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3D SIMULATION OF ALLOY SOLIDIFICATION IN THE NUSCAS SYSTEM

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Abstract. The authors present the capabilities of the authorial software in the field of engineering simulation. This system uses the finite element method. It enables the performance of simulations of phenomena described by partial differential equations. Currently the NuscaS system consists of: a library of finite elements, a finite elements mesh generator as well as modules for performing simulations of heat transfer and solidification. The module of solidification enables one to conduct simulations of equilibrium solidification of two-component alloys for three-dimensional problems. This paper presents the results of exemplar simulations that illustrate the capabilities of the described tool. These results consist of cooling curves, charts of part of the solid phase in the cast, fields of temperature in the cast and casting mould. The paper concludes with remarks and discussion of the obtained results.

Introduction

This article presents the capabilities (functionality) of the authorial software in the field of cast solidification simulations. The issue of cast simulation has been discussed in numerous scientific works [1, 2], however, this topic also attracts the attention of commercial firms [3, 4]. The work on this software was started at the Czestochowa University of Technology in 1996 by N. Sczygiol. At the same time, it was decided that this software would be named the NuscaS system [5].

The NuscaS system is dedicated to conducting numerical simulations of the casting process. This software is based on the Finite Element Method (FEM). At the present time, it enables one to conduct simulations for two- and three-dimensional areas.

The NuscaS system is divided into three main parts: pre-processor (preparation of simulation tasks that are to be solved), processor (computational part) and post-processor (graphical presentation of the obtained results). Currently, the NuscaS software is constantly being developed. There are scientific works concentrated on the improvement of existing solvers and developing new solvers for the NuscaS software.

Presently, the NuscaS system is being developed by PhD students and scientists from the Department of Applied Computer Science and Software Engineering

which belongs to the Institute of Computer and Information Sciences of the Czestochowa University of Technology.

1. Description of approach, assumptions and work methodology

The solvers of the NuscaS system are based on the finite element method. The solidification solver that is presented in this work is based on the heat transfer equation with the term of heat source. The term of the heat source is associated with the phenomena of latent heat evolution [6]:

$$\nabla \cdot (\lambda \nabla T) + \rho c \frac{\partial T}{\partial t} = q, \quad (1)$$

where λ is the thermal conductivity coefficient, T is the temperature, c is the specific heat, ρ is the density, t is the time and q is the heat source term, which in the case of solidification, is related to the phase change phenomena.

Solution of the heat transfer equation with the source term uses not only the finite element method [7], but also the apparent heat formulation (AHC) [8]:

$$\nabla \cdot (\lambda \nabla T) = c^* (T) \frac{\partial T}{\partial t}, \quad (2)$$

where c^* is the effective heat capacity, which can be obtained with the use of specific approximation formulas [9].

In the case presented in this paper, the effective heat capacity is obtained directly from the differentiating enthalpy formula with respect to the temperature. The system of linear equations, which emerges from semi-discretization over space with the finite element method and discretization over time with the Euler backward scheme, is solved with use of the conjugate gradients method [10]. To conduct the simulations presented in this paper, it was assumed that the casting solidifies in a way that can be modelled with the equilibrium model [11]:

$$f_s(T) = \frac{1}{1-k} \frac{T_L - T}{T_M - T}, \quad (3)$$

where k is the partition coefficient, T_L is the liquidus temperature and T_M is the melting temperature of pure metal.

All of the solvers that belong to the NuscaS system are developed with the use of C++ programming language. Advanced features of this language, such as templates or exceptions, are used.

At present, visualization of the obtained solution is performed with the use of GiD software [12]. GiD software has been chosen because it is a very configurable tool that provides a wide spectrum of possibilities to adapt to the needs of a given user.

2. Examples of numerical simulation

In this paper are presented the results obtained for the cast shown in Figure 1. The cast is shaped like a cube with edges 200 mm in length. The thickness of the casting mould is equal to 20 mm. Figure 1 also presents the location of the test points. In these points the changes of temperature in time were read. These points, indicated by cross-points, are named $P1$, $P2$ up to $P5$.

