Computer Simulation of Thermal Processing of Steel

B Smoljan¹, D Iličić², K Hajdek¹ and W Sitek³
¹University North, Department of Packaging, Recycling and Environmental Protection, Trg dr. Žarka Dolinara 1, 48000 Koprivnica, Croatia
²University of Rijeka, Faculty of Engineering, Department of Materials Science and Engineering, Vukovarska 58, 51000 Rijeka, Croatia
³Silesian University of Technology, Faculty of Mechanical Engineering, Division of Biomedical Engineering, Institute of Engineering Materials and Biomaterials, ul. Konarskiego Street 18a, 44-100 Gliwice, Poland

E-mail: bozo.smoljan@gmail.com

Abstract. The review of the numerical modelling of casting and welding of steel workpieces was studied. The contemporary industry needs tools to optimize and control parameters of processes by considering the favourite chemical composition of steel. In recent time, very efficient tool for optimizing and controlling of the process parameters is numerical modelling of engineering processes. At casting and welding numerical modelling is focused on optimization of distribution of microstructure contents, mechanical and physical properties distribution and tolerated distortions and residual stresses. Mechanical properties and prevention of distortion and cracking can be accomplished by prediction and control of residual stresses and microstructure distribution. The numerical modelling of thermal processing of metals consists of the research of multi-scale processes and multi-physics processes, such as phase transformations, heat transfer and mechanics of materials, and research of numerical methods for computer interpretation of the problem. By means of the numerical modelling and computer simulation of thermal processing should calculate the transient temperature field, melting and solidification processes, as well as, to calculate distribution of mechanical and physical properties and microstructure composition. In this work, the numerical models of studied thermal processes are based on the finite volume method. Values of surface heat transfer coefficient, heat capacity and heat conductivity coefficient were obtained by the inversion method. The microstructures composition has been predicted by CCT diagrams and additionally improved by the kinetic equations. The mathematical model has accomplished to solve thermal processing of 3-D axially symmetric specimens.

1. Introduction

Welding and casting are very important processes in the engineering of metal materials. At the welding and casting of metals, numerous physical processes are taking place at once. There are heat transfer and heat conduction, melting and solidification, diffusion and phase transformation, as well as, mechanical stressing and distortion, [1–4].

Modern technology needs precise prediction of results of metal processing. By numerical modelling can successfully predict the results of metal processing. Today in computer simulation of welding and casting there is many very good and useful computer software, which gives an opportunity to calculate the kinetics of solid-state transformation, grain structure, porosity, residual
stresses and distortion generation [5-7]. However, there are many questions, which should be answered.

Usually, numerical modelling of welding and casting of metals consists of definition of melting and solidification processes, distribution of microstructure and mechanical properties, as well as, prediction of residual stresses and distortions.

The numerical model should describe processes at all phases of metal heating and cooling. Proper input data and boundary conditions should be involved in the numerical model [8]. By the inputs data, geometry, physical and mechanical characteristics should be defined. To predict thermal properties of metals today is very useful an inverse heat transfer analyses based on experimental results. The thermodynamic state of the system is defined by initial and boundary conditions. Boundary conditions could be kinematic or thermal.

It is known that a finite volume method is a suitable tool for numerical calculations in heat conduction, heat transfer, diffusion and fluid flow processes. In recent times, the finite volume method was successfully applied in solving of a large range of thermoplastic problems [9, 10].

