3D simulations of solidification with liquid phase flow

E Gawronska and R Dyja
Faculty of Mechanical Engineering and Computer Science, Czestochowa University of Technology, Armii Krajowej 21, 42-201 Częstochowa, Poland
E-mail: gawronska@icis.pcz.pl, dyja@icis.pcz.pl

Abstract. The work discusses issues related to 3D coagulation simulations including liquid phase flow. The approach chosen by the authors is based on the numerical solution of the enthalpy solidification formula and the Navier-Stokes equation, in which the buoyancy force approximation was added. Both of these equations are discretized in space using Finite Element Method, and in both cases time integration utilizes the Theta scheme, which is a generalized form of Euler Backward approach. The presence of the Navier-Stokes equation in the model forces the use of special techniques to ensure the convergence of the solution. From a number of available methods, the method of adding stabilizing elements in the FEM formulation was chosen, i.e. the stabilization formulas PSPG/SUPG (Pressure Stabilized Petrov Galerkin/Streamline Upwind Stabilized Petrov Galerkin). The occurrence of large temperature gradients, however, made it necessary to use the so-called lumped mass matrix in the energy equation. The work presents the results obtained using a model implemented by the authors in the form of a computer program written in C++ programming language. The use of this language and appropriate libraries made it possible to obtain sufficient performance to perform 3D solidification simulations.

1. Introduction
Solidification remains one of the most troublesome phenomena in numerical modeling. The number and variety of physical processes that take place between microscale and macroscale pose a significant dare to the scientists working on a suitable calculation model connected with diffusion and convection. The problem of mass transfer with energy transfer is quite prevalent thus the Navier-Stokes equations are useful because of describing the physics of many scientific phenomena and problems, and in their full and/or simplified forms help with the design of aircraft and cars [1], the study of blood flow [2], the analysis of pollution [3], and many other things. Solidification is not an exception [4] in this context. A great many different models have been proposed over the years that offered reasonable results [5, 6], but each of them assumed some simplifications. None of the results included all of the problems occurring during modeling of this complicated phenomenon. Many of the computation models are subject to some restrictions. For instance, one such restriction is the omission of convection force in liquid metal. Unfortunately, their omission in a numerical model may cause crucial differences between the temperature range achieved in computer simulations, and the temperature of the real casting itself. What is more, due to such a simplification it is not possible to model certain phenomena which are essential factors influencing the quality of castings – for example, dopant distribution in the casting or shrinkage during solidification [7, 8].
Simulation tools become indispensable for engineers who are interested in tackling increasingly more complex problems or the ones who are interested in searching larger phase space of process and system variables to find the optimal design. Advances in hardware allow not only to solve the larger tasks (using more detailed grids) but also to describe the problem more accurately. Increasing capacity of computer memory makes it possible to consider growing problem sizes. At the same time, increased precision of simulations triggers even greater load. The increasing complexity of models (by including a more significant number of processes in them) causes problems with the implementation of the models. A solution to the transfer equations causes numerical problems regardless of the chosen discretization method. What is more, numerical methods of solving the Navier-Stokes equations are characterized by the significant time of calculations. That is why modern models must be implemented with the use of technology such as parallel computers [9], accelerated architectures or by using a specific organization of calculations [10, 11].

The Navier-Stokes equations depend on the simulated phenomenon. There may be a need to include a wide range of fluid motion speeds. Whether the focus is on the very convection or the flow of metal in the gating system, due to the high density of the metal, it is not possible to overlook fluid inertia effects. In our work, we propose the use of the stabilized finite element method (FEM) form to solve the Navier-Stokes equations without considering the classic Ladyzhenskaya-Babuska-Brezzi (LBB) consistency condition which can impede obtaining a solution of these equation [12].

In the paper, the results obtained using a model implemented by the authors in the form of a computer program written in C++ programming language are presented. The use of this language and appropriate libraries made it possible to obtain sufficient performance to perform 3D solidification simulations.

