Archives of Materials Science and Engineering
Volume 78
Issue 1
March 2016
Pages 23-28
International Scientific Journal published monthly by the World Academy of Materials and Manufacturing Engineering

Computer simulation of hardness and microstructure of casted steel 100Cr6

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ABSTRACT

Purpose: The research purpose is to upgrade the mathematical modelling and computer simulation of casting of steel.

Design/methodology/approach: Based on theoretical analyses of physical processes which exist in casting systems the proper mathematical model is established and computer software is developed.

Findings: On the basis of control volume method, the algorithm for prediction of mechanical properties and microstructure distribution in steel casting has been developed.

Research limitations/implications: The computer simulation of casting of steel is consisted of two parts: numerical calculation of transient temperature field in process of solidification and cooling of casting to the final temperature, and of numerical calculation of mechanical properties.

Practical implications: The hardness and microstructures of casting has been predicted based on CCT diagrams. Physical properties that were included in the model, such as heat conductivity coefficient, heat capacity and surface heat transfer coefficient were obtained by the inversion method.

Originality/value: The algorithm is completed to solve 3-D situation problems such as the casting of complex cylinders, cones, spheres, etc. The established model of steel casting can be successfully applied in the practice of casting

Keywords: Steel casting; Computer simulation; Hardness; Microstructure

Reference to this paper should be given in the following way:

B. Smoljan, D. Iljkić, M. Maretić, Computer simulation of hardness and microstructure of casted steel 100Cr6, Archives of Materials Science and Engineering 78/1 (2016) 23-28.

METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

1. Introduction

The numerical simulation of mechanical properties distribution in castings and ingots has one of the priorities in simulation of phenomena of casting. 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 [1-7].

Many very useful software are exist for the calculation of grain structure, porosity, hot tearing, and solid-state transformation. For example there are coupled modules MAGMASOFT, ProCAST, NovaCast, PowerCAST, CalcoSOFT, SOLIDCast, PAM-CASTSIMULOR, ConiferCAST, MAVIS2000, FLOW-3D, CAPCAST, SUTCAST, dieCAS, ADSTEFAN, MICRESS that can be used for computer simulation of casting. But, there are still questions on which answers should be given to satisfy all industry needs in mathematical modelling and simulation of casting [8-10]. Computer programs for simulation of the casting can be developed by considering the issues such as achievement of tolerable casting defects, desired hardness distribution, microstructure distribution and required workpiece shape [11].

Process 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. Simulation of heat transfer is thermodynamical problem. 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 [12].

Proposed numerical model of casting 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. Recently, FVM is used as a simple and effective tool for the solution of a large range of problems in the thermoplastic analysis [13,14]. 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 [13]. Simulations of microstructural transformations are based on the both, CCT diagrams and actual chemical composition.

2. Computer modelling

Numerical simulation of solidification gives consideration to both the motions of molten metal during the mould cavity filing process and convective motions after pouring. Hot liquid is poured into colder mould and both, specific heat and heat of fusion of the solidifying metal pass through a series of thermal resistances to the cold mould until solidification is complete (Fig. 1).

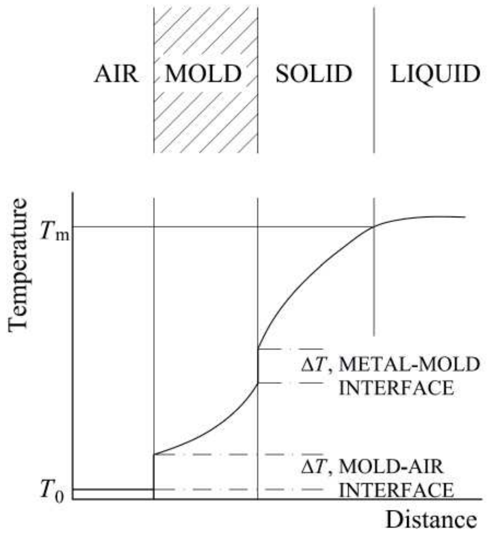

Fig. 1. Temperature profile in solidification of a pure metal

Complete process of solidification and cooling of casting is based on the following system of differential equations [2,3,15]:

- the Navier-Stokes equations

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

- the continuity equation

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

- the Fourier's heat conduction equation 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 is:

