1. Introduction

The heat treatment of hot-work tool steel is a technological process, in which thermal phenomena, phase transformations and mechanical phenomena are dominant. Models, which describe processes mentioned above, don’t take into consideration the many important aspects. As a result of the complexity of phenomenon of heat treatment process, there are many mathematical and numerical difficulties in its modelling. For this reason there hasn’t a model which includes phenomenon accompanying heat treatment and hardening of hot-work tool steel [1-6].

The numerical analysis of the heat treatment processes is the important problem for the modern lab which designs for the industry. The special attention on the development this branch of the numerical methods is inspired by the industry, which due to the modern technology and reduces the cost, requires the tools to improve the heat treatment processes. The research works including the issue of the heat treatment can be divided into those that in the complex way analyze the presented phenomena, as well as those that focus only on the one phenomena of the heat treatment process. The phenomena occurring during the heat treatment are very complex and still incompletely described. The model of the hardening process should contain at least three coupling elements: thermal, structural and mechanical [3,4,7-11]. Determination of the composition of each phases, their kinetics and obtained structures during the cooling process of iron alloys is necessary to calculate the stresses for the hardening process. In the heat treatment process the significant stresses are generated and cause, in most cases, the plasticize of the material. Therefore, in the modeling of mechanical phenomena the use of the models of elastic-plastic materials is required. Additionally, to ensure the reliability of the results of numerical simulations of mechanical phenomena, except thermal, structural and plastic strains the transformation induced plasticity should be taken into account [3,12-18].
The element which has the significant influence on the results of numerical simulation of the hardening is the appropriate choice of the cooling conditions which are modeled by the boundary conditions. This is important in the case of quenching the hot-work tool steel, which is easily hardened [6]. Therefore, in the paper paid attention to this problem by comparing the results from numerical simulation for the two rate of cooling, although both are relatively small. To implement this type of algorithms one usually applies the FEM, which makes it possible to take into account both nonlinearities and inhomogeneity of thermally processed material [1,3,10,13,19,20].

2. Model of heat transfer phenomena

The fields of temperature are determined from heat transfer equation:

\[ \text{div}(\lambda \text{grad}(T)) - C \frac{\partial T}{\partial t} = -Q, \quad T = T(x_a, t) \]  

where \( \lambda = \lambda(T) \) is the heat conductivity coefficient [W/(mK)], \( T = T(x, t) \) temperature [K], \( C = C(T) \) is an effective heat capacity [J/(m3K)], \( Q \) is intensity of internal sources in which the heat of phase transformations are taken into account [W/m3], \( x_a \) are the coordinates [m] and \( t \) is time [s].

The equation (1) is supplemented by initial conditions

\[ T(x_a, t_0) = T_0(x_a), \quad Q(x_a, t_0) = Q_0(x_a) = 0 \]  

and boundary conditions:

a) On the part of the edge \( \Gamma = \Gamma_q \) the heat flux is given \( q = q^* \), Neumann condition (type II). A condition of this type the thermal insulation is modeled.

\[ -\lambda \frac{\partial T}{\partial n} = q = 0 \]  

b) On the part of the edge \( \Gamma = \Gamma_n \) the heat flux (\( q_n \)) is determined by the difference between the temperature of edge and the surrounding medium, Newton condition (type III). In the paper by this type of boundary condition the heating and cooling process is modeled.

\[ -\lambda \frac{\partial T}{\partial n} = q_n = \alpha(T)(T_\Gamma - T_\infty) \]  

where \( \alpha(T) \) is the heat transfer coefficient [W/(m2K)], \( \Gamma \) is surface, from which the heat is taken over, \( T_\infty \) is temperature of the medium rounded.

Heat of phase transformations \( \dot{Q}^{ph} \) take into account in source unit of conductivity equation (1) calculate by formula [3,10,21]:

\[ \dot{Q}^{ph} = \sum_k \dot{Q}_k^{ph} = \sum_k H_k^{ph} \eta_k \]  

where: \( H_k^{ph} \) is volumetric heat of \( k \) - phase transformations [J/m3] (k=2..5 appropriate for the bainite, ferrite, martensite and pearlite), \( \eta_k \) is rate of change fractions of \( k \) - phase.

This internal heat source could be taken into account by enthalpy changes. The following enthalpy changes for the diffusional and diffusionless transformations were used [11,21]:

\[ \Delta H_B = 314 \times 10^6, \quad \Delta H_M = 630 \times 10^6, \quad \Delta H_P = 800 \times 10^6 \]  

where \( \Delta H_B, \Delta H_M \) and \( \Delta H_P \) indicate the enthalpy changes during austenite-bainite, austenite-martensite and austenite-pearlite transformations, respectively.