2. Mathematical and numerical derivations

The governing equation for modeling solidification process is based on heat transfer equation with source term:

$$\rho c \frac{\partial T}{\partial t} + \rho c \left( u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial z} \right) = \lambda \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \frac{q}{\rho c}$$

(1)

where $T$ is temperature, $u$ is velocity from convection force, $\lambda$ is thermal conductivity, $\rho$ is density, $c$ is specific heat, $q$ is heat source along with the heat of solidification and $t$ is time. In the model solving equation (1) the Newton boundary condition on the outer sides of the mold was implemented (heat exchange between the mold and the environment) also, the contact condition for the heat exchange between the mold and the casting. Apparent heat capacity formulation can be written as the following equation (1):

$$c^* \frac{\partial T}{\partial t} + \rho c \left( u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial z} \right) = \lambda \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right)$$

(2)

where $c^*$ is the approximation of the effective heat capacity. From different methods of this approximation, the DelGiudice method was chosen:

$$c^* = \frac{\frac{\partial H}{\partial x} \frac{\partial H}{\partial y} \frac{\partial H}{\partial z}}{\frac{\partial H}{\partial x} \frac{\partial H}{\partial y} \frac{\partial H}{\partial z}} = \frac{H}{T_f - T_f}$$

(3)

where $H$ is enthalpy:

$$H(T) = \int_{T_{ref}}^{T} cpdT + (1 - f_s)\rho V L$$

(4)

Due to the assumption that liquid metal is a Newtonian fluid in this model it possible to write Navier-Stokes set of equations as:

$$\rho \frac{\partial u_x}{\partial t} + \rho \left( \frac{\partial (u_x)}{\partial x} + \frac{\partial (u_y u_x)}{\partial y} + \frac{\partial (u_z u_x)}{\partial z} \right) - \frac{\partial p}{\partial x} + \rho \mu \left( \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right) + \rho \mu \frac{f_1}{K} u_x = 0$$

(5)
\[
\rho \frac{\partial u_x}{\partial t} + \rho \left( \frac{\partial (u_x u_x)}{\partial x} + \frac{\partial (u_y u_x)}{\partial y} + \frac{\partial (u_z u_x)}{\partial z} \right) = \frac{\partial p}{\partial x} + \rho \mu \left( \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right) + \rho \mu \frac{f_1}{K^2} u_y = \rho f_y
\]  

(6)

\[
\rho \frac{\partial u_x}{\partial t} + \rho \left( \frac{\partial (u_x u_x)}{\partial x} + \frac{\partial (u_y u_y)}{\partial y} + \frac{\partial (u_z u_z)}{\partial z} \right) - \frac{\partial p}{\partial z} + \rho \mu \left( \frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \right) + \rho \mu \frac{f_1}{K^2} u_z = 0
\]  

(7)

\[
\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} = 0
\]  

(8)

where \( p \) is pressure, \( \mu \) is viscosity, \( f_1 \) is a liquid fraction, and \( K \) is the permeability of the mushy zone approximated by The Kozeny-Carman equation and \( f_1 \) is vertical force connected with buoyancy by Boussinesq formula:

\[
f_y = -\beta g(T - T_0)
\]  

(9)

where \( \beta \) is expansion coefficient, \( g \) is gravitational acceleration and \( T_0 \) is reference temperature.

The proper set of initial and boundary conditions complements the above equations. Firstly, \( u \) is set as an initial condition, and secondly, the no-slip condition is used between the mold and the cast. After spatial discretization using the finite element method [13], it can be written as:

\[
M^S \dot{T} + (N^S(u) + K^S)T = 0
\]

\[
M\dot{u} + (N(u) + K)u - Gp + Du = F
\]

\[
G^T u = 0
\]  

(10)

where \( M \) is a mass matrix, \( K \) is stiffness matrix, \( N \) is a matrix of shape function connected with velocity \( u \), and \( G \) is matrix connected with basic functions of the finite elements [14].

