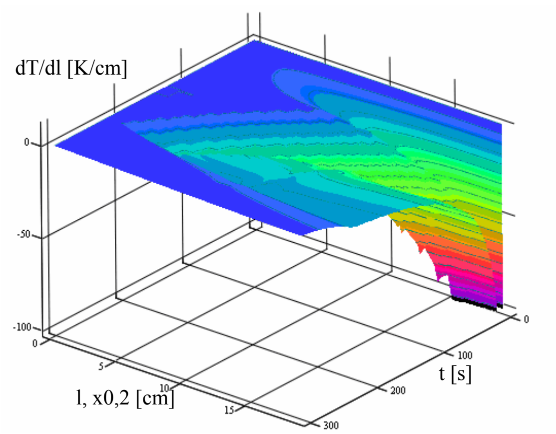
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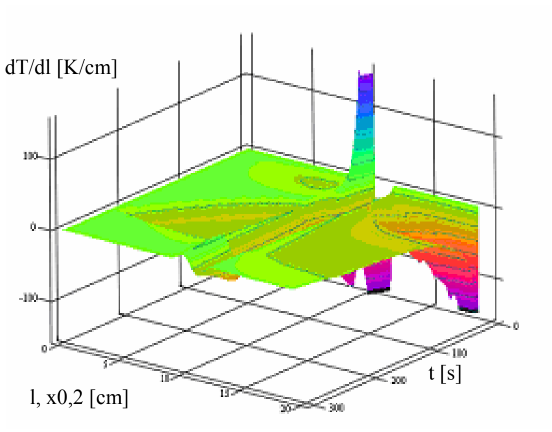
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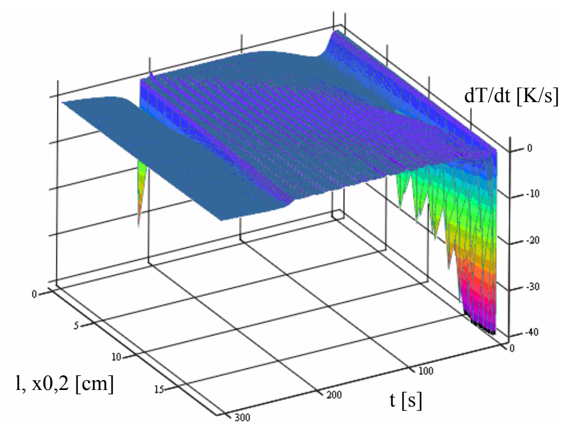
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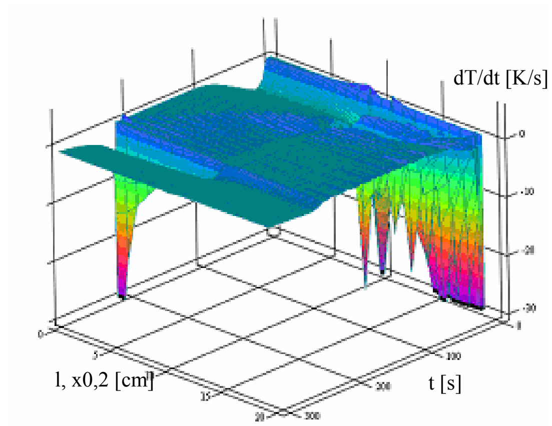
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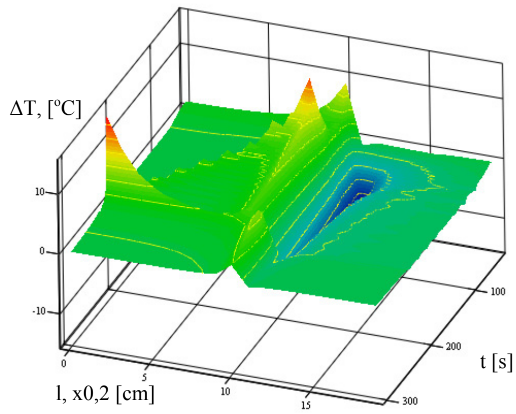
f)



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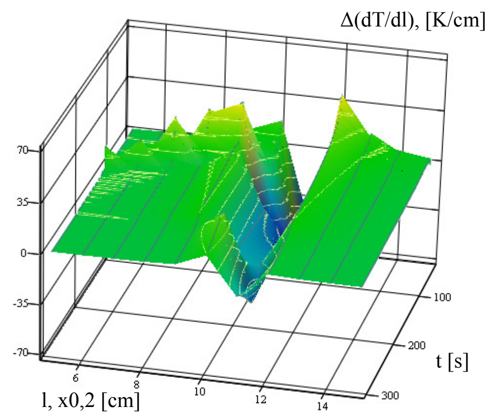

