## ARCHIVES

Of

# FOUNDRY ENGINEERING

ISSN (1897-3310) Volume 11 Special Issue 2/2011 135–138

26/2

Published quarterly as the organ of the Foundry Commission of the Polish Academy of Sciences

# Modelling of phenomena in solid state for the steel casting cooled by liquid

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Received 11.04.2011; Approved for print on: 26.04.2011

## Abstract

In this paper a mathematical model of cooling process for steel castings is presented. Effect of convective motion of the coolant on material structure after cooling process is investigated. Mathematical and numerical model based on Generalized Difference Method for axysimmetric elements is used. To solve the Navier-Stokes equation the characteristic based split scheme (CBS) has been applied. The solution of the heat transport equation with the convective term has been obtained by a stabilized meshless method. To determine of the phase transformation the macroscopic model built on the basis of Time Temperature Transformation diagrams for continuous cooling of medium-carbon steel has been used. The temporary temperature fields, the phase transformation, thermal and structural strains for the cooled element and the fields of temperature and velocity for the coolant have been determined.

Keywords: heat treatment, phase transformation, convection, cooling of liquid coolant

#### **1. Introduction**

In casting processes the appropriate control of the cooling process of steel parts is important. Trough this treatments the right phase composition is obtained. The control of these phenomena yields the desired mechanical and physical characteristics used in the design of machines and equipment. Predicting the characteristics of the material is particularly important in the casting process. Phase transformations in such the process could lead not only to the improvement of the properties of the workpiece, but also can cause significant temporary stresses leading to cracking of the material [1, 2].

The phenomena of cooling of castings process are difficult to model numerically because of their complexity and mutual coupling. The most important of these phenomena include the thermal, mechanical and phase transformations.

The modelling of the cooling castings process should devote significant attention to the model of thermal phenomena, because their quality is connected with the final results. In the modelling of the thermal phenomena it is usually assumed that the cooling conditions are approximated by the appropriate boundary conditions, with more or less closer to the real process conditions. However, this approach, especially in the modelling of liquid cooling processes, may lead to a large error of approximation. This occurs when the coolant is liquid, and also for geometrically complex parts of machines. The identical cooling conditions for all boundaries are unacceptable. The effects of gravity and the forced movement of the coolant cannot be ignored. Therefore, the model of heat transport for heat treatment processes should take into account the movements of the liquid cooling [3,4].

In the modelling phenomena of a cooling process, it is important to take into account the phase transformations. The paper presents the macroscopic model based on an analysis of TTT diagrams. Analysis of these diagrams allows to determine final parts of structures in cast element [1].

### 2. Heat transfer model

In presented paper a model of heat transfer for the coolant and the cooled axisymmetric element in the cooling process is described. The temperature fields are determined on the basis of



the heat transfer equation with convection term, which for axially symmetric space take the following form:

$$\frac{\lambda}{r}\frac{\partial T}{\partial r} + \frac{\partial}{\partial r}\left(\lambda\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right) - \rho C\left(V_r\frac{\partial T}{\partial r} + V_z\frac{\partial T}{\partial z}\right) + (1)$$
$$-\rho C\frac{\partial T}{\partial t} = q_r$$

where T [K] is the temperature, t [s] is the time,  $\lambda = \lambda(T)$  [W/mK] is the thermal conductivity,  $\rho$  [kg/m<sup>3</sup>] is the density, C [J/kgK] is the specific heat, V [m/s] is the velocity,  $q_v$  [J/m<sup>3</sup>s] is the volumetric heat source, r – is a distance from the symmetry axis.

In the thick-walled castings during cooling process occur the temperature changes induced particularly by the pearlite transformation. In equation latent heat of the phase transformation as volumetric heat source in heat transfer equation is introduced.

For the modelling of heat flow the generalized finite difference method was used. So that a function of temperature has been developed into Taylor series with an accuracy to the second derivative. The temperature in nodes was determined by the solution of the heat transfer equation with the convective term based on GFDM. This solution in a nonlinear implicit time scheme is applied [4].

Because the presented system matrix is highly asymmetric, it was solved by using the biconjugated gradients method. In this iterative method was used the Jacobi preconditioner [5].

#### **3. Model of fluid motion**

In modelling of the hardening process, especially when the coolant is a liquid, should be considered the behavior of the cooling medium. In this process the large changes in the intensity occurring in cooling were caused by convection or forced movement of liquid. The basis for the mathematical description of this movement is the Navier-Stokes equation with the free convection term.