To solve, presented above, the heat transfer phenomena, i.e. heat transfer equation (1) with completed initial (2) and boundary conditions (3), (4), the finite element method in Galerkin formulation was used [3,22].

3. Model of phase transformations in the solid state

In the paper the macroscopic model for calculation of the created fractions of the phases in solid state, for hot-work tool steel (W360), is used for following chemical composition (Table 1) [6]:

| Steel | C% | Mn% | Si% | Cr% | Mo% | V% |
|-------|----|-----|-----|-----|-----|----|
| W360  | 0.50 | 0.25 | 0.20 | 4.50 | 3.00 | 0.55 |

The continuous cooling diagram (CCT) is used to determine the significant parameters of phase transformations model (the time and the temperature of start and end of transformations) (Fig. 1) [6].

![Continuous Cooling Transformation diagram (CCT) for the hot-work tool steel W360](image_url)

Fig. 1. The Continuous Cooling Transformation diagram (CCT) for the hot-work tool steel W360 [6]

To calculate the kinetic of phase transformation of heating (transformation to austenite) the diagram of continuous heating (CHT) is used. Whereas to determine the phase transformations in the cooling process the new defined diagram of continuous
cooling (CCT) for the higher temperature of austenitization (offset CCT diagram) are taken into account (Fig. 2). The offset of the diagram to the left side, in reference to the original graph (Fig. 1), is the result of the changes in method of CCT diagram analysis. It was assumed that the start point of cooling curve is in the point of intersection of the two lines - cooling curve and the temperature line in 800°C. In this way can avoid, in the simulation of the kinetic of cooling transformations, the offset all lines on the CCT diagram for the different heating temperatures [6].

Fig. 2. The Continuous Cooling Transformation diagram (CHT) and shifted CCT diagram with marked cooling rate for the hot-work tool steel W360

The kinetics of phase transformation in solid state i.e. during heating process - austenitization, cooling - austenite to pearlite or bainite in model are calculated by JM formula. The changes of content of martensite are defined by the empirical kM equation [3,13,23,24]:

\[
\eta_{A}^M(T,t) = \frac{\alpha}{\alpha_{s}(T)} \frac{\eta_{A}^{M_{s}}}{\eta_{M_{s}}^{M}} (T) \]

where \(\eta_{A}^M(T,t)\) is the fraction of forming austenite after heating, \(\eta_{M}^{M_{s}}\) is maximal phase fraction for established cooling rate estimated on the basis of CCT diagram, \(b_{s}(t)\) and \(a(t)\) are coefficients calculated assuming the initial fraction (\(\eta_{A}(t_{s})=0.01\)) and the maximum value of fraction (\(\eta_{A}(t_{f})=0.99\)), \(\eta_{A}^{M_{s}}\) and \(\eta_{A}^{M_{s}}\) is maximal phase fraction for established cooling rate estimated on the basis of CCT diagram, \(b_{s}(t)\) and \(a(t)\) are coefficients calculated assuming the initial fraction (\(\eta_{A}(t_{s})=0.01\)) and the maximum value of fraction (\(\eta_{A}(t_{f})=0.99\)), \(\eta_{A}^{M_{s}}\) is the fraction of forming austenite after heating, \(\eta_{M}^{M_{s}}\) is a constant from experiment; for considered steel \(m = 3.5\), the start temperature of martensite transformation amount \(M_{s}=548\) K, and final temperature of transformation is equal \(M_{f}=123\) K [14,16].

Increases of the isotropic deformation \(\varepsilon^{ph}\) caused by changes of the temperature and phase transformation in the heating and cooling processes are calculated using the following relations for heating and cooling respectively[3,10]:

\[
\varepsilon^{ph} = \varepsilon^{ph}_{A} + \varepsilon^{ph}_{M} = \sum_{n=0}^{k} a_{n} \varepsilon^{T}_{n} + \sum_{n=0}^{k} b_{n} \varepsilon^{S}_{n} + \sum_{n=0}^{k} c_{n} \varepsilon^{P}_{n}
\]

where \(a_{n} = \eta_{n}^{A} / \eta_{M}^{M_{s}}\) are coefficients of thermal expansion of: austenite, bainite, ferrite, martensite and pearlite, respectively, \(\varepsilon^{ph}_{A}\) is the isotropic deformation accompanying transformation of the input structure into austenite, whereas \(\varepsilon^{ph}_{M}\) are isotropic deformations from phase transformation of: austenite into bainite, ferrite, martensite, or of austenite into pearlite, respectively.

