Three-dimensional numerical model of solidification with motion of the liquid phase

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Abstract

The paper presents numerical modeling of solidification process with convective motion of the liquid phase, generated both in the liquid and mushy zones. The transition region between the areas filled with liquid and solid is treated as a porous medium, which incorporates the suppression of fluid motion caused by the solid phase growth. Mathematical and numerical models of the phenomenon for three-dimensional domain are presented. To solve the problem Finite Element Method is used. The results obtained from numerical simulation are presented and discussed.

Keywords: Solidification; Binary alloy; Natural convection; Numerical modeling; Finite Element Analysis;

1. Introduction

Numerical modeling of physical phenomena is intensively developed in recent years. The reason is the huge increase in computing power. The results of numerical simulations of complex physical processes in three-dimensional areas are presented more often in the literature. Solidification phenomenon undoubtedly belongs to the group of such complex processes. Binary alloy solidification process, which takes into account convective motion of the liquid phase is intensively investigated for years [1–3].

Many commercial software packages, such as MAGMA, PROCAST, NOVAFLOW or FIDAP offer extensive possibilities for simulation of foundry processes. Unfortunately, these programs are very expensive, and user-defined modifications of their functionality are rather limited. In-house programs are solution of this problem. They give complete flexibility in changing the source code, so they have almost unlimited ability to modify and expansion. Presented work is based on the results obtained using such a program, made on the basis of the Finite Element Method.

The starting point of the process in the presented model is an area filled with a liquid alloy, overheated above the liquidus temperature to a value of ΔT. Properly adopted boundary conditions determine the rate of cooling process. Already at this stage, the convective motion of the fluid appears due to vertical temperature differences. The process of solidification begins after reaching the liquidus temperature. At this point the solid phase growth is observed. It leads to expansion of the mushy zone. In this zone, convection is suppressed by solid matrix of dendrites and grains. The shape and evolution of this mixed region depend significantly on the intensity of convective motion of the liquid. The process ends when all the material cool down below the solidus temperature.
2. Mathematical model

During the solidification process (Fig. 1), there are three regions separated by the isotherms of liquidus and solidus. Their evolution depends on the shape and dimensions of the casting as well as the cooling parameters.

The set of differential equations which governs the mathematical model of the process consists of the heat transport equation with convective term (1), Navier-Stokes equations with buoyancy and Darcy’s viscous terms (2) and the continuity equation (3).

\[
\text{div} (\lambda \nabla T) = \rho \left[ \frac{\partial (c_e T)}{\partial x} + v \frac{\partial (c_e T)}{\partial y} + w \frac{\partial (c_e T)}{\partial z} \right]
\]

\[
\text{div} (\rho \nu \vec{u}) = \frac{\partial \rho}{\partial x} + G_s + D_z = \rho \left[ \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right]
\]

\[
\text{div} (\rho \nu \vec{v}) = \frac{\partial \rho}{\partial y} + G_y + D_y = \rho \left[ \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right]
\]

\[
\text{div} (\rho \nu \vec{w}) = \frac{\partial \rho}{\partial z} + G_z + D_z = \rho \left[ \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right]
\]

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0
\]

where: \( T \) [K] is temperature, \( t \) [s] - time, \( \lambda \) [W/(m·K)] - coefficient of thermal conductivity, \( \rho \) [kg/m\(^3\)] - density, \( c_e \) [J/(kg·K)] - effective heat capacity, \( u, v, w \) [m/s] - components of the velocity vector, \( x, y, z \) [m] - Cartesian coordinates, \( p \) [Pa] - pressure, \( \mu \) [kg/(m·s)] - dynamic viscosity of liquid phase, \( G_s, G_y, G_z \) - components of the buoyancy term, \( D_s, D_y, D_z \) - components of the Darcy’s term.

Components of the buoyancy and Darcy’s term are calculated as follows

\[
G_s = \rho g_s \beta (T - T_{ref}) \quad D_s = \frac{M_u}{K}
\]

\[
G_y = \rho g_y \beta (T - T_{ref}) \quad D_y = \frac{M_v}{K}
\]

\[
G_z = \rho g_z \beta (T - T_{ref}) \quad D_z = \frac{M_w}{K}
\]

where: \( g_s, g_y, g_z \) [m/s\(^2\)] are components of the gravitational acceleration vector, \( \beta \) [K\(^{-1}\)] - volumetric thermal expansion coefficient, \( T_{ref} \) [K] - reference temperature, \( K \) [m\(^2\)] - permeability of porous medium.