2. Numerical modelling of heat transfer and solidification

Numerical modelling of solidification of molten metal considers both the motions of liquid metal during the filing of the cavity and convective motions. During the solidification, molten metal goes through a many of thermal resistances. Figure 1 schematically shows the process of solidification of molten metal.

\[
\begin{align*}
\mu \left( \frac{\partial^2 v}{\partial r^2} + \frac{1}{r} \frac{\partial v}{\partial r} + \frac{\partial^2 v}{\partial z^2} \right) - \frac{\partial p}{\partial r} + \rho g \beta (T - T_s) &= \frac{d\rho}{dt} \\
\mu \left( \frac{\partial^2 v}{\partial r^2} + \frac{1}{r} \frac{\partial v}{\partial r} + \frac{\partial^2 v}{\partial z^2} \right) - \frac{\partial p}{\partial z} + \rho g \beta (T - T_a) &= \frac{d\rho}{dt}
\end{align*}
\] (1)

The following system of differential equations describes processes of solidification and cooling in solid state at the welding or casting process [1-4, 11]:

Figure 1. Temperature diagram of solidification of molten metal.
\[\frac{\partial v_r}{\partial r} + \frac{v_r}{r} + \frac{\partial v_z}{\partial z} = 0\]  \hfill (2)

\[\frac{\lambda}{r} \frac{\partial T}{\partial r} + \frac{\partial}{\partial r} \left( \frac{\lambda}{r} \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( \frac{\lambda}{c_{\text{ef}}} \frac{\partial T}{\partial z} \right) = \rho c_{\text{ef}} \left( \frac{\partial T}{\partial t} + v_r \frac{\partial T}{\partial r} + v_z \frac{\partial T}{\partial z} \right)\]  \hfill (3)

where: \(T/K\) is the temperature; \(t/s\) is the time; \(T_\infty/K\) is the reference temperature; \(c/J\text{kg}^{-1}\text{K}^{-1}\) is the specific heat; \(c_{\text{ef}} = c + L(T_\beta - T_\alpha)/K\text{kg}^{-1}\text{K}^{-1}\) is the effective specific heat; \(L/J\text{kg}^{-1}\) is the latent heat of solidification; \(\lambda/W\text{m}^{-1}\text{K}^{-1}\) is the thermal conductivity coefficient; \(\rho = \rho(T)\text{kgm}^{-3}\) is the density; \(\mu(T)/\text{Nm}^{-2}\) is viscosity coefficient; \(v_r, v_z/\text{ms}^{-1}\) are the \(r\)- and \(z\)-component of velocity; \(p/\text{Nm}^{-2}\) is the pressure; \(g_r, g_z/\text{ms}^{-2}\) are the \(r\) and \(z\)-component of gravitational acceleration; \(\beta/K^{-1}\) is the coefficient of thermal expansion; \(r, z/m\) are the coordinates of the vector of the considered position.

Boundary condition:

\[-\lambda \frac{\partial T}{\partial n_s} = \alpha(T_s - T_\infty)\]  \hfill (4)

where \(\alpha/W\text{m}^{-2}\text{K}^{-1}\) is heat transfer coefficient, \(T_s/K\) is air temperature \(T_\infty/K\) is surface temperature

Dependence of physical properties involved in equations (1) to (4) on temperature should be known [9, 10]. It was accepted that liquid metal flow does not exist after the cavity is fulfilled, and the convection term was neglected [12]. Finite volume method is a very suitable numerical method to solve the system equations from equations (1) to (3). By the integration over the control volume surfaces discretization system of \(N\) linear algebraic equations can be established with \(N\) unknowns. Figure 2 shows the liquid-solid interface in control volume and cavity or mould.

**Figure 2.** Liquid-solid interface: (a) control volume, (b) cavity or mould.

Quantity of growth of solidified part of liquid metal was predicted by calculation of solidified quantity in control volumes. Quantity of solidified part in the control volume is equal to:

\[f_i = \frac{m_i}{m_{\text{vol}}} = \frac{c_m(T_i - T_{z_i})}{L}\]  \hfill (5)

