Analysis of three-dimensional binary alloy solidification with shrinkage cavity formation

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Abstract

The paper focuses on modeling of binary alloy solidification process with using Finite Element Method (FEM). The process is characterized by liquidus and solidus temperatures which are constant because solutal segregation is neglected. Analysed region is three-dimensional and consists of casting and riser. Mathematical and numerical models of solidification process are presented in the paper. The main focus is put on the algorithm of shrinkage cavity creation process. On the base of mathematical and numerical model computer program has been made. It is capable to simulate shrinkage cavity formation. Two examples show the results of different calculations performed by the program. The first example shows shrinkage cavity created during fast cooling of the top part of the riser while the second one was performed by significantly slower cooling. The shape and localization of shrinkage cavity obtained from simulation is compared to defect which was created during experiment.

Keywords: Shrinkage cavity, Binary alloy, 3D numerical modeling, Finite Element Method

1. Introduction

Contraction of the melted metal goes ahead in three main stages but only one of them is considered. As the temperature reduces the first noticed contraction is that in the liquid state. The volume of the liquid metal decreases linearly with falling temperature. The amount of this contraction is usually barely noticed.

The contraction on solidification starts at the liquidus temperature. It is caused by greater density of the solid compared to that of the liquid. The same amount of solid has a smaller volume than liquid phase. Lack of material is responsible for creation of shrinkage cavities. This type of contraction is taken into account.

The last stage of contraction occurs during cooling process in the solid state and is neglected.

At the beginning surface of the casting solidifies while the core remains liquid. In the final stage of solidification shrinkage cavity appears there. Its shape and localization is variable and depends on the shape of casting and cooling parameters. Phenomenon of shrinkage cavity formation is often discussed in the literature [1-4].

Investigations shows that structural defects of castings can take concentrated or distributed shapes.
2. Mathematical description

Solidifying casting with raiser is considered. The mould is neglected in the description but its influence on heat transport through the side and bottom surfaces of the casting is modeled by appropriate boundary conditions. Considered region consists of few zones which are identified by amount of liquid, solid and gas (fig. 1). Main domains of solidifying casting are solid region $\Omega_S$, liquid region $\Omega_L$ and region $\Omega_A$ filled with gas. Besides that mixture of mentioned phases appears. During solidification solid-liquid area $\Omega_{S+L}$ is observed as well as mixture of solid and gas $\Omega_{S+A}$ or compound of three of them $\Omega_{S+L+A}$.

![Fig. 1. Solidifying volume contains different zones](image)

The governing equation for the model is equation of transient heat diffusion (1). The emission of heat during solidification is contained in equation as effective heat $\rho \lambda$, where $\rho [\text{kg/m}^3]$ is density, $\lambda [\text{W/(mK)}]$ – coefficient of thermal conductivity, $T [\text{K}]$ is temperature, $t [\text{s}]$ - time, $\rho \lambda$, $\alpha_1$, $\alpha_2$ [W/(m$^2$K)] are heat convection coefficients on the top and side boundary respectively, $T_\infty [\text{K}]$ – ambient temperature, $T_0 [\text{K}]$ – initial temperature of the liquid alloy, $n$ – outward pointing normal vector at the casting external boundaries.

$$c_{ef} = \begin{cases} c_s, & \text{dla } T < T_s \\ c + \frac{L}{T_L - T_s}, & \text{dla } T_s \leq T \leq T_L \\ c_l, & \text{dla } T > T_L \\ \end{cases}$$

Equation (1) is supplemented by the boundary conditions of the third kind

$$\begin{align} x & \in \Gamma_T: -\lambda \n \cdot \mathbf{grad} T = \alpha_1 (T - T_\infty) \\
 x & \in \Gamma_S: -\lambda \n \cdot \mathbf{grad} T = \alpha_2 (T - T_\infty) \end{align}$$

The plane of symmetry is thermally insulated

$$x \in \Gamma_{sym}: -\lambda \n \cdot \mathbf{grad} T = q = 0$$

The initial condition is used as follows

$$t = 0: T|_{\Omega_L} = T_0$$

3. Numerical model

Numerical modeling of shrinkage cavities formation is not often discussed in the literature. The examples of papers considering that phenomenon are articles [6-10].