Effective heat capacity \( c_e \) takes into account of heat of solidification [3] and is calculated as follows

\[
c_e = \begin{cases} c_s, & \text{dla } T < T_S \\ c_f, & \text{dla } T_S \leq T \leq T_L \\ c_i, & \text{dla } T > T_L \end{cases}
\]

where: \( c_s, c_f, c_i \) [J/kg] are the specific heats of solid, liquid and mushy zone respectively, \( L \) [J/kg] - latent heat of solidification, \( T_s, T_L \) [K] - liquidus and solidus temperature.

Material properties are averaged using solid-phase \( f_s \) and liquid-phase \( f_l \) fractions

\[
\lambda = f_s \lambda_s + f_l \lambda_l \\
\rho = f_s \rho_s + f_l \rho_l \\
c = f_s c_s + f_l c_l
\]

In the above relations \( f_s \) is obtained according to the following formula [3] as linear function of temperature, while \( f_l = 1 - f_s \).

\[
f_s = \begin{cases} 1 & \text{if } T < T_S \\ \frac{T - T_S}{T_L - T_S} & \text{if } T_S \leq T \leq T_L \\ 0 & \text{if } T > T_L \end{cases}
\]

Permeability \( K \) is calculated using Carman-Kozeny relation [4]

\[
K = \frac{d^2 \varphi^3}{180(1 - \varphi)^2}
\]

where: \( d \) [m] is average pore diameter in mushy zone, \( \varphi [-] \) - porosity coefficient, but in this case \( \varphi = f_l \).

Equations (1-3) are supplemented by appropriate boundary conditions

\[
x, y, z \in \Gamma_{ext} : -\lambda \cdot \nabla T = \alpha (T - T_w)
\]

\[
x, y, z \in \Gamma_{avg} : -\lambda \cdot \nabla T = q_{ext} = 0
\]

\[
x, y, z \in \Gamma_{ext} : u = v = w = 0
\]

\[
x, y, z \in \Gamma_{avg} : T = T_s
\]

\[
x, y, z \in \Gamma : T = T_L
\]

\[
x, y, z \in \Gamma : T = T_S
\]
and initial conditions
\[ t = 0 : T_{i_{kL}} = T_0 \]
\[ t = 0 : u, v, w \big|_{i_{kL}} = 0 \quad (10) \]

where: \( a \) [W/m\(^2\)K] is the substitute heat transfer coefficient which replaces the influence of the mold, \( T_0 \) [K] – ambient temperature, \( T_0 \) [K] – initial temperature of the alloy, \( n \) – vector normal to the casting boundaries.

### 3. Numerical model

Using the criterion of the method of weighted residuals [5, 6], equation (1) was multiplied by the weighting function \( \phi \) and integrated over the entire volume

\[ \int_{\Omega_{L,5+L,5}} \phi \left( \int_{\Omega_{L,5+L,5}} \left( \frac{\partial \phi T}{\partial x} + v \frac{\partial \phi T}{\partial y} + w \frac{\partial \phi T}{\partial z} \right) dV \right) \rho c_v dV = 0 \quad (11) \]

Above equation was written in a weak form

\[ \int_{\Omega_{L,5+L,5}} \lambda \int_{\Omega_{L,5+L,5}} \frac{\partial \phi}{\partial x} \left( \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) dV + \int_{\Omega_{L,5+L,5}} \lambda \int_{\Omega_{L,5+L,5}} \frac{\partial \phi}{\partial y} \left( \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) dV + \]
\[ + \int_{\Omega_{L,5+L,5}} \lambda \int_{\Omega_{L,5+L,5}} \frac{\partial \phi}{\partial z} \left( \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) dV = \int_{\Omega_{L,5+L,5}} \phi \partial \phi T \frac{\partial T}{\partial t} dV \quad (12) \]

The weak form was space-discretized using the Streamline Upwind Petrov-Galerkin (SUPG) method [7-10]. This choice was dictated by the need to ensure the stability of the numerical solution of heat transport equation with convective term. As a result of backward Euler time-integration scheme and the aggregation procedure a global FEM equation was obtained

\[ \left( K + \frac{1}{\Delta t} A \right) T^{f+1} = \frac{1}{\Delta t} M T^f + B \quad (13) \]

where: \( K \) denotes heat conductivity matrix, \( A \) – convection matrix, \( M \) – heat capacity matrix, \( B \) – right hand side vector.