where \(T_i/K\) and \(T_{z_i}/K\) are the temperatures at the beginning and the end of time step \(\Delta t\), respectively, \(m/\text{kg}\) is mass quantity of solidified part of the control volume, \(m_{\text{vol}}/\text{kg}\) is control volume mass, \(c_m/J\text{kg}^{-1}\text{K}^{-1}\) is heat capacity of the mixture of liquid and solid part of the control volume. The mass of solidified part in the control volume will grow up until the \(\Sigma f_i = 1\).
The transient temperature field in an isotropic body is determined by (equation 3), or Fourier’s law of conductivity [9, 10, 13]. In the calculation of the heating process during the welding, it was assumed that the heating arc on the top side of the welding joint has a Gaussian distribution:

\[ Q = q_0 \int_0^r e^{-\frac{d}{r_0^2}} 2\pi r dr \]  

where \( Q/W \) is the heat input, \( r_0/m \) is the distance of the arc centre, \( d \) is the factor and \( q_0/Wm^{-2} \) is the energy generation rate [13, 14].

Numerical modelling of the temperature transient field is in the root of mathematical modelling of thermal processes. Results of numerical modelling of the temperature transient field directly affects the calculations of steel properties, the kinetics of microstructure transformation, and calculations of residual stresses and distortions.

In the mathematical model it can be accepted that variable \( \rho \) for steel is constant and equal to 7800 \( kgm^{-3} \). Accepted dependence of specific heat capacity, \( c \) of steel on microstructure composition and temperature is shown in table 1 [15].

### Table 1. Dependence of specific heat capacity of steel on temperature and microstructure composition.

| Temperature, \( T/°C \) | 0   | 300 | 600 | 800 | 950 |
|---------------------------|-----|-----|-----|-----|-----|
| Ferrite + Pearlite (Bainite) | 378 | 446 | 509 | 570 | 596 |
| Austenite                 | 415 | 440 | 467 | 490 | 520 |
| Martensite                | 376 | 445 | 507 | -   | -   |

Table 2 shows the accepted values of heat conductivity coefficients [10].

### Table 2. Dependence of heat conductivity coefficients of steel on temperature and microstructure composition.

| Temperature, \( T/°C \) | 0   | 300 | 600 | 800 | 950 |
|---------------------------|-----|-----|-----|-----|-----|
| Ferrite + Pearlite (Bainite) | 49  | 42  | 34  | 27  | 21  |
| Austenite                 | 15  | 18  | 22  | 25  | 28  |
| Martensite                | 43  | 37  | 30  | -   | -   |

Table 3 shows the heat transfer coefficients of ordinary air [10].

### Table 3. Heat transfer coefficient of air.

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

3. Numerical modelling of the distribution of microstructure composition and hardness

Microstructure composition and mechanical properties of steel after some thermal processing depend on the regime of cooling process. The regime of continues cooling can be approximate by small steps of cooling. Continues cooling transformations, in this case, can be expressed as the sum of isothermal transformations increments. Avrami’s equation for calculation of isothermal microstructure transformations can be applied to calculate kinetics of continuous cooling transformations in solid state, which exist during the welding and casting. The transformed fraction of austenite, \( \Delta x \) can be expressed in incremental form by [16, 17]:

\[ r = \frac{2}{\pi} \int_0^r e^{-\frac{d}{r_0^2}} 2\pi r dr \]
where $Tm/K$ is the characteristic temperature, $\Delta t_m/s$ is the characteristic time step. The Schéil’s additivity rule defines that microstructure transformation is finished when the sum of transformed portions of microstructure, $\Sigma \Delta x_m$ is equal to unity:

$$\sum_{m=1}^{M} n_x(\frac{1}{1-x_{m-1}})^{\frac{1}{n}} (1-x_{m-1}) \Delta t_m = 1$$  \hspace{1cm} (8)

Parameters $k$ and $n$ in equation 7 and 8 can be determined based on the characteristic time of isothermal transformation.

$$k = \frac{\ln(1-x)}{t_T}$$ \hspace{1cm} (9)

This characteristic time $t_T$ can be predicted from experimentally evaluated IT diagram of steel. Additionally characteristic time $t_T$ should be adduced in accordance with the real chemical composition of studied steel. It can be done by using kinetic equations.