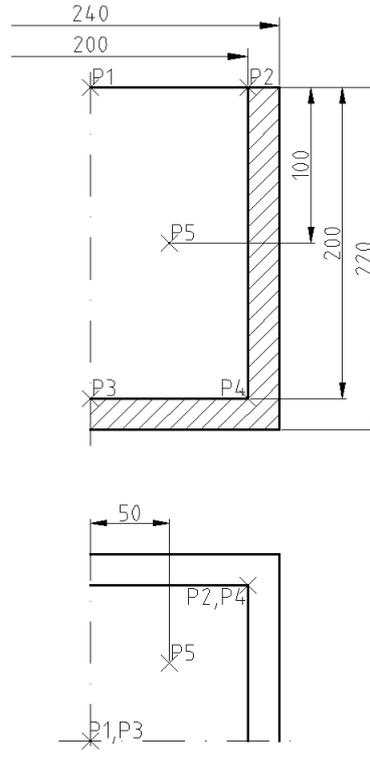


Fig. 1. Shape and dimensions of mould

The shape of the solid, for which the calculations were conducted, is presented in Figure 2. Because the cast is symmetric, the computations were performed on a quarter of the real casting solid. Figure 2 also presents the finite elements mesh. This mesh consists of 251 045 elements and 47 062 nodes (in the whole area - both cast and mould). 156 240 elements and 28 730 nodes lie inside the cast volume and the rest of the elements lie inside the casting mould volume and some elements are contact elements. The calculations were performed with use of tetrahedral elements in the whole area. Contact between the casting mould and cast was modelled with the use of prism elements. Those elements have a triangular basis and height equal to zero.

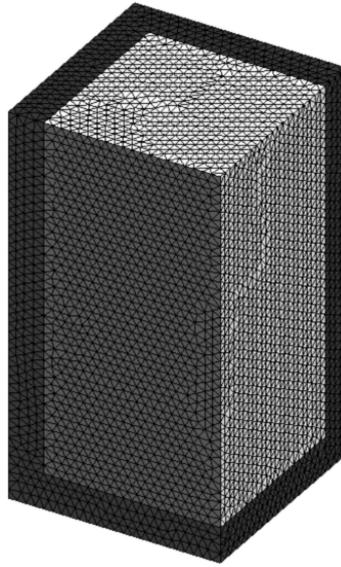


Fig. 2. Finite element model for computations of solidification process

Boundary conditions have a significant impact on the modelled process. In this specific case, the third type of boundary condition (Newton's condition) was used to model heat exchange with the environment. It was assumed that the ambient temperature, used in the third type of boundary condition, equals 300 K. The heat exchange coefficient on the side faces of the casting mould equals 100 W/Km^2 and on the bottom face equals 50 W/Km^2 . The heat exchange coefficient is lower on the bottom face, because it was assumed that the heat exchange with the base is difficult.

It was assumed that the top face of the casting and mould is buried with an isolating layer. This assumption allows us to set the heat exchange coefficient at 10 W/Km^2 . The heat exchange between the cast and the casting mould was modelled with the use of the fourth type of boundary condition with non-ideal contact. The conductivity of the separating layer was assumed to be equal to 1000 W/Km .

The values of the casting material properties used in the calculations are presented in Table 1. Table 2 contains the material properties of the casting mould material. The initial temperature of the liquid alloy was 1000 K. It was assumed that the casting mould was heated to 600 K. The filling of mould with liquid metal was not considered in the presented simulation. At 0 s the mould was completely filled with liquid metal. The phenomenon connected to the movement of liquid metal in the mould (for example: convection) was not considered in the simulation. The simulation continues until 1000 s counted from filling casting mould with liquid metal. After 1000 s the temperature ranges reached the following values: from 740.28 K up to 766.74 K in the cast and from 615.53 K up to 760.49 K in the casting mould.

Table 1

Physical properties of cast material

Quantity	Unit symbol	Value
Thermal conductivity coefficient - solid phase	W/Km	200
Thermal conductivity coefficient - liquid phase	W/Km	90
Density - solid phase	kg/m ³	2800
Density - liquid phase	kg/m ³	2500
Specific heat - solid phase	J/Kkg	980
Specific heat - liquid phase	J/Kkg	1050
Solidus temperature	K	853
Liquidus temperature	K	923
Melting temperature of pure metal	K	933
Latent heat of solidification	J/Kkg	390000

Table 2

Physical properties of casting mould material

Quantity	Unit symbol	Value
Thermal conductivity coefficient	W/Km	24
Density	kg/m ³	7200
Specific heat	J/Kkg	600

At the time of 1000 s, the cast was solid in the whole area (in entire area of casting the solid phase fraction equals 1). A nonzero value of the solid phase fraction was first observed at 5 s. For the first time in the simulation, the solid phase fraction equals 1 in the entire casting after 760 s.