Equations (2) were solved in the areas \( \Omega_i \) i \( \Omega_{5+L,5} \) with using Characteristic Based Split (CBS) method, based on the Chorin’s projection method [11] described and expanded by Taylor, Zienkiewicz and Codina [6, 12]. Since this method involves the initial solution of equations (2) without pressure, values of velocity components are not correct. Therefore, it shall be an artificial field velocity and marked with star \( u^*, v^*, w^* \). For example, the difference between \( u^* \) and \( u^* \) was calculated as follows

\[ \Delta u^* = u^* - u^f = \]
\[ = \Delta t \left[ div(\mu \nabla u) - \rho \left( \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) G_s - D_s \right] \bigg|_{i_{kL}} \quad (14) \]

Differences \( \Delta u^* \), \( \Delta v^* \) were calculated analogously. Of course, due to presence of the convective term in (14), it requires stabilization, i.e. with use of SUPG. Correction of the velocity field was performed after calculation of the pressure.

\[ u^{f+1} - u^* = -\frac{\Delta t}{\rho} \left( \frac{\partial P}{\partial x} \right)^{f+1} \]
\[ v^{f+1} - v^* = -\frac{\Delta t}{\rho} \left( \frac{\partial P}{\partial y} \right)^{f+1} \]
\[ w^{f+1} - w^* = -\frac{\Delta t}{\rho} \left( \frac{\partial P}{\partial z} \right)^{f+1} \quad (15) \]

Pressure was determined from Poisson’s equation, which was obtained after calculating the divergence of (15)

\[ \Delta t \left[ div(\nabla p) \right]^{f+1} = \rho \left( \frac{\partial u^*}{\partial x} + \frac{\partial v^*}{\partial y} + \frac{\partial w^*}{\partial z} \right)^{f+1} \quad (16) \]

Equations (14-16) were space-discretized using standard Galerkin procedure.

Numerical model used tetrahedral finite elements. Volume \( \Omega = \Omega_{L,5+L,5} \) was divided into \( N \) tetrahedrons

\[ \Omega = \bigcup_{j=1}^{N} \Omega_j \quad (17) \]

Normalized tetrahedron (Fig. 2) satisfies the following conditions

\[ -1 \leq r, s, t \leq 1 \]
\[ r + s + t \leq -1 \quad (18) \]

Fig. 2. Normalized tetrahedron in the coordinate system r, s, t
Then continuous Galerkin (CG) formulation was used with orthonormal basis functions $\phi_{ijk}$, proposed by Dubiner [14]. Components of the orthonormal base were defined as follows

$$
\phi_{ijk}(r,s,t) = \frac{P^{n}(\alpha)}{2} \left( \frac{1-\beta}{2} P_{j}^{2l+1}(\beta) \right) \left( \frac{1-\gamma}{2} P_{i}^{2m+1}(\gamma) \right) \left( \frac{1-\zeta}{2} P_{k}^{2n+1}(\zeta) \right) \tag{19}
$$

where $P^{n}(\alpha)$ is Jacobi polynomial of the $n$-th order defined on the interval $[-1,1]$.

### 4. Examples of calculation

Casting geometry is presented in Fig. 4.

On the plane of symmetry condition of thermal insulation was introduced. The remaining external surfaces of the domain were associated with Newton’s boundary conditions, where coefficient of heat convection $\alpha = 100$ [W/m^2K] and the ambient temperature $T_\infty = 300$ [K]. Initial temperature $T_0$ was equal 1800 [K]. Material properties of the alloy are presented in Table 1.

<table>
<thead>
<tr>
<th>Material property</th>
<th>Liquid phase</th>
<th>Solid phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$ [W/(mK)]</td>
<td>23</td>
<td>35</td>
</tr>
<tr>
<td>$\rho$ [kg/m^3]</td>
<td>6915</td>
<td>7800</td>
</tr>
<tr>
<td>$c$ [J/(kgK)]</td>
<td>837</td>
<td>644</td>
</tr>
<tr>
<td>$\mu$ [kg/(ms)]</td>
<td>0.006 94</td>
<td>-</td>
</tr>
<tr>
<td>$\beta$ [K^{-1}]</td>
<td>0.000274</td>
<td>-</td>
</tr>
<tr>
<td>$d$ [m]</td>
<td>0.0002</td>
<td>-</td>
</tr>
</tbody>
</table>

### Table 1. Material properties used in the calculations

<table>
<thead>
<tr>
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<tbody>
<tr>
<td></td>
<td>270000</td>
<td>1766</td>
<td>1701</td>
</tr>
</tbody>
</table>

The area of casting was divided into 953696 tetrahedral finite elements, which resulted in 169519 nodes. The calculations were carried out with variable time step, dependent on the highest velocity in the domain, but not more than 0.01 [s]. The calculation process was stopped when the temperature decreases below the solidus temperature $T_S$.