Martensitic transformation can be expressed by [18]:

$$x_m = (1-x_p - x_n)(1 - \exp(-0.01 (M_S - T)))$$ \hspace{1cm} (10)

The martensite increment is equal to:

$$\Delta x_m = x_m(T_m) - x_M(T_m)$$ \hspace{1cm} (11)

Critical temperatures of austenite decomposition can be expressed as a function of hardenability properties [16].

Hardness at different specimen’s points can be predicted based on time of cooling from 800 to 500 °C, $t_{8/5}$. Time $t_{8/5}$ was evaluated from the CCT diagrams, which should be adjusted taken into account the real chemical composition of steel [16, 19].

Since steel welding joints or casting could be additionally reheated during processing, the influence of reheating on microstructure composition and mechanical properties should be calculated [16, 20, 21]. With reheating, some kind of tempering is going on. Characteristic tempering temperature, $T_t$ can be expressed by:

$$T_t = \frac{T_r(C + a \ln \Delta t)}{C}$$ \hspace{1cm} (12)

where constants $a$ and $C$ have the same meaning as have in Hollomon-Jaffe expression [14].

4. Applications

4.1. Computer simulation of casting

The established numerical model of hardness and microstructure distribution of casted steel was applied in computer simulation of the casting of steel EN42CrMo4. The computer simulation was done by the software BS-CASTING. The chemical composition of studied steel EN42CrMo4 was: 0.44% C; 0.14% Si; 0.62%; Mn; 0.011% P; 0.025% S; 1.19% Cr; 0.23% Mo; 0.16% V.

Figure 3 shows the mould and steel casting design. The temperature of liquid metal was 1580 °C and temperature of metal mould was 105 °C. The molten metal was poured from the open top of the cavity. Figure 4 and figure 5 show hardness distribution and distribution of ferrite, pearlite, bainite and martensite of casted steel.
Figure 3. Geometry of: (a) mould, (b) casting.

Figure 4. As-casted hardness.

Figure 5. Distributions of: (a) ferrite, (b) pearlite, (c) bainite, (d) martensite.
4.2. Computer simulation of welding
Welded joints were made of normalized steels EN42CrMo. Figure 6 shows the geometry of the welding joint.

![Figure 6. Welding joint geometry.](image)

Heat input was 4.8 kJ/cm and welding rate was 30 cm/min. The base metal and filler metal has the same chemical composition of 0.44% C; 0.14% Si; 0.62% Mn; 0.011% P; 0.025% S; 1.19% Cr; 0.23% Mo; 0.16% V. Welding joints are tempered at 380 °C for one hour.

The numerical simulation of welding joint hardness and microstructure distribution was done by using BS-WELDING computer software. Figure 7 shows the distribution of microstructure composition of welding joint.

![Figure 7. Distribution of microstructure composition: (a) ferrite, (b) pearlite, (c) bainite, (d) martensite.](image)
Figure 8 shows the distribution of hardness of welding joint

![Figure 8](image-url)

**Figure 8.** Distribution of hardness of welding joint: (a) as-welding hardness, (b) hardness after tempering.

5. Conclusions

The numerical model and computer software have been developed to simulate thermal processes at casting and welding of steel. During the welding and casting many physical processes are going on. In numerical modelling of welding and casting should be focused on solidification, transient temperature field, microstructure transformation in solid state, mechanical properties.

Numerical modelling of thermal processing of steel could be performed by the application of the finite volume method. By the developed computer software the hardness and microstructure distribution in steel casting and welding joint can be estimated.

The numerical model has been applied in computer simulation of casting and welding of workpieces made of steel EN42CrMo4. Physical properties, i.e., steel density, the specific heat capacity of steel, heat transfer coefficient and heat conductivity coefficient of steel which were included in numerical models of casting and welding, were accepted from literature and additionally experimentally adjusted by inversion method.