For the considered steel, the values of thermal expansion coefficients for the initial structure (spheroid), described in the articles, have the values depend on the temperature: 100°C - 11.1×10^{-6} 1/K, 400 °C - 12.3×10^{-6} 1/K and 700°C - 13.6×10^{-6} 1/K. The thermal expansion coefficient for the austenite is equal 22×10^{-6} 1/K [6].

Therefore, that the thermal expansion coefficient is not a line function, it is approximated by square function, which passed through the points described above:

\[
\alpha_{ph}(T) = 5.5556 \times 10^{-13} T^2 + 3.4189 \times 10^{-9} T + 9.7475 \times 10^{-6}
\]

Isotropic structural strains are calculated on the base of literature review and analysis of numerical dilatometric tests obtained for different cooling rate. These tests are made for the large range of cooling rate for the austenite to pearlite, to bainite and to martensite transformations. The values of structural strain coefficient are equal: 2.2, 6.0, 8.2 and 2.85 (×10^{-3}) for austenite, bainite, martensite and pearlite respectively [6,10].

The comparison of results from the simulation of cooling process with different established cooling rate (the average cooling rate in the range of 800 - 500°C (see Fig. 2)) is presented on the figure 3. To calculate the dilatometric curve the equation (8) is used. The displacement on figure 3 are referred to base length equal 10 mm (most applied length of the dilatometric specimen).

Fig. 3. Calculate dilatometric curves for established cooling rate (see Fig. 2)
4. Model of thermo-elasto-plastic stress and strain

The stresses and strains are calculated by the solution of equilibrium equations and constitutive relations in the rate form, i.e.:

$$\text{div}\sigma(x, t) = 0, \quad \sigma = \sigma^T, \quad \sigma = D \cdot \dot{\varepsilon} + D \cdot \varepsilon$$

(10)

where $\sigma = \sigma$ ($\sigma_{\alpha\beta}$) is stress tensor, $D = D(v, E)$ is the tensor of material constants (isotropic materials), $v$ is Poisson ratio, $E = E(T)$ is the Young’s modulus, however $\varepsilon^r$ is tensor elastic strains.

The equation (10) is completed by initial conditions

$$\sigma(x, t_0) = 0, \quad \varepsilon^r(x, t_0) = 0, \quad t_0 = 0$$

(11)

and boundary conditions which provide external statically determinate

$$\dot{U}(x_0, t) = \dot{U}, \quad \begin{{bmatrix} \dot{U} = 0 \end{bmatrix}$$

(12)

where $U$ is the vector of displacement, $\dot{U}$ - remove degrees of freedom.

Total strains in the around considered points are result of the sum (assumed the rule of additivity of strain):

$$\varepsilon = \varepsilon^r + \varepsilon^{pl} + \varepsilon^p$$

(13)

where $\varepsilon^{pl}$ are isotropic of temperature and structural strains, $\varepsilon^p$ are transformations plasticity, and $\varepsilon^p$ are plastic strains.

For the Huber-Misses plasticity condition the flow function ($f$) has the form [3,8,10,13]:

$$f = \sigma - Y(T, \sum \eta(T) \varepsilon^p + \varepsilon^r) = 0, \quad Y = \sum Y_0(T) \eta_k, \quad k = 1, 2, 3, 4, 5$$

(14)

where $\sigma$ is effective stress, $\varepsilon^p$ is effective plastic strain, $Y$ is a plasticized stress of material on the phase fraction ($\sum \eta_k$) in temperature ($T$) and effective strain ($\varepsilon^p$):

$$Y(T, \sum \eta(T) \varepsilon^p) = Y_0(T, \sum \eta(T) \varepsilon^p) + Y_0(T, \sum \eta(T)) \sum \eta(T) = \sum Y_0(T) \eta_k$$

(15)

$Y_0(T, \sum \eta_k)$ is a yield points of material dependent on the temperature and the phase fraction, however $Y_0(T, \sum \eta(T) \varepsilon^p)$ is a surplus of the stress resulting from the material hardening $Y_0(T, \sum \eta(T) \varepsilon^p) = Y_0(T, \kappa(T), \varepsilon^p)$ wherein the $\kappa(T)$ is the hardening modulus.

The plastic strains is determined by nonisothermic plastic flow law [3, 11,22]:

$$\varepsilon^p = \dot{\varepsilon}^p \frac{\partial f}{\partial \sigma}, \quad \dot{f} = 0, \quad \dot{\varepsilon}^p = \dot{\varepsilon}^p \frac{3S}{2Y}$$

(16)
where $S$ is the deviatoric part of stress tensor ($S = \sigma - I\sigma_{kk}/3$).

