COMPUTER SIMULATION OF STEEL CASTING

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Abstract

The mathematical model and computer simulation for prediction of mechanical properties of cast steel was developed. Because of wide range of applicability and ease of use of finite volume method (FVM), this numerical method was suitable to create integrated computer program for simulation of transient temperature field in process of solidification and cooling of casting.

Distribution of hardness of cast steel has been predicted by conversion of calculated cooling times from 800 to 500 °C to the hardness. The algorithm for prediction of hardness in casting is based on real chemical composition. The established procedure was applied in computer simulation of cast steel properties.

Keywords: Computer simulation; steel casting; hardness; microstructure

1. INTRODUCTION

During the casting, many different physical processes, such as, solidification, solid state phase transformation, evolution of microstructure, diffusion, heat conduction, and mechanical stressing and distortion are at once taking place inside metal [1-5].

Computer simulation of the casting can be done by considering the issues such as achievement of tolerable casting defects, desired hardness distribution, microstructure distribution and required workpiece shape. Many very useful software are exist for the calculation of grain structure, porosity, hot tearing, and solid-state transformation. But, there are still questions on which answers should be given to satisfy all industry needs in mathematical modelling and simulation of casting [6-7].

Simulation capabilities have been extended beyond thermal and flow modelling for casting. The input of the simulation is composed of the following categories: geometry of casting, physical characteristics of the alloy and the moulds, kinematic boundary conditions and thermal boundary conditions. It is necessary to establish the appropriate algorithm which describes cooling process and to involve appropriate input data in the model. Inverse heat transfer problems should be solved to determine thermal properties for casting based on experimentally evaluated cooling curve results [8].

Proposed numerical model of casting in this work is based on finite volume method (FVM). The finite volume method (FVM) has been established as a very efficient way of solving fluid flow and heat transfer problems. The key feature of the FVM approach is that the FVM is based on flux integration over the control volume surfaces. The method is implemented in a manner that ensures local flux conservation, regardless of the grid structure [9].

2. COMPUTER MODELLING OF HEAT TRANSFER AND SOLIDIFICATION

Numerical simulation of solidification gives consideration to both the motions of molten metal during the mould cavity filing process and convective motions after pouring.

Complete process of solidification and cooling of casting is based on the following system of differential Equations (1-4) [2, 3, 10-12]:

- the Navier-Stokes Equations (1):

$$\mu\left(\frac{\partial^2 v_r}{\partial r^2}+\frac{1}{r}\frac{\partial v_r}{\partial r}+\frac{\partial^2 v_r}{\partial z^2}-\frac{v_r}{r^2}\right)-\frac{\partial p}{\partial r}+\rho g_r \beta\left(T-T_\infty\right)=\rho\frac{\mathrm{d}v_r}{\mathrm{d}t}$$
$$\mu\left(\frac{\partial^2 v_z}{\partial r^2}+\frac{1}{r}\frac{\partial v_z}{\partial r}+\frac{\partial^2 v_z}{\partial z^2}\right)-\frac{\partial p}{\partial z}+\rho g_z \beta\left(T-T_\infty\right)=\rho\frac{\mathrm{d}v_z}{\mathrm{d}t} \quad (1)$$

- the continuity Equation (2):

$$\frac{\partial v_r}{\partial r}+\frac{v_r}{r}+\frac{\partial v_z}{\partial z}=0 \quad (2)$$

- the Fourier's heat conduction Equation (3) including the convection term

$$\frac{\lambda}{r}\frac{\partial T}{\partial r}+\frac{\partial}{\partial r}\left(\lambda\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)=\rho c_{\mathrm{ef}}\left(\frac{\partial T}{\partial t}+v_r\frac{\partial T}{\partial r}+v_z\frac{\partial T}{\partial r}\right) \quad (3)$$