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

where T/K is the temperature, t/s is the time, $\rho = \rho(T)$/kgm^{-3} is the density, λ/Wm^{-1}K^{-1} is the thermal conductivity coefficient, T_s/K is surface temperature, T_a/K is air temperature, α/Wm^{-2}K^{-1} is heat transfer coefficient, v_r, v_z/ms^{-1} are the r- and z-component of velocity, respectively, $\mu(T)$/Nsm^{-2} is dynamical viscosity coefficient, $c_{ef} = c + L/(T_\beta - T_\alpha)$/Jkg^{-1}K^{-1} is the effective specific heat of a mushy zone, L/Jkg^{-1} is the latent heat of solidification, c/Jkg^{-1}K^{-1} is the specific heat, p/Nm^{-2} is the pressure, g_r, g_z/ms^{-2} are the r- and z-component of gravitational acceleration, respectively, β/K^{-1} 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 in control volume can be calculated by:

$$f_i = \frac{m_i}{m_{vol}} = \frac{c_m(T_1 - T_2)}{L} \qquad (5)$$

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/Jkg^{-1}K^{-1} 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 was presumed that convection term has no relevant role and that liquid metal flow could be neglected after pouring [16]. Equations (1) to (3) was found out using the finite volume method, but physical properties included in equations (1) to (5) should be defined [11,13,14]. 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 were additionally adjusted. Accepted values of specific heat capacity, c are shown in Table 1 [17]. Values of variable λ for different microstructures of steel are shown in Table 2 [12].

Total heat conductivity coefficients of steel at some temperature, T can be estimated by:

$$\lambda_T = \left(x_F\lambda_{(F+P)T} + x_P\lambda_{(F+P)T} + x_B\lambda_{BT} + x_M\lambda_{MT} + x_A\lambda_{AT}\right)/100 \qquad (6)$$

where x_F, x_P, x_B, x_M, x_A are contents ferrite + pearlite, bainite, martensite and austenite at temperature, T, respectively. Heat transfer coefficients of air are given in Table 3.

Quantity of growth of solidified part of casting was predicted by calculation of solidification rate in control volume (Fig. 2).

When $\Sigma f_i = 1$, the mass of solidified part of casting will grow up for mass of control volume.

Table 1.
Specific heat capacity of different microstructural compositions of steel

	Temperature, T/°C	Ferrite + Pearlite (Bainite)	Martensite	Austenite
Specific heat capacity, c/Jkg^{-1}K^{-1}	0	378	376	415
	300	446	445	440
	600	509	507	467
	800	570	-	490
	950	596	-	520

Table 2.
Heat conductivity coefficients

	Temperature, T/°C	Ferrite + Pearlite (Bainite)	Martensite	Austenite
Heat conductivity coefficients, λ/Wm^{-1}K^{-1}	0	49	43	15
	300	42	37	18
	600	34	30	22
	800	27	-	25
	950	21	-	28

Table 3.
Calibrated values of heat transfer coefficient of air

Temperature, T/°C	20	100	200	400	600	800	1000
Heat transfer coefficient, α/Wm^{-2}K^{-1}	12	15	21	33	50	84	113

