NUMERICAL SIMULATION OF THE HEAT TREATMENT PROCESS FOR 100Cr6 STEEL

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Abstract
The success of quenching process depended heavily on the suitable choice of a quenching media. In this work, a numerical simulation of the process of quenching C-ring sample of 100Cr6 steel was discussed. The results showed an overview of the phase transformation, residual stress, distortion and hardness on the specimen throughout quenching process to the end. The simulation results also revealed that the sample is not cracked and the highest residual stress located on the inner and outer at the bottom edge of the C-ring with C-ring model being quenched in PVP-12 solution. At the same time, the obtained hardness was qualified the working requirements.

Keywords: numerical simulation, heat treatment, 100Cr6 steel, hardness

1 Introduction
Simulation of metal heat treatment
Nowadays, there has been an increasing fundamental interest in understanding the simulation of metal heat treatment. However, the simulation of 100Cr6 steel heat treatment is still an on-going research topic. There are few researches focused on the simulation of fully mechanical – physical – metallurgical behaviour due to the limitation of the simulation software. Among the commercial simulation software today, Sysweld software is considered as the strongest and the most complete application for the heat treatment of metals. For deformation problems, Sysweld not only calculates the distortion due to thermal expansion like other software, but also calculates the distortion caused by the phase transformation [1]. Success or failure of heat treatment affected manufacturing costs and determines product quality and reliability. For this reason, modelling of heat treatment processes has been of a great importance to engineers and scientists. Many researchers, such as Mukai et al. [2], Brimacombe et al. [3], have done many valuable works on modelling of phase transformations during quenching of steel.

Aqueous polymer solutions used as cooling media and their properties
Water and oil quenchants have conventionally been the most frequently used quenching media in the heat treating industry, particularly for crack-sensitive steel parts [4]. Oil, however, possesses several substantial disadvantages: relatively limited variability in quench rates, fire hazards, and smoke emissions [5]. Thus, aqueous polymer quenchant solutions have been developed to replace quench oils in some applications, in order to fill the gap between the cooling rates of water and oils, so that steels of lower hardenability could be quenched [6,7].
The use of water-soluble polymers as quenching media for hardening steels is gradually growing. Economical advantage, safety, cleanliness, and adaptability to a large range of steels are the most important attractions of utilization in the recent years [7]. Poly vinyl pyrrolidone (PVP) has similar performance compared to mineral oil, with good stability in use, high solubility in water, and higher drag-out than poly alkylene glycol (PAG) at similar viscosity [8]. The characteristic of normal solubility modifies the conventional three-stage quenching mechanism in vaporizable liquids (vapour blanket or film boiling stage, nucleate boiling stage, and convective cooling stage), and offers the mechanism of cooling hot metal by surrounding it with high polymer concentration gradient that governs the rate of heat extraction. Once the metal has been cooled, the slight film of polymer surrounds the probe [8]. In this work, we have focused on the numerical simulation of the process of quenching C-ring sample of 100Cr6 steel in poly (N-vinyl-2-pyrrolidone) aqueous solution at concentration 12% wt. (PVP-12).

2 Experimental materials and methods

Modelling of the quenching process
The shape and dimensions of the C-ring specimen are given in Fig. 1. The material employed for the C-ring specimen was a 100Cr6 (DIN 17230) with the nominal chemical composition (certified by the supplier) of 1.04% C, 0.26% Si, 0.33% Mn, 0.31% Ni, 1.53% Cr, 0.01% Mo. Using the Sysweld software to discrete the C-ring model in Fig. 1, the finite element model is obtained as shown in Fig. 2. Because of the curves in the cross section of the model, in order to ensure the accuracy when meshing the model, we applied the element type with curved edges. On the other hand, in the direction of the thickness, the model has a uniform cross-section shape, so the element type with the straight edge will fit in this direction.

![Fig. 1 Geometry and dimensions of C-ring (mm)](image)

![Fig. 2 FEM model of the C-ring](image)

Incorporating two features mentioned above, we used the element type which included 5 faces and 15 nodes in combination with straight and curved edges to mesh the C-ring model. In order to achieve a necessary precision, the size of the elements must be small enough [9]. In this study, the elements with the biggest edge of 2 mm were modeled in the simulation.

2.2 Material properties assignation
For the numerical simulation, the FEM model as shown in Fig. 2 must be clearly defined all of the material properties, this means that it must be assigned a full set of physical properties of the material.
It should be noted that, the quenching simulation problem will be studied in the continuous change of material properties from the state at quenching temperature (850°C) to the state at completed cooling temperature (30°C). In this study, 100Cr6 steel was used which has the physical properties as shown in Fig. 3 to 6 [1].