Characteristic boundary condition Equation (4) is:

$$-\lambda\frac{\delta T}{\delta n}\bigg|_{\mathrm{s}}=\alpha\left(T_{\mathrm{s}}-T_{\mathrm{a}}\right) \quad (4)$$

where T (K) is the temperature, t (s) is the time, $\rho = \rho(T)$ (kg / m^3) is the density, λ (W / (m·K)) is the thermal conductivity coefficient, T_s (K) is surface temperature, T_a (K) is air temperature, α (W / (m^2·K)) is heat transfer coefficient, v_r, v_z (m / s) are the r- and z-component of velocity, respectively, $\mu(T)$ (N·s / m^2) is dynamical viscosity coefficient, $c_{ef} = c + L / (T_\beta - T_\alpha)$ (J / (kg·K) is the effective specific heat of a mushy zone, L (J / kg) is the latent heat of solidification, c (J / (kg·K)) is the specific heat, p (N / m^2) is the pressure, g_r, g_z (m / s^2) are the r- and z-component of gravitational acceleration, respectively, β (1 / K) is the volume coefficient of thermal expansion, r, z/m are the coordinates of the vector of the considered node's position, T_∞ (K) is the reference temperature $T_\infty = T_{in}$, r (m) is the radius.

Increment of solidified part, f_i in control volume can be calculated by Equation (5):

$$f_{\mathrm{i}}=\frac{m_{\mathrm{i}}}{m_{\mathrm{vol}}}=\frac{c_{\mathrm{m}}\left(T_1-T_2\right)}{L} \quad (5)$$

where m_i (kg) is mass quantity increase of solidified part in control volume, m_{vol} (kg) is mass quantity of control volume, c_m (J / (kg·K)) is heat capacity of liquid and solid mixture, T_1 (K) is the temperature at the beginning and T_2 (K) is the temperature at the end of time step Δt. In proposed model, it was presumed that convection term has no relevant role and that liquid metal flow could be neglected after pouring [13]. Equations (1) to (3) were found out using the finite volume method. Physical properties included in Equations (1) to (5) should be defined [9, 14]. Accuracy of the heat transfer prediction directly influences to the accuracy of both, calculations of phase transformation kinetics and calculations of mechanical properties of steel. Involved variables in model should be additionally adjusted.

Quantity of growth of solidified part of casting was predicted by calculation of solidification rate in control volume. When $\Sigma f_i = 1$, the mass of solidified part of casting will grow up for mass of control volume.

3. COMPUTER MODELLING OF HARDNESS AND MICROSTRUCTURE COMPOSITION

Hardness and microstructure properties can be estimated based on isothermal transformation (IT) diagrams, continuous cooling transformation (CCT) diagrams and characteristic cooling times from 800 to 500 °C.

When using isothermal transformation (IT) diagrams, in accordance to the Scheil's additivity rule, characteristic microstructure transformation is completed when transformed part of microstructure, X is equal to one [15] according to Equation (6):

$$\int_0^t \frac{dt}{\tau(X_0, T)} = 1 \tag{6}$$

where $\tau(X_0, T)$ represent the isothermal transformation time for $X = X_0$ at a temperature T, and t is the total transformation time. Time of isothermal transformation could be calculated by thermo-kinetic equations or could be found out by using IT diagram [15].

Transformed part of microstructure, X can be calculated by Avrami's isothermal Equation (7):

$$X = 1 - \exp(-k \cdot t^n) \tag{7}$$

For purpose of numerical analysis by computer, it is convenient when kinetics of austenite decomposition is defined in an incremental form of Avrami's isothermal equation. By differentiating the Avrami's equation it follows that

$$\frac{dX}{dt} = \exp(-k \cdot t^n) \cdot n \cdot k \cdot t^{n-1} \tag{8}$$

and by extracting the time component from Equation (8) it follows that

$$\frac{dX}{dt} = n \cdot k^{\frac{1}{n}} \cdot \left(\ln \frac{1}{1-X}\right)^{1-\frac{1}{n}} \cdot (1-X). \tag{9}$$

Equation (9) can be written in an incremental form and the volume fraction ΔX of austenite transformed in the time interval Δt_i at temperature T_i can be calculated as follows:

$$\Delta X_{(N)} = n \cdot k^{\frac{1}{n}} \cdot \left(\ln \frac{1}{1-X_{(N-1)}}\right)^{1-\frac{1}{n}} \cdot \left(1 - X_{(N-1)}\right) \cdot \Delta t_{(N)}. \tag{10}$$

Dependence of kinetic parameters k and n from Equation (10) on chemical composition of steel can be determined inversely by using data from IT diagrams, CCT diagrams and Jominy test results.