Using the Leblond model, completed by decreasing functions $(1 - \eta)$ which has been proposed by the authors of the work [7,10,12,15], transformations plasticity are calculated as following:

$$
\varepsilon^{pl} = \begin{cases} 
0, & \text{for } \eta_k \leq 0.03, \\
-3 \sum_{i=1}^{k+1} (1 - \eta_k) \epsilon_i^{vol} \frac{S}{Y_i} \ln(\eta_i) \eta_i, & \text{for } \eta_k \geq 0.03
\end{cases} \quad (17)
$$

where $\epsilon_i^{vol}$ are volumetric structural strains when the material is transformed from the initial phase „1” into the $k$-phase, $Y_i$ is a actual yield points of input phase (in cooling process it is austenite).

The equations (10) are solved by using the FEM [3,22]. The system of equations used for numerical calculation is:

$$
[K][U] = \left( \begin{bmatrix} \eta_k \\ \varepsilon \end{bmatrix} - \left[ \begin{bmatrix} t^{\rho} \end{bmatrix} \right] \right) + \left[ \begin{bmatrix} t^{\rho} \end{bmatrix} \right] \quad (18)
$$

where $K$ is the element of stiffness matrix, $U$ is the vector of nodal displacement, $t^{\rho} = \{t^{\rho}\}$ is the vector of nodal forces resulting from thermal and structural strains, $t^{\rho} = \{t^{\rho}\}$ is the vector of nodal forces resulting from plastic strains and transformation plasticity.

The final displacements, strains and stresses are resulting integration with respect to time, from initial $t = t_0$ (see (11)) to actual time $t$, i.e.

$$
U(x_o, t) = \int_0^t \dot{U}(x_o, \tau) d\tau, \quad \varepsilon(x_o, t) = \int_0^t \dot{\varepsilon}(x_o, \tau) d\tau, \quad \sigma(x_o, t) = \int_0^t \dot{\sigma}(x_o, \tau) d\tau
$$

(19)

The rate vectors of loads in the brackets in (17) are calculated only once in the increment of the load, whereas the vector $t^{\rho}$ is modified in the iterative process.

In the numerical model the integrals (19) are approximate by following formula:

$$
U(x_o, t^{s+1}) = \sum_{s=0}^{s} \sum_{t^{s+1}} U(x_o, \Delta t) \Delta t + \sum_{s=0}^{s-1} \sum_{t^{s+1}} \dot{U}(x_o, \Delta t) \Delta t + \sum_{s=0}^{s-1} \sum_{t^{s+1}} \delta t \sum_{s=0}^{s-1} \dot{U}(x_o, \Delta t) \Delta t
$$

$$
\varepsilon(x_o, t^{s+1}) = \sum_{s=0}^{s} \sum_{t^{s+1}} \varepsilon(x_o, \Delta t) \Delta t + \sum_{s=0}^{s-1} \sum_{t^{s+1}} \dot{\varepsilon}(x_o, \Delta t) \Delta t + \sum_{s=0}^{s-1} \sum_{t^{s+1}} \delta t \sum_{s=0}^{s-1} \dot{\varepsilon}(x_o, \Delta t) \Delta t
$$

$$
\sigma(x_o, t^{s+1}) = \sum_{s=0}^{s} \sum_{t^{s+1}} \sigma(x_o, \Delta t) \Delta t + \sum_{s=0}^{s-1} \sum_{t^{s+1}} \dot{\sigma}(x_o, \Delta t) \Delta t + \sum_{s=0}^{s-1} \sum_{t^{s+1}} \delta t \sum_{s=0}^{s-1} \dot{\sigma}(x_o, \Delta t) \Delta t
$$

(20)

where $s + 1$ is the actual time step, $s$ - previous time step, $mit$ is the number of iteration in the increase of time $\Delta t$. In the iterative process of evaluation of plastic strains, the modified Newton-Raphson algorithm is used [22,25].

5. Example of numerical calculations

The simulation of hardening process for axisymmetric element made of hot-work tool steel (W360) was performed. The dimension of the element was equal $\phi 50 \times 100$ mm (Fig. 5).
The cooling was modelled with the Newton condition and the value of heat transfer coefficient assumed equal 20 W/(m²K) (cooling in the air [6,27]). The simulations of cooling process were performed for the two different sets of the boundary conditions. “Task 1”: the temperature of coolant was constant and equalled $T_\infty=300$ K. “Task 2”: the temperature of surrounding medium ($T_\infty$) was variable and taken the value on the level of 150 K less than average temperature of hardening element. When the average temperature of cooled element was below 450 K it was assumed that the temperature of coolant equalled 300 K. In the second task the cooling process was realized by using the constant heat flux with the value of 3000 W/m².