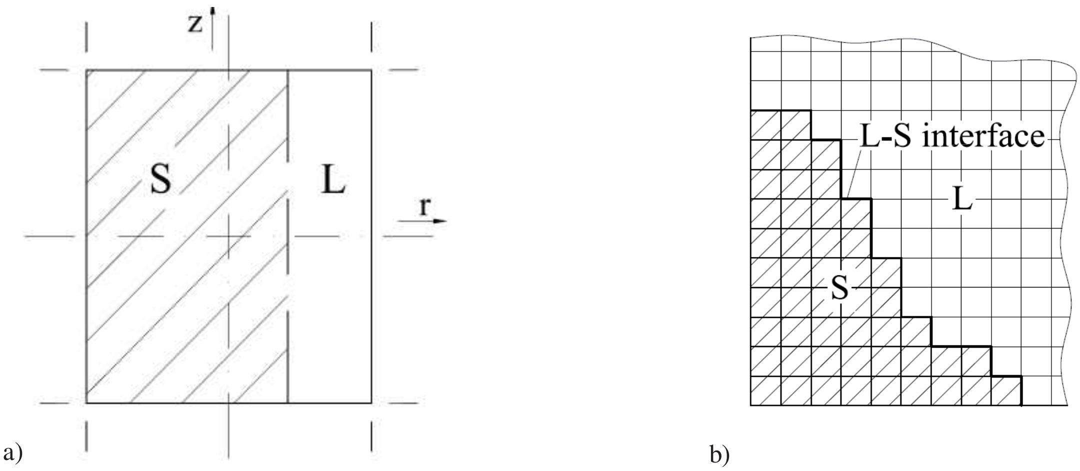

Fig. 2. Liquid-solid interface, a) control volume, b) casting

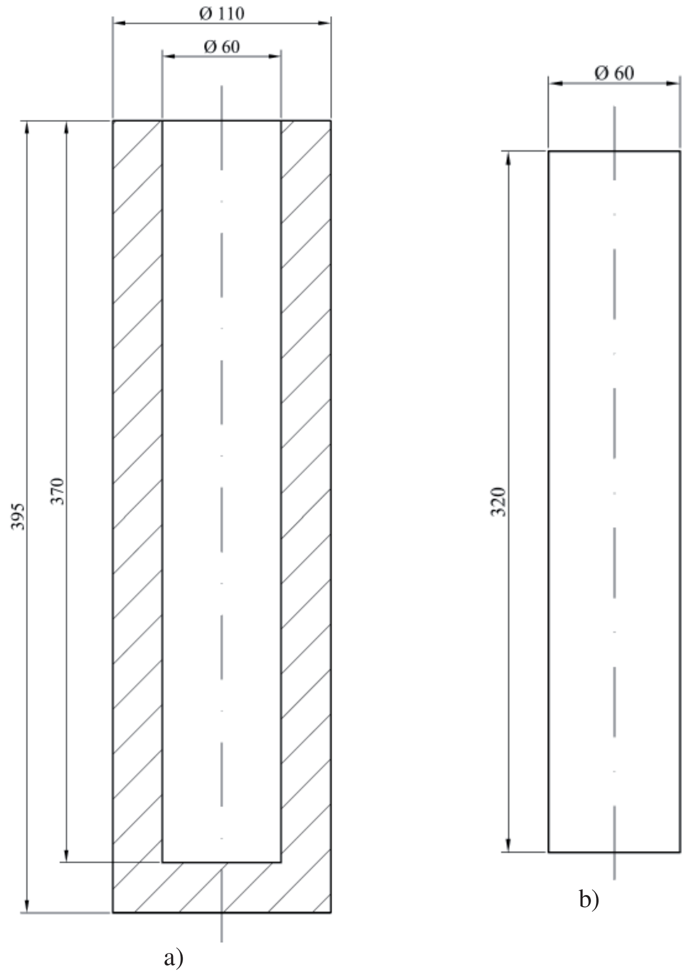

Fig. 3. Geometry, a) mould, b) steel casting

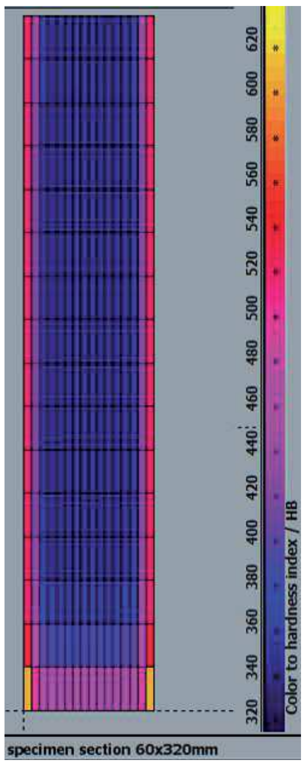

Fig. 4. Distribution of hardness of steel casting

In the developed computer simulation of casting, the hardness and microstructure composition at different workpiece points is estimated by the conversion of the calculated cooling time $t_{8/5}$ to the hardness and microstructure composition based on CCT diagrams using linear alignment with the actual chemical composition. Final estimation of microstructure composition was improved using the thermo-kinetic expressions [11,18].