Equations in that form can be solved with precisely selected finite elements [15]. The strategy which is described in this paper is based on the use of the stabilized Finite Element Method [16]. It makes it possible to avoid limits imposed by the Ladyzhenskaya-Babuska-Brezzi condition. SUPG (Streamline Upwind Petrov-Galerkin) and PSPG (Pressure Stabilized Petrov-Galerkin) techniques supply stabilization. Despite the fact that SUPG should reduce solution oscillations occurring due to high velocities, it is still possible to obtain these oscillations because of high gradients of temperature. Thus additionally, it is popular to use a diagonal mass matrix to avoid oscillations caused by high gradients during solidification simulations.

Consideration of the drag force part in stabilization requires special efforts [17]. An approach used in this paper determines stabilization coefficient values by the velocity of the liquid and limits it proportionally to the volume of liquid fraction. During the calculations, the authors assumed a small time step which allowed to use temperature from the previous time step when the temperature was needed to determine actual material properties values. That approach permits to treat solidification equation as linear, which makes for better overall performance. What is more, such an approach allows using a lumped mass matrix in solidification equation [14]. Bearing described assumptions in mind and using \( \Theta \) scheme for time integration, the final form of equations solved in the applied model is:

\[
\left[ M^S + M^S_{SUPG} + \Delta t \Theta (N^S_{SUPG} + K^S) \right] \dot{T}^{t+1} = \left[ M^S + M^S_{SUPG} + \Delta t (1 - \Theta) (N^S_{SUPG} + K^S) \right] T^t
\]  

(11)

\[
\left[ M + M_{SUPG} + \Delta t \Theta (N_{SUPG} + K + D + D_{SUPG}) \right] \dot{u}^{t+1} - \Delta t Gp^{t+1} + \left[ M + M_{SUPG} + \Delta t (1 - \Theta) (N_{SUPG} + K + D + D_{SUPG}) \right] u^t = \Delta t \Theta (F + F_{SUPG}) + (1 - \Theta) (F + F_{SUPG})
\]  

(12)

\[
\left[ M_{PSPG} + \Delta t \Theta (G_T N_{PSPG} + D_{PSPG}) \right] \dot{u}^{t+1} - \Delta t Gp^{t+1} + \left[ M_{PSPG} + \Delta t (1 - \Theta) (G + N_{PSPG} + D_{PSPG}) \right] u^t = \Delta t \Theta F_{PSPG} + (1 - \Theta) F_{PSPG}
\]  

(13)

where matrices with SUPG and PSPG are terms supplied by stabilization, \( \Delta t \) is time step \( \Theta \) is parameter determining type of time integration scheme.
3. Results
The model described in section II was implemented by authors hereof in C++ language with the use of TalyFEM finite element routines library [18] and PETSc, as a provider of linear algebra algorithms and data structures [19]. The results of calculations taking into account convection are shown for the domain presented in figure 1 and finite element mesh presented in figure 2. The boundary conditions utilized the following parameters: Newton boundary condition with the environment temperature equal to 300 K, the heat exchange coefficient equals to 10 W m⁻¹K⁻¹ on the all walls except for the bottom wall of the mold where the heat exchange coefficient equals to 40 W m⁻¹K⁻¹. Continuity condition assumed a value of 1000 W m⁻¹K⁻¹ for heat transfer through a separation layer between the mold and cast.

A summary of the material properties can be found below in table 1 (for casting) and table 2 (for mould). That properties correspond on a binary alloy Al-2%Cu.

![Figure 1](image1.png)
![Figure 2](image2.png)

**Figure 1.** Side view of the cast and mould with dimensions.  
**Figure 2.** View a finite element mesh of the cast and mould.