Starting with weighted residuals method [11, 12] equation (1) is multiplied by weighting function $w$ and integrated over entire domain $\Omega$

$$\int_\Omega \left( \lambda T \right)_t w \frac{\partial T}{\partial t} \, d\Omega = 0$$

The weak form is obtained with using Greens theorem to lower the order of equation (7)

$$\int_\Omega \lambda \mathbf{w} \cdot \mathbf{grad} T \, d\Omega + \int_\Omega \rho c \frac{\partial T}{\partial t} \, d\Omega = \int_\Gamma \mathbf{w} q \, d\Gamma$$

Above equation was space-discretized with use of tetrahedral elements. Considered volume $\Omega$ is divided into $N$ tetrahedrons

$$\Omega = \bigcup_{j=1}^N \Omega_j$$
Normalized tetrahedron shown in the fig. 2 fulfills following conditions in the space $T$:

$$-1 \leq r, s, t \leq 1$$
$$r + s + t \leq -1$$ (10)

Fig. 2. Tetrahedron in the coordinate system $r, s, t$

Next the normalized tetrahedron is mapped into cube (fig. 3) with use of following exchange of coordinates [13]

$$r = \frac{(1 + \alpha)(1 - \beta)(1 - \gamma)}{4} - 1$$
$$s = \frac{(1 + \beta)(1 - \gamma)}{2} - 1$$
$$t = \gamma$$ (11)

where $\alpha, \beta, \gamma$ are so called Duffy coordinates and they fulfill the condition

$$-1 \leq \alpha, \beta, \gamma \leq 1$$ (12)

Rys. 3. The transformation of coordinates $r, s, t$ into Duffy coordinates

Finally the continuous Galerkin formulation is used with orthonormal basis functions $w_{a,b}$ introduced by Dubiner [14]. They are defined in the following way

$$w_{a,b}(r,s,t) = \frac{P_{a,b}^{(a,b)}(r)}{\sqrt{2l+1}} \sqrt{\prod_{i=0}^{a-1} \frac{1 - \beta^i}{2}} \sqrt{\prod_{i=0}^{b-1} \frac{1 - \gamma^i}{2}} \sqrt{\prod_{i=0}^{b-1} \frac{1 - \gamma^{2l+j+i}}{2l+j+i+2}}$$ (13)

where $P_{n}^{(a,b)}(x)$ is Jacobi polynomial of the n-th order defined on the interval $[-1,1]$.

After time discretization procedure (Euler backward scheme) in relation to time derivative and aggregation of the discrete model, global finite element equation is obtained

$$\left( K + \frac{1}{\Delta t} M \right) \mathbf{T}^{f+1} = \frac{1}{\Delta t} \mathbf{M} \mathbf{T}^{f} + \mathbf{B}$$ (14)

where $K$ denotes heat conductivity matrix, $M$ – heat capacity matrix, $B$ – right hand side vector.

The algorithm of shrinkage cavity calculation starts by sorting nodes according to decreasing vertical coordinate. It means that nodes located at the top of the casting are in the first positions in the sorted list. In the next step nodal volumes of the liquid are calculated

$$\sum_{i=1}^{n} V_{li} = V_{li}, \sum_{i=1}^{n} V_{si} = 0, \sum_{i=1}^{n} V_{a(i)} = 0$$ (15)

where $n$ is total number of nodes, $V_{li}$, $V_{si}$, $V_{a(i)}$ [m$^3$] – volume of liquid, solid and gas in the i-th node.