The Navier-Stokes equation is defined as follows [6]:

$$\mu \left( \frac{\partial^2 V_r}{\partial r^2} + \frac{1}{r} \frac{\partial V_r}{\partial r} + \frac{\partial^2 V_r}{\partial z^2} - \frac{V_r}{r^2} \right) - \frac{\partial p}{\partial r} = \rho \left( \frac{dV_r}{dt} + V_r \frac{\partial V_r}{\partial r} + V_z \frac{\partial V_r}{\partial z} \right)$$

$$\mu \left( \frac{\partial^2 V_z}{\partial r^2} + \frac{1}{r} \frac{\partial V_z}{\partial r} + \frac{\partial^2 V_z}{\partial z^2} \right) - \frac{\partial p}{\partial z} + \rho a_z \beta \left( T - T_{ref} \right) =$$

$$= \rho \left( \frac{dV_z}{dt} + V_r \frac{\partial V_z}{\partial r} + V_z \frac{\partial V_z}{\partial z} \right)$$

$$(2)$$

where V [m/s] is the velocity component in the r or z-direction,  $\mu$  [kg/ms] is the dynamic viscosity, p [N/m<sup>2</sup>] is the pressure,  $a_z$  [m/s<sup>2</sup>] is the acceleration component in the z-direction,  $\beta$  [1/K] is the volumetric thermal expansion coefficient,  $T_{ref}$  [K] is the reference temperature.

The Navier-Stokes equation (2) is supplemented by the continuity equation taking the form:

$$\frac{\partial V_r}{\partial r} + \frac{V_r}{r} + \frac{\partial V_z}{\partial z} = 0$$
(3)

Equations (2) and (3) are complemented by appropriate boundary and initial conditions.

The Navier-Stokes equation (2) is solved only in a region filled with the coolant by means of a characteristic based split (CBS) scheme [2-4]. In this method an auxiliary velocity field V\* is introduced to uncouple equations (2) and (3).

$$\frac{V_r^* - V_r^k}{\Delta t} = \frac{\mu}{\rho} \left( \frac{\partial^2 V_r}{\partial r^2} + \frac{1}{r} \frac{\partial V_r}{\partial r} + \frac{\partial^2 V_r}{\partial z^2} - \frac{V_r}{r^2} \right) - \left( V_r \frac{\partial V_r}{\partial r} + V_z \frac{\partial V_r}{\partial z} \right) \\
\frac{V_z^* - V_z^k}{\Delta t} = \frac{\mu}{\rho} \left( \frac{\partial^2 V_z}{\partial r^2} + \frac{1}{r} \frac{\partial V_z}{\partial r} + \frac{\partial^2 V_z}{\partial z^2} \right) + a_z \beta \left( T - T_{ref} \right) + \\
- \left( V_r \frac{\partial V_z}{\partial r} + V_z \frac{\partial V_z}{\partial z} \right)$$
(4)

where  $V_{\alpha}^{k}$  is the velocity component in the r or z-direction for the previous time step.

The final velocity field is corrected by the pressure increment so that is divergence free:

$$V_{\alpha} - V_{\alpha}^{*} = -\frac{\Delta t}{\rho} p_{,\alpha}$$
(5)

By taking the divergence of (5) the following Poisson equation for the pressure is obtained:

$$\frac{\Delta t}{\rho} \left( \frac{\partial^2 p}{\partial r^2} + \frac{1}{r} \frac{\partial p}{\partial r} + \frac{\partial^2 p}{\partial z^2} \right) = \frac{\partial V_r^*}{\partial r} + \frac{V_r^*}{r} + \frac{\partial V_z^*}{\partial z}$$
(6)

The final velocity field is corrected by the pressure increment:

$$V_{a} = V_{a}^{*} + \Delta V_{a}^{*}, \ \Delta V_{a}^{*} = -\frac{\Delta t}{\rho} (p_{,a})$$

$$\tag{7}$$

The momentum and Poisson equations were solved by GDFM using an implicit time scheme for i-th node of the grid.