Fig. 5. Evolution of temperature field

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1. Experiment for KBN project no. 7 TO7 00917, Polish Foundrymen’s Technical Association, AGH, Cracow, 2002.
Fig. 5 shows the evolution of temperature field in the solidifying area. The initial phase takes place rapidly due to the intense convection of liquid material. After 10 [s] from the beginning of the process colder streams of the liquid are observed, and thus denser liquid rising off the top of the riser and flows downwards. In the lower part of the cast, begins to form a zone of lower temperature. The heat in the raiser after 40 [s] is uniformly distributed as a result of convective mixing, while in the lower part of the cast notable temperature gradient is observed. Significant difference in the temperature between fast solidifying casting and riser, where liquid material dominates is noticed after 160 [s]. After 260 [s] from the beginning the heat transfer takes place almost exclusively by diffusion.

![Solid phase fraction - after 10 [s]](image1)

![Solid phase fraction - after 40 [s]](image2)

![Solid phase fraction - after 160 [s]](image3)

![Solid phase fraction - after 260 [s]](image4)

Fig. 6. Solid phase growth

Solidification phenomenon is observed a few seconds after the start of the cooling process. The solid phase appears at the beginning near the edges of the casting (Fig. 6). The lower part solidifies much faster than the top, due to the geometry as well as the influence of convection. Liquid with a lower temperature flows to the bottom area where it is further cooled by heat removal through the cooled external surfaces. The solid phase grows rapidly from the bottom and side walls of the casting, which is clearly seen after 160 [s]. After 260 [s] from the beginning only a narrow funnel-shaped volume is in semi-liquid state.

![Solid phase fraction - after 10 [s]](image5)

![Solid phase fraction - after 40 [s]](image6)

![Solid phase fraction - after 160 [s]](image7)

![Solid phase fraction - after 260 [s]](image8)

Fig. 7. Evolution of velocity field

The evolution of the velocity field is presented in Fig. 7. The highest speeds are recorded at the initial stage, when the influence of convection on the heat transport is most intense. Convection disappears gradually, according to development of mushy zone.

![Velocity [m/s] after 10 [s]](image9)

![Velocity [m/s] after 40 [s]](image10)

![Velocity [m/s] after 160 [s]](image11)

![Velocity [m/s] after 260 [s]](image12)

Fig. 8. Final temperature field

Fig. 8 presents the temperature distribution at the end of the solidification process. It shows a significant shift of the heat core to the top of the riser, which was caused by the convection. After 365 [s] all the material passed to the solid state.
5. Summary

Building three-dimensional models, taking into account the coupling between the physical phenomena is nowadays a standard engineer's work. An efficient FEM application was created to enable simulating the solidification process including the convective motion of the liquid phase in three-dimensional areas. Parallel computing in terms of the most time consuming calculations enabled a significant acceleration of the calculation process and better utilization of multicore processors. Presented numerical model and calculation results show the possibility of using in-house computer program to simulate solidification process. Inclusion of the mold area, solute distribution, and shrinkage cavity formation will enrich it in the future.

References


Trójwymiarowy model numeryczny procesu krzepnięcia stopu dwuskładnikowego z uwzględnieniem ruchów fazy ciekłej

Streszczenie

W pracy przedstawiono model matematyczny i numeryczny procesu krzepnięcia z uwzględnieniem ruchów konwekcyjnych fazy ciekłej, generowanych zarówno w strefie ciekłej jak i stało-ciekłej. Strefa przejściowa pomiędzy obszarem cieczy i ciała stałego traktowana jest jako ośrodek porowaty, w którym uwzględniono tłumienie ruchu cieczy wywołane narastaniem fazy stałej. Przedstawiono model matematyczny i numeryczny rozważanego procesu dla obszaru trójwymiarowego. Do rozwiązania zagadnienia wykorzystano metodę elementów skończonych. Przedstawiono i omówiono uzyskane wyniki.