According to additivity rule, the non-isothermal transformation kinetics can be described as the sum of a series of the small isothermal transformations. **Figure 1** shows the scheme for microstructure prediction based on cooling curve and IT diagram. In **Figure 1**, the temperature range is divided into a series of small finite steps. Maintaining the time interval, Δt_i to sufficiently short times permits the assumption that the conditions are isothermal over each time step. It was assumed that each time step produces such a transformation as occurs in the IT diagram at the same temperature and microstructure composition.

After calculation of microstructure composition at different location of cast steel, hardness can be estimated by:

$$\mathrm{HRC} = X_P \mathrm{HRC}_P + X_F \mathrm{HRC}_F + X_B \mathrm{HRC}_B + X_M \mathrm{HRC}_M \tag{11}$$

where X_P, X_F, X_B, X_M are contents of ferrite, pearlite, bainite, martensite respectively, and HRC_P, HRC_F, HRC_B, HRC_M are HRC hardness of ferrite, pearlite, bainite, martensite respectively.

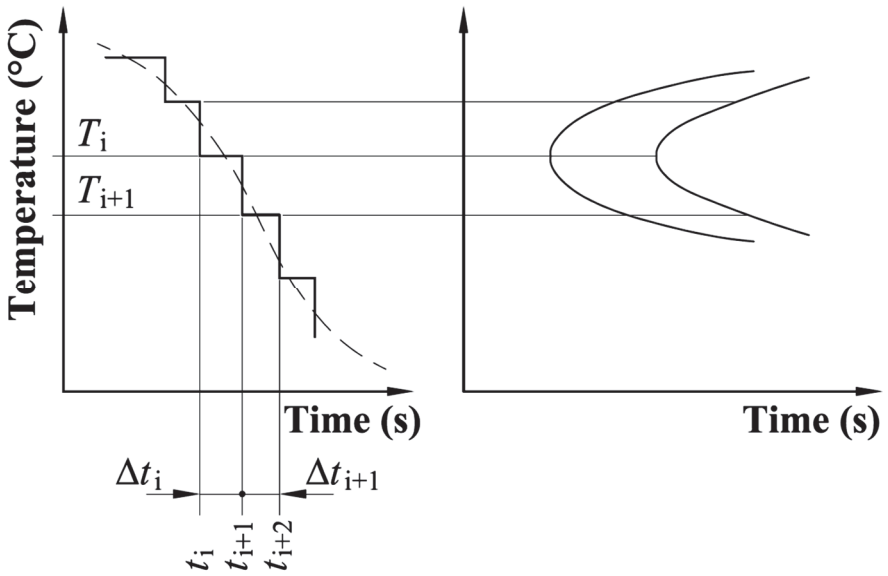

Figure 1 Prediction of microstructure composition from cooling curve and IT diagram

When using continuous cooling transformation (CCT) diagrams, hardness and microstructure composition at different location of cast steel can be estimated by drawing the cooling curves in the CCT diagram. This is a very simple method which is often used.

Also, hardness at different location of cast steel can be estimated by the conversion of the calculated characteristic cooling times from 800 to 500 °C, $t_{8/5}$ to the hardness by using CCT diagram or Jominy hardenability curve.

Hardness, microstructure composition of characteristic steel microstructure and characteristic temperature of austenite decomposition were calculated based on all three explained methods [16].

4. APPLICATION

The developed method for prediction of mechanical properties and microstructure distributions were applied in design of two different castings. Computer simulation of mechanical properties of cast steel was done using the computer software BS-CASTING. The castings were made of steel EN 42CrMo4 and steel EN 100Cr6. The chemical composition of castings is shown in **Table 1**.

Table 1 Chemical composition of steel castings

Steel	Chemical composition (wt.%)									
	C	Si	Mn	P	S	Cr	Ni	Mo	Cu	V
EN 42CrMo4	0.44	0.14	0.62	0.011	0.025	1.19	-	0.23	-	0.16
EN 100Cr6	1.05	0.25	0.33	0.030	0.020	1.53	0.31	0.01	0.20	0.01

The geometry of the mould and castings is shown in **Figure 2**. Pouring temperature during the casting was 1580 °C and the temperature of the mould was 105 °C. The steel castings are poured from the open top of the mould. The hardness distribution of the castings is shown in **Figure 3**.