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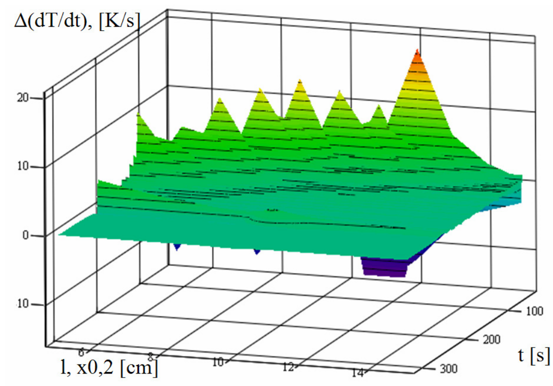

i)

Fig. 5. Collected results for temperature and its derivatives in region without a particle (a, c, e) and with a particle (b, d, f) in solidification range. Reinforcing particle has initial temperature higher than the matrix (T_z=820 ^oC, T_o=720 ^oC). a), b) - temperature distribution, c), d) - temperature derivative after direction, e), f) - temperature derivative after time, g) - temperatures difference between the systems: composite and alloy, h) thermal gradients difference between the systems: composite and alloy, i) - temperature derivatives difference between the systems: composite and alloy

and in consequence its gradient is highest at particle/matrix interface. Heat penetration depth into the particle is smaller than into the matrix, what is connected with thermal conductivity. The greater the matrix thermal conductivity, the changes range is bigger and smaller the extreme values are. Differences in temperature and thermal gradient decrease with time and they result from different initial temperatures for components. Nevertheless, even equal initial temperatures generate almost immediate diversification in matrix and reinforcement temperatures and gradients. Difference in temperature shown in Fig. 5. g), except value of thermal mismatch shows also range of thermal changes in matrix in function of time and space. Gradient relation shows space of structural changes. The changes number, temperature derivative after time variation is relatively smaller than registered variation connected with heat effects of crystallization. Crystallization effects in regions with and without particle are similar. In both cases they are overlaid decreasing influence of the reinforcement. In case of temperature derivative difference in derivative modulus can be taken into consideration. Nevertheless, thermal gradient in investigated cases has got great influence on local structure morphology.

4. Summary

With use of different calculating methods in two different software systems the heat flow kinetics was studied. Thanks to performed analysis it was shown that changes character for temperature and its gradient can be described in a proper way.

This can be obtained by simple means of 2D simulation. Its results can be easy utilize was shown above. Minimization of components interactions can be obtained by selecting materials with similar thermophysical properties.

Ideal state is practically out of reach. Necessity of primal structure shaping forces use of components with similar thermal properties. More pure the metal is or closer to eutectic, the smaller the solidification range is. Faster the heat flow and quicker the composite creation time is, smaller the solidification interval is. Composition of all elements, that is reinforcement, matrix, transition phases, wetting, and casting mould influence the matrix structure and its possible changes. Thermophysical mismatch of components can be described by temperature distribution and its derivative after time and direction. Complexity of proceeding phenomena forces analysis of every composite material separately.

Developed concept of quantitative forecasting of components matching is composed by following steps [28]:

1. Morphological modulus determination for statistically represented particles,
2. 2D simulation of solidification process for region with and without particle,
3. Temperature derivative after time and direction determination, its ratio or product for both elementary regions,
4. Determination of selected structural properties and assumption of relations describing structural properties,
5. Determination of differences between temperature in region with and without particle and its derivatives.

5. Conclusions

1. Solidification process simulation allows quantitative determination of the thermophysical diversification of components.
2. There is a possibility to take particle geometry into account and thus quantitative determination of geometry influence.
3. There is a possibility for taking into account the thermal and geometrical influence of transition phases and wetting.

Obtained results confirm purposefulness for components selection criteria sharpen and indicate need for control of following composite technological process elements:

- reinforcement wetting by alloy matrix by shaping the surface enrgy of phases,
- nucleation and growth of phases, mainly in relation to Al-Si eutectic.

Use of thermal verification procedure for solidifying composite gives a possibility to cast composite properties control.

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