3. Application

The developed method for prediction of mechanical properties and microstructure distributions were applied in design of casting. Computer simulation of mechanical properties and microstructure distribution of steel casting was done using the computer software BS-CASTING.

The casting was made of steel EN 100Cr6. The chemical composition of casting was: 1.05 %C, 0.25 %Si, 0.33 %Mn, 0.030 %P, 0.020 %S, 1.53 %Cr, 0.31 %Ni, 0.01 %Mo, 0.20 %Cu, 0.01 %V. The geometry of the mould and casting is shown in Figure 3.

Pouring temperature during the casting was 1580°C and the temperature of the mould was 105°C. The steel casting is poured from the open top of the mould.

The hardness distribution of the casting is shown in Figure 4. The distributions of ferrite, pearlite, bainite and martensite of steel casting are shown in Figure 5.

4. Conclusions

The mathematical model of steel casting has been developed to predict the mechanical properties and microstructure distribution in a casted steel specimen. The numerical model of casting is based on the finite volume method and 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 and microstructure composition in specimen points was calculated by the conversion of calculated time of cooling from 800 to 500°C to hardness and microstructure composition using the CCT diagram. Additionally, predictions of microstructure composition are improved bay calculations based on actual chemical composition.

A developed mathematical model has been applied in computer simulation of casting of ingot made of high hardenability steel EN 100Cr6. It can be concluded, that hardness and microstructure composition in casted steel can by successfully calculated by proposed method.

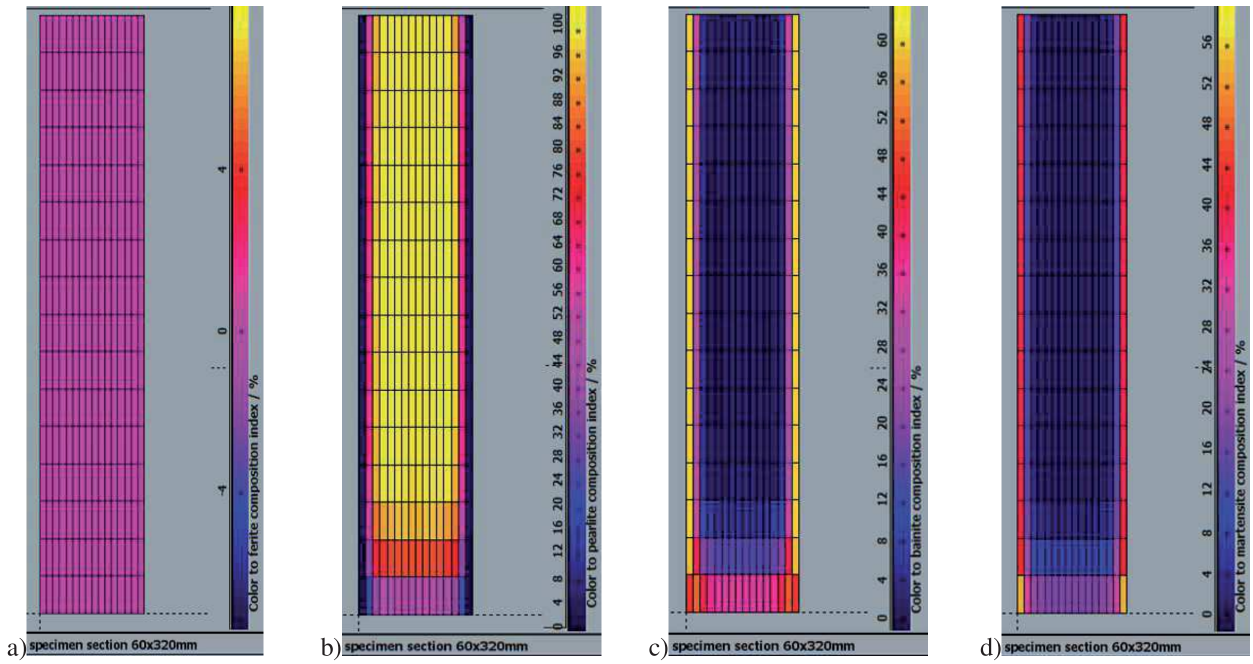

Fig. 5. Distributions of a) ferrite, b) pearlite, c) bainite, d) martensite of steel casting

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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