Hardened zones in the cross sections of the element, after cooling for both of task, are presented in figures 7, 8 and 9.

Distributions of the simulated fractions in the cross-section A-A (Fig. 5) after hardening are presented in figure 10.
In the simulation on the mechanical phenomena the Young’s and tangent modulus ($E$ and $E_t$) were dependent on temperature, whereas the yields stress ($Y_\sigma$) was dependent on temperature and phase composition. Assumed, that Young’s and tangent modulus are equal $2 \times 10^5$ and $4 \times 10^3$ MPa ($E_t=0.05E$), yield points 150, 500, 1200 and 300 MPa for austenite, bainite, martensite and pearlite, respectively, in the temperature 300 K. In the temperature of solidus Young’s modulus and tangent modulus equalled 100 and 10 MPa, respectively, whereas yield points equalled 5 MPa. The discrete values of thermophysical properties depends on the temperature [3,13] were include by using the approximation with square spline functions (Fig. 11).

Fig. 11. The graph of the assumed functions of the material properties, depend on the temperature, used in model of stress: Young’s modulus $E(T)$, tangent modulus $E_t(T)$ and yield point for each of phase $Y_\sigma(T, \eta_k)$.

The distributions of the residual stresses, after the hardening process were presented in the figures 12÷16. In the figures a) the results from the first task were shown, whereas in the figures b) from the second task.

Fig. 12. Residual radial stresses, a) Task 1, b) Task 2

Fig. 13. Residual circumferential stresses, a) Task 1, b) Task 2

Fig. 14. Residual axial stresses, a) Task 1, b) Task 2

Fig. 15. Residual shear stresses, a) Task 1, b) Task 2
Fig. 16. Distributions of residual stresses in the cross sections B-B and A-A (Fig. 5), a) Task 1, b) Task 2

In the figure 17 the changes of stresses in the time of the hardening process in the superficial layer (point 2, Fig. 5) were presented.

Fig. 17. The stresses according to the time (point 2, Fig. 5), a) Task 1, b) Task 2

The distributions (after the cooling process) of effective plastic strains were shown in the figure 18. Also the distributions of effective transformations induced plasticity were presented in the figure 19.

Fig. 18. The distributions of the effective plastic strains ($\times 10^{-3}$)

Fig. 19. The distributions of the transformations plasticity ($\times 10^{-3}$)
6. Conclusions

On the basis of simulated dilatometric curves can see that the considered steel is hardened very easy. To obtain the bainite-martensite structure the cooling rate can’t be greater than 3.2 K/s (see Figs 1, 2 and 3).

On the basis of obtained results from simulations of the superficial heat treatment can be concluded that the cooling in the heated air is much more preferred than in the air with room temperature. For these reasons, in the technology of hardening process of hot-work tool steel, the appropriate selection of the cooling rate is very important. The cooling in the air was applied and the cooling rate was equals: 0.234 and 0.222 K/s in the point 1 and 2 respectively “task 1” (Fig. 5). After the cooling process in the air the domination of martensite phase in structure of material is obtained (Figs 7 and 10). The cooling in the heated air was applied and the cooling rate was equals: 0.055 and 0.054 K/s in the point 1 and 2 respectively “task 2” (Fig. 5). After the cooling process in the heated air the domination of bainite phase in structure of material is obtained (Figs 8 and 10).

The distributions of the residual stress after the hardening process are more favorable for the example with the heated air. In the both tasks (1, 2) the circumferential and axial stresses are compressive, but after the cooling in the heated air the level of stresses in the second task is significantly lower (Figs 12+15 and 16b).

The deposition of compressive circumferential and axial stresses (the most meaningful stresses) is superficial (Figs 13, 14 and 16). The regular distributions of the stresses are obtained. Unfavorable is the distribution of shear stresses after the cooling process in the air with room temperature (Fig. 15a). The values of these stresses are much higher than the level of stresses obtained in second task. (see Fig. 15b). It can cause the cracking already in the hardening process.

It can be claimed that in the numerical simulation of such hardening the fact that transformation plasticity is included in the model of mechanical phenomena brings about the changes in obtained results [10,11,16]. The phase transformations significantly effect on the changes of the temporary stresses (Fig. 17) and in consequence on the residual stresses after hardening of the element considered.

The distributions of the effective plastic strains (Fig. 18) and effective transformations plasticity (Fig. 19) are comparable. Insignificantly differences in the solutions are occurred, but the area of distribution of strains is similar. It is independent on the type of cooling.

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