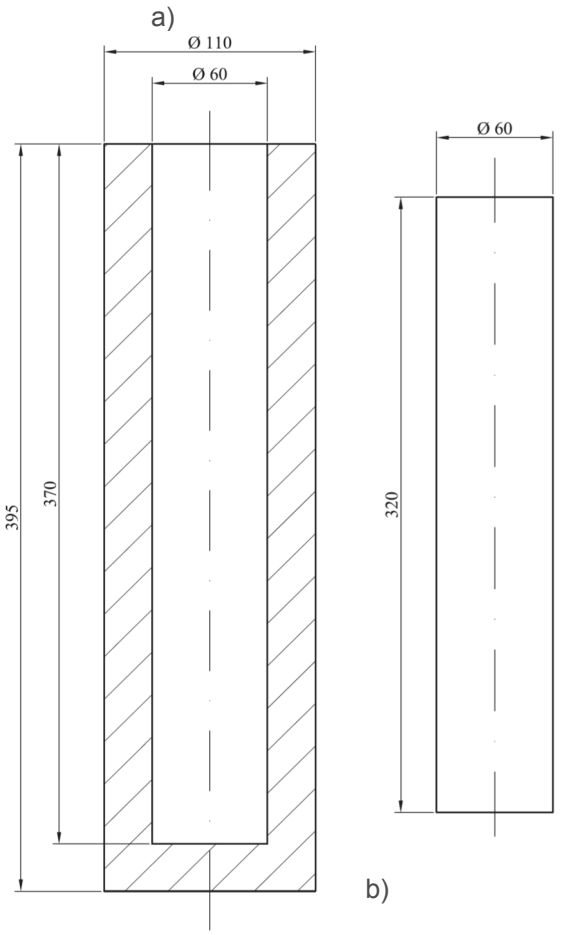

Figure 2 Geometry, a) mould, b) steel casting

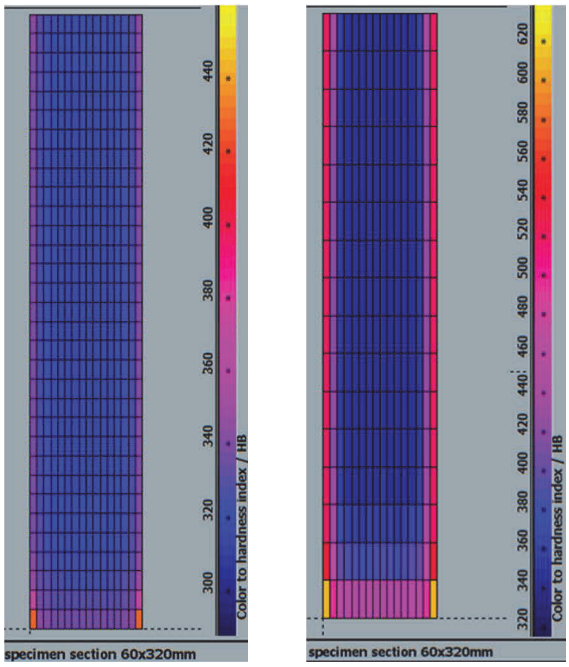

Figure 3 Distribution of hardness of, a) EN 42CrMo4, b) EN 100Cr6 steel casting

5. CONCLUSION

The mathematical model of steel casting has been developed to predict the hardness distribution in a cast steel specimen. The numerical model of casting is based on the finite volume method. The model is consisted of numerical modelling of solidification, numerical modelling of transient temperature field, microstructure transformation in solid state, numerical modelling of hardness

Input material properties involved in mathematical model of casting are additionally adjusted with experimental work by inversion method.

Hardness in cast steel specimen points was calculated by the conversion of calculated cooling times from 800 to 500 °C.

A developed mathematical model has been applied in computer simulation of casting of two ingots made of steel EN 42CrMo4 and steel EN 100Cr6. It can be concluded, that hardness in cast steel can by successfully calculated by proposed method.

ACKNOWLEDGEMENTS

This work has been supported in part by Croatian Science Foundation under the project 5371.

This work has been supported in part by University of Rijeka, Support No 13.09.1.1.02.

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