#### 4. Model of phase transformations

The Time-Temperature-Transformation (TTT) diagram for C45 steel is used in presented model of phase transformations. Temporary values of temperature, time and maximum participation of the particular phase in the current cooling cycle are obtained from them. Kinetics of the ith-phase is calculated from empiric Avrami equation for cooling process [1,2,7,8]:

$$\eta_{(i)}(T,t) = \min\left\{\eta_{(i\%)}, \widetilde{\eta}_{\gamma} - \sum_{j\neq i} \eta_{j}\right\} \cdot \left(1 - \exp\left(-b(T)t^{n(T)}\right)\right)$$
(8)

where:  $\tilde{\eta}_{\gamma}$  denotes volumetric participation of the austenite,  $\eta_{j}$  is volumetric participation of the phases created during cooling process,  $\eta_{(i\%)}$  is final participation of the ith-phase estimated from the TTT diagram, b(T) and n(T) are coefficients depend on the temperature and time (t<sub>s</sub>, t<sub>t</sub>) of the beginning and end of phase transformation.

$$n(T) = 6,12733/\ln\left(\frac{t_{f}(T)}{t_{s}(T)}\right), \qquad b(T) = \frac{0,01005}{t_{s}^{n(T)}}$$
(9)



Fig. 1. Sample temperature curve on the TTT diagram

Participation of created martensite is evaluated on the base of empiric Koistinen-Marburger equation [1,9]:

$$\eta_{M}(T,t) = \left(\tilde{\eta}_{A} - \sum_{\alpha \neq M} \eta_{\alpha}\right) (1 - \exp(-k(M_{s} - T))),$$

$$k = -\ln\left(\sum_{\alpha} \eta_{\alpha}\right) / (M_{s} - M_{f})$$
(10)

where:  $M_s$  denotes initial temperature of the martensitic transformation estimated on the base of TTT diagram.

From the method of calculation of phase fractions by using TTT diagrams follows that timeline in the diagram does not represent the actual time of continuous transformation. Real time transformation is determined from the equation [1]

$$t = \sum_{i} \Delta t_{i} + \sum_{i} \Delta t_{i}^{cor}$$
(11)

where correction time is defined as follow

$$t_i^{cor} = t_{(i-1)} - \left(\frac{-\ln(\eta_{\gamma})}{b(T_i)}\right)^{\left(\frac{1}{n(T_i)}\right)}$$
(12)

The kinetics of the phase transformations during cooling strongly depend on austenisation temperature, therefore model, which exploits two TTT diagrams for C45 steel (880 [°C] and 1050 [°C] austenisation temperature) was developed [10,11]. The constructed application uses a pairs of corresponding points of both TTT diagrams. Each of the points located at the curve determining the end of transformation must have the maximum value of transformation.

Increment of the temperature and phase transformations dependent strain  $d\varepsilon^{Tph} = d\varepsilon^{T} + d\varepsilon^{ph}$  is obtained from following relation:

$$d\varepsilon^{T} = \sum_{i} \alpha_{i}(T) \eta_{i} dT, \quad d\varepsilon^{ph} = \sum_{i} \gamma_{i}(T) d\eta_{i}$$
(13)

where:  $\alpha_i$  is linear thermal expansion coefficient of the ith-phase,  $\gamma_i = \delta V_i / (3V)$  denotes coefficient of volume change during ithphase transformation.

#### 5. Examples

In the paper the calculation for the cooling axisymmetric element was presented. The dimensions of the steel element are r=0.04 [m], h=0.06 [m], the radius of the container with the coolant is 0.12 [m], height is 0.12 [m]. The effect of coolant motion on distribution of bainite, martensite, thermal and structural strains was investigated. In the presented examples only natural convection is taken into account. Material properties of steel element taken as for C45 steel and for coolant assumed as for liquid sodium. Following initial conditions were assumed: initial temperature of cooled element  $T_E=1200$  [K], initial temperature of coolant  $T_C=300$  [K], ideal contact between element and coolant. Sample results obtained from calculations are shown in figures 2 and 3.



Fig. 2. Sample fields of motion vectors, after time *t*=1 [s]

#### 6. Conclusions

Presented model may be used to estimate of kinetics and distribution of phases in the solid state, after solidification process for axisymmetric medium-carbon steel element. The results from this model may be used to prediction of technological conditions for casting process. The solutions of the numerical model of phase transformations, temperature and coolant flow are in good conformity with the reference results (analytical solution, numerical benchmarks and experimental researches).



Fig. 3. The fields of a) ferrite, b) pearlite, c) bainite, d) martensite, e) structural and thermal strain after cooling

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