Both, microstructure composition and hardness were predicted by the conversion of calculated time of cooling from 800 to 500°C, \( t_{8/5} \) to the corresponding values of microstructure composition or hardness. Time of cooling from 800 to 500°C, \( t_{8/5} \) has been evaluated based on standard CCT diagrams. By the relations for microstructure transformations kinetics, specific time \( t_{8/5} \) has been additionally adjusted in accordance with chemical composition of studied steel. The hardness of the steel after welding calculated by the considering effects of the reheating processes during the welding.

It can be concluded, that hardness and microstructure composition of welded joints and castings made of steel can be successfully calculated by the proposed method.

6. References

[1] Tseng T C and Kobayashi S 1989 *Int. J. Mach. Tools Manuf.* **29** 121–140
[2] Smoljan B, Ilikić D, Smokvina Hanza S, Štic L and Jokić M 2018 Proc. 12th Int. Seminar Numerical Analysis of Weldability (Graz - Castele Seggau) (Verlag der Technischen Universität Graz) p 167
[3] Rosso M 2008 *Modelling of Casting*, in *Handbook of Thermal Process Modelling Steels* (Boca Raton, FL: CRC Press, Taylor & Francis Group)
[4] Vanaparthy N M and Srinivasan M N 1998 *Modell. Simul. Mater. Sci. Eng.* **6** 237–249
[5] Dobrzański L A, Śliwa A and Tanski T 2009 *Archives of Computational Materials Science and Surface Engineering* **1** 25–28.
[6] Sommerfeld A, Böttger B and Tonn B 2008 *J. Mater. Sci. Technol.* **24** 321–324
[7] Schneider M and Beckermann C 1995 Metallurgical and Materials Transactions A 26 2373–2388
[8] Gur C H and Pan J 2008 Handbook of Thermal Process Modelling Steels (Boca Raton, FL: CRC Press, Taylor & Francis Group)
[9] Smoljan B, Iljkić D and Novak H 2013 Proc. 2nd Mediterranean Conf. on Heat Treatment and Surface Engineering (Dubrovnik-Cavtat) (Zagreb: Croatian Society for Heat Treatment and Surface Engineering) p 399
[10] Patankar S 1980 Numerical Heat Transfer and Fluid Flow (New York: McGraw Hill Book Company)
[11] Sowa L 2014 Journal of Applied Mathematics and Computational Mechanics 13 123–130
[12] Flemings M 1984 Solidification Processing (McGraw-Hill Book Company)
[13] Smoljan B, Iljkić D, Štic L, Tomašić N and Smokvina Hanza S 2016 Proc. 41st Int. Conf. WELDING 2016 (Opatija) (Zagreb: Croatian Welding Society)
[14] Demirdžić I 1984 Zavarivanje 27 481–489 (in Croatian)
[15] Bhadeshia H 2002 Material Factors, in Handbook of Residual Stress and Deformation of Steel (ASM International)
[16] Smoljan B, Iljkić D, Smokvina Hanza S, Jokić M, Štic L and Borić A 2019 Materials Performance and Characterization 8 17–36
[17] *** 1991 Heat Treating, ASM Handbook Vol. 4 (Materials Park, OH: ASM International)
[18] Koistinen D P and Marburger R E 1959 Acta Metall. 7 59–60
[19] Smoljan B, Iljkić D and Tomašić N 2015 Proc. 28th ASM Heat Treating Society Conference, Heat Treating 2015 (Detroit, MI) (ASM International, Materials Park, OH) p 266
[20] Reti T, Felde I, Guerrero M and Sarmiento S 2009 Int. Conf. on New Challenges in Heat Treatment and Surface Engineering (Conference in honour of Prof. Božidar Liščić) (Dubrovnik-Cavtat) (Zagreb: Croatian Society for Heat Treatment and Surface Engineering) p 333
[21] Smoljan B, Iljkić D and Smokvina Hanza S 2009 Journal of Achievements in Materials and Manufacturing Engineering 34 152–156

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