![CCT diagram of 100Cr6 steel](image)

**Fig. 3** CCT diagram of 100Cr6 steel

![Thermal conductivity of 100Cr6 steel](image)

**Fig. 4** Thermal conductivity of 100Cr6 steel
2.3 Setup the computing conditions

As for the quenching process, in general, there are two heat transfer processes available: a) heat transfer within the internal part of the quenching specimen by heat conduction which is characterized by the thermal conductivity \( K \) as presented in Fig. 4 and b) heat transfer from the specimen to the quenching medium through the heat exchange surface between a specimen and quenching medium. In this numerical simulation, the heat exchange surface or skin of the model with quenching medium are 2D elements which are constructed and declared prior to computation as in Fig. 7. The heat transfer coefficient (HTC) at this surface is the boundary condition of the simulation problem. The value of the heat transfer function at the model’s surface is determined by experiment and will be inserted in the Sysweld for computation.
To determine the cooling curve in the PVP-12 (Fig. 8) aqueous solution, the test probe was conducted in accordance with ISO 9950 and both of parts were made of Inconel 600. We used a similar measurement system to IVF SmartQuench which includes: Naberthem furnace from Germany, Portable Data Acquisition Module USB – 4718. On the other hand, because the model is symmetrical, it has modelized one-half only and it has one symmetric surface (cross-section). This would save a lot of computing time and computing resources, while computational accuracy would not change [9].

3 Results and discussion

Simulation results of phase transformation in quenched specimen

The simulation results of the phase transformation when quenching the C-ring specimen in our homemade PVP-12 are presented in Fig. 9. The computed results showed that the C-ring specimen with 2 mm thickness is heated to 850°C and then immersed in PVP-12 homogeneous medium will receive a two phases structure, consist of martensite (phase 3) and residual austenite (phase 6).
The amount of martensite that obtained after quenching in the PVP-12 medium was 87.75% and the residual austenite content was about 12.25%. Because the model was too thin, all the nodes in the model had a cooling rate exceeding the critical value (40 °C/s), which means that when the C-ring specimen was quenched in PVP-12 the martensite would be completely transformed.

**Computation results of stress field in quenched specimen**

The computer not only can simulate the phase transformation in specimen, but also compute the evolution of the residual stress formation in quenched specimen. Fig. 10 presents the computed results of Von Mises Stress field, $\sigma_{eq}$, which was the vector sum of the six stress components ($S_{11}$, $S_{22}$, $S_{33}$, $S_{12}$, $S_{23}$, $S_{31}$). It can also be calculated according to the three principal stresses as following:

$$\sigma_{eq} = \frac{1}{\sqrt{2}} \sqrt{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2}$$

(1.)

Where $\sigma_1$, $\sigma_2$, $\sigma_3$ are the three principal stresses in the three directions x, y, z respectively.
The results revealed that the residual equivalent stress has a minimum value of 0.7452 MPa obtained at the top of the C-ring and inside the model. On the entire cross section of the C-ring specimen, the residual equivalent stress value tended to increase from the core to the outer edge of the specimen. The results also demonstrated that the residual equivalent stress (Seqv) had the greatest value at the inner and outer edges, at the thickest part of the model - meaning that this area was the most vulnerable place to be cracked when quenching.

**Fig. 11** displays a representation of the process of residual stress formation at the nodes 480, 705, 439, and 432 from the time the model was immersed into the PVP-12 aqueous solution until the stress at the survey nodes is unchanged (residual stress).

**Fig. 11** The evolution of the stress formation process at some survey nodes 480, 705, 439, 432

The figure showed that the "active time" was 0-11s, after about 11 seconds, the stress values at the nodes did not change anymore - residual stress remaining. On the other hand, the simulation results also indicated that, during the "active time" (0-11s), the equivalent stress values changed continuously: initially the equivalent stress at the nodes increased because the specimen was shrank when dipped into the quenched medium, then the stress values reduced caused by the swelling effect of the volume change during phase transformation. Among the survey nodes, node 439 had the highest equivalent stress (290 MPa at 3.5s), meaning that when quenching the C-ring sample in the PVP-12 quenchant, node 439 was the most susceptible location to be cracked. In this case, because the maximum residual stress on the C-ring model was 290 MPa which was much smaller than the yield strength of 100Cr6 steel (1324 MPa), the quenched specimen was not cracked.

**3.3 Simulation results of hardness of quenched specimen**
At the time of the specimen was immersed in the solution 3.18s, the maximum hardness value on the model was 397 HV - reached at the node 480. The lowest hardness is 100 HV at the cross section and at the thickest bottom of the model (**Fig. 12** left). When the model was in the solution for about 119 seconds, the hardness at the nodes of the whole model was 784.4 HV (**Fig. 12** right). That is, after quenching 119s in the PVP-12 solution, the martensite transformation was finished.
4 Conclusions

The numerical simulation can predict the formation of the microstructure and the hardness of the specimen after quenching. At the same time, it also specifies the residual stress and its changing in the model, which is especially important to select an appropriate quenchant for a specific material and specimen shape.

Simulation results of the quenching process of C-ring specimen of 100Cr6 steel in PVP-12 aqueous solution showed that the microstructure of the sample consisted of martensite and approx. 12.25% residual austenite, the residual stress was small and the hardness was achieved 784.4 HV. Therefore, it is possible to use PVP-12 aqueous solution as a quenchant for C-ring specimen made of 100Cr6 steel.

References


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