Solid phase fraction $f_s$ is calculated as linear function of temperature

$$f_s = \begin{cases} 1 & \text{for } T < T_s \\ \frac{T_l - T}{T_l - T_s} & \text{for } T_s \leq T \leq T_L \\ 0 & \text{for } T > T_L \end{cases}$$ (16)

During cooling process in the liquid state the nodal temperature is monitored at each time step. Decreasing the temperature in any node below liquidus temperature $T_l$ starts the procedure of introducing a gas into nodes. The amount of gas depends on the value of contraction on solidification coefficient $\Delta_a$. On the base of known $f_s$ at the moment $t$ and $t + \Delta t$, volumetric increment of the solid phase is calculated in the following way

$$\Delta V_{si} = [f_{si}(t + \Delta t) - f_{si}(t)]V_{si}(t)$$ (17)

Actual nodal volume of the solid is calculated using below equation

$$V_{si}(t + \Delta t) = V_{si}(t) + \Delta V_{si}$$ (18)

Total volumetric increment of the solid is obtained as a sum of the nodal increments

$$\Delta V_s = \sum_{i=1}^{n} \Delta V_{si}$$ (19)

The nodal volume of liquid is actualized according to below formula

$$V_{li}(t + \Delta t) = V_{li}(t) - \Delta V_{li}$$ (20)
Corrected nodal content of the solid phase is calculated in the following way

\[ f_{i(j)} (t+\Delta t) = \frac{V_{i(j)} (t+\Delta t)}{V_{(i)}} \]  

(21)

Total increment of the gas is determined as a result of multiplication \( \Delta V \) by shrink coefficient \( S_h \)

\[ \Delta V_g = \Delta V_s S_h \]  

(22)

Calculated volume of the gas is distributed over nodes according to the algorithm described in the paper [15].

4. Examples of calculations

The geometry of domain\(^1\) used in calculations is presented in the fig. 4. Because of the symmetry only half casting was modeled.

Material properties of liquid, solid and gas are presented in the tab. 1.

<table>
<thead>
<tr>
<th>Material property</th>
<th>Liquid</th>
<th>Solid</th>
<th>Gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda ) [W/(mK)]</td>
<td>23</td>
<td>35</td>
<td>0.027</td>
</tr>
<tr>
<td>( \rho ) [kg/m(^3)]</td>
<td>6915</td>
<td>7800</td>
<td>1.1</td>
</tr>
<tr>
<td>( c ) [J/(kgK)]</td>
<td>837</td>
<td>644</td>
<td>1000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter of solidification</th>
<th>L [J/kg]</th>
<th>( T_L ) [K]</th>
<th>( T_S ) [K]</th>
<th>( S_h ) [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>270000</td>
<td>1766</td>
<td>1701</td>
<td>0.0575</td>
</tr>
</tbody>
</table>

The volume of casting was discretized into 557672 tetrahedral finite elements. Total number of nodes in the mesh was equal to 100366. The calculations were performed with constant time step \( \Delta t = 0.05 \) [s] until the temperature decreased below \( T_S \). The results of calculations are visualised side by side to comparison. First variant is shown on the left while the second one is on the right.

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\(^1\) Experiment for KBN project no. 7 TO7 00917, Polish Foundrymen’s Technical Association, AGH, Cracow, 2002
Temperature field changes according to the time during solidification. Temperature decreasing is presented in the fig. 4-6. Significant differences between the cases of simulation are noticeable in the top part of the raiser. When the cooling rate is low, the thermal centre is located shallow compared to second case. The localization of thermal centre affects shrinkage cavity vertical size.

Fig. 7-9 give interesting data about changes of solid phase distribution in the casting. Differences in the solid phase distribution are undetectable in the bottom part of the investigated element. Significant differences are visible in the top part of the raiser, which is affected by the heat convection through the top boundary. If the raiser is cooled slowly, final shrinkage cavity looks like a shallow cone, but if the cooling rate is high, defect is slightly deeper. In both cases bottom part of the shrinkage cavity lies near the thermal centre of the casting.
Vertical section through the cast is presented in the fig. 10a where the shape and localization of the defect is visible. The differences between shrinkage cavities obtained during simulations are compared in the fig. 10b-c.

5. Conclusions

The shapes and localizations of shrinkage cavities obtained during simulation in comparison with the defect arisen in the experiment shows that simulation without the mould taken into account leads to rough accuracy in predicting structure of the macroscopic defects.

Proprietary computer program implemented on the base of presented numerical model is useful in quick prediction of the positions and shapes of shrinkage cavities. Accuracy of the calculations will be better if the mould is taken into account.

References