| Quantity name                          | Unit         | Value  |
|----------------------------------------|--------------|--------|
| Density $\rho_S$                       | kg m⁻³       | 2824   |
| Density $\rho_L$                       | kg m⁻³       | 2498   |
| Specific heat $c_S$                    | J kg⁻¹K⁻¹    | 1077   |
| Specific heat $c_L$                    | J kg⁻¹K⁻¹    | 1275   |
| Thermal conductivity $\lambda_S$      | W m⁻¹K⁻¹     | 262    |
| Thermal conductivity $\lambda_L$      | W m⁻¹K⁻¹     | 104    |
| Solidus temperature $T_S$             | K            | 853    |
| Liquidus temperature $T_L$            | K            | 926    |
| Solidification temperature of pure component $T_M$ | K | 933 |
| Eutectic temperature $T_E$            | K            | 821    |
| Heat of solidification $L$            | J kg⁻¹       | 390000 |
| Solute partition coefficient $k$       | -            | 0.125  |
| Viscosity $\mu$                       | kg m s⁻¹     | 0.004  |
| Expansion coefficient $\beta$         | K⁻¹          | 0.0001 |
| Secondary dendrite arm spacing $K_0$  | m            | 1.4\times 10⁻¹ |

**Table 1.** Material properties for casting.
Table 2. Material properties for mold.

| Quantity name          | Unit       | Value |
|------------------------|------------|-------|
| Density $\rho$         | kg m$^{-3}$| 7500  |
| Specific heat $c$      | J kg$^{-1}$K$^{-1}$ | 620   |
| Thermal conductivity $\lambda$ | W m$^{-1}$K$^{-1}$ | 40    |

The computational domain comprised of 62546 nodes and 354162 tetrahedron finite elements. Time step used in time integration was equal to 0.025 s, and time integration used a value of $\Theta$ equal to 1 (Euler Backward). Total run time for our simulation was 120 s. The results of the computer simulation are presented only for the first 50 s after which most samples showed no significant convection.

The first series of results present temperature maps for the cast and mould after 6.25 s (figure 3), after 12.5 s (figure 4), 18.75 s (figure 5), 25 s (figure 6), 37.5 s (figure 7), 50 s (figure 8). Corresponding solid fraction and velocity maps are presented in figures 9–14, and in figures 15–20, respectively. It can be seen that the temperature and velocity decreasing over time what is comply with the physical principles. An increasingly lower temperature produces that alloy transforms from a liquid phase by a solid-liquid to solid phase. The liquid phase movement is visually and mechanically observable during the solidification process and influence on it.
Figure 7. Temperature distribution after 1500 steps duration of the solidification simulation.

Figure 8. Temperature distribution after 2000 steps duration of the solidification simulation.

Figure 9. Solid phase fraction distribution after 250 steps duration of the solidification simulation.

Figure 9. Solid phase fraction distribution after 500 steps duration of the solidification simulation.

Figure 10. Solid phase fraction distribution after 750 steps duration of the solidification simulation.

Figure 11. Solid phase fraction distribution after 1000 steps duration of the solidification simulation.
Figure 12. Solid phase fraction distribution after 1500 steps duration of the solidification simulation.

Figure 13. Solid phase fraction distribution after 2000 steps duration of the solidification simulation.

Figure 14. Velocity vectors distribution after 250 steps duration of the solidification simulation.

Figure 15. Velocity vectors distribution after 500 steps duration of the solidification simulation.

Figure 16. Velocity vectors distribution after 750 steps duration of the solidification simulation.

Figure 17. Velocity vectors distribution after 1000 steps duration of the solidification simulation.
Figure 18. Velocity vectors distribution after 1500 steps duration of the solidification simulation.

Figure 19. Velocity vectors distribution after 2000 steps duration of the solidification simulation.

4. Conclusion
The paper discusses the problem of convection in 3D solidification simulations. It presents the influence of liquid phase movement on the solidification process. Included data obtained from a proprietary tool for solidification simulations and give physical correct results. During casting solidification, the movement of the liquid metal affects the local composition and solidification conditions. The internal sources of fluid movement include i.a. shrinkage (solidification contraction), natural convection, and deformation of solid phases because of thermal stress and pressure. Therefore, the inclusion of convection in numerical modeling is very important. All tools for numerical computing should be i) fast, ii) cheap (simulations on workstations), iii) flexible (general-purpose solver), and iv) accurate (adaptive error control) [20]. Though the authors’ software is still in development it satisfies all of these conditions. Future work plans include an experimental comparison of results as the presented model has so far been checked only against benchmark problems.

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