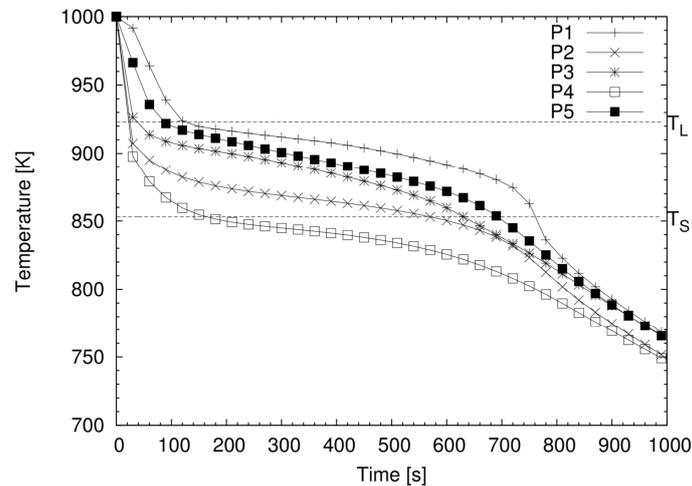


Fig. 3. Cooling curves obtained from selected points

In Figure 3 are presented the cooling curves obtained for the selected points (points annotated $P1...P5$ in Figure 1). In Figure 3 the liquidus temperature (T_L) and solidus temperature (T_S) are drawn with dotted lines. The shape of the presented cooling curves indicates that between the liquidus and solidus temperature solidification occurred. Cooling of the cast was fastest in the area where the cast and the casting mould was in contact, especially in the area of the side faces (where points $P2$ and $P4$ were). In that region the fastest heat exchange occurred.

The cooling curves obtained for points $P1$ and $P3$ show that heat exchange was difficult, because the isolation layer had an impact on the heat exchange (point $P1$) or because heat exchange with the ground proceeded at slower rate (point $P3$).

Because point $P5$ was located at some distance from the casting mould faces, the cooling curve of that point has a similar shape to the cooling curves of the $P1$ and $P3$ points, where heat exchange with the environment was difficult.

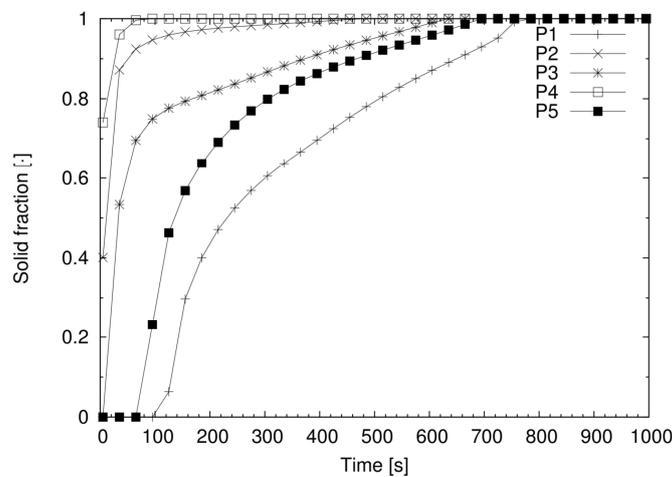


Fig. 4. Solid phase growth curves obtained from selected points

In Figure 4 the solid phase growth curves are presented. These curves were obtained for the same points as in the case of the cooling curves. The solid phase fraction was calculated with use of formula (3).

In Figure 5 the temperature field in the casting is presented. This temperature field was obtained at 125 s. To improve the readability of these figures only the outline of the casting mould is drawn. In Figure 6 the solid phase fraction distribution at 125 s is presented. As in the case of the figure with the temperature field, the casting mould is transparent. The maximum temperature in the casting mould was 800.92 K at that time and this maximum value occurred in the faces near the casting.

As could be observed, in Figures 3 and 4 and Figures 5 and 6, the cast first solidified in the bottom part and the process of solidification ended in the top part of the cast. This phenomena occurs mainly due to the very low value of heat ex-

change coefficient assumed for the isolating layer located on the top faces of the casting mould and cast.

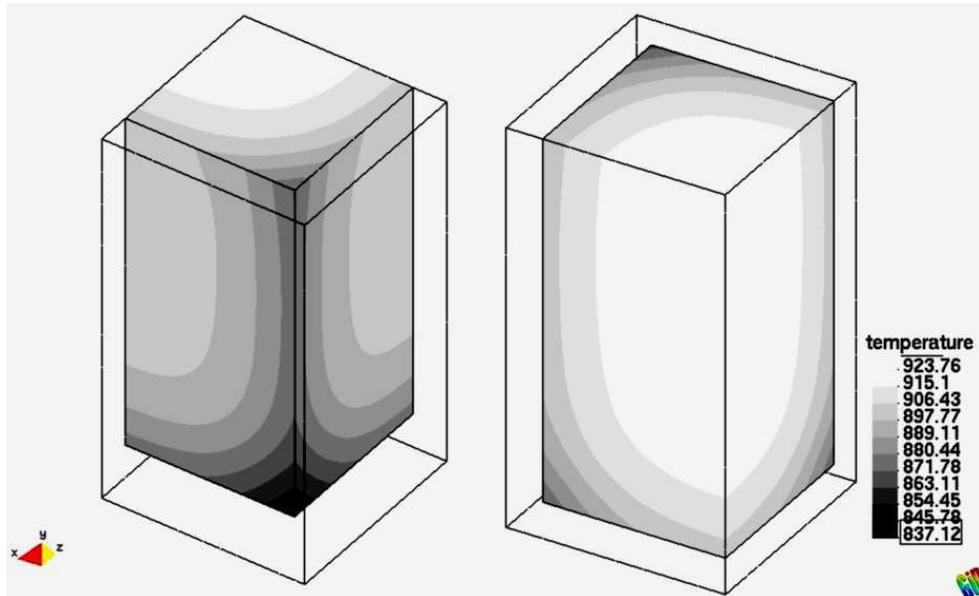


Fig. 5. Temperature field in casting 125 s after pouring

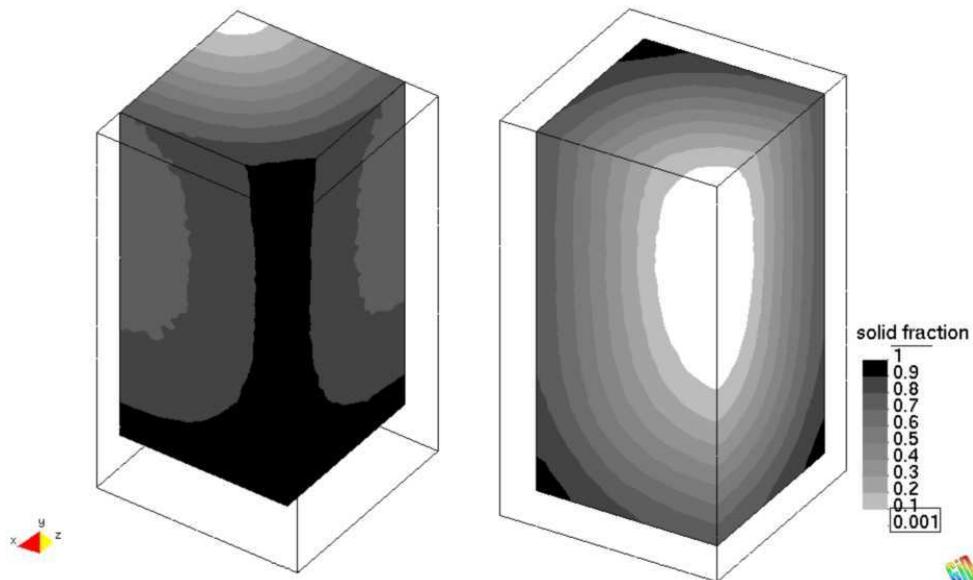


Fig. 6. Solid phase fraction distribution 125 s after pouring

Conclusions

The paper presents the capabilities of the NuscaS software in the field of engineering computations. As could be observed from the presented results, currently NuscaS software enables one to perform a simulation of equilibrium solidification for a 3D model.

The modular design of the NuscaS software allows for the independent development of various solvers designed for heat exchange or solidification simulations. All the solvers use one library that contains classes intended for file operations or helping with complex calculations (for example solving huge linear equations systems). This library also reduces the time required for work related to assembling the global system of equations in the finite element method.

The presented example, despite the fact that it has very a simple shape, allows thorough testing of the developed software. Analysis of the obtained results, especially cooling curves, enables us to conclude that the results obtained from NuscaS are correct at least from the physical nature of the simulated process.

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