Numerical simulation of phase transformation during gas quenching after low pressure carburizing

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Abstract. Low pressure carburizing followed by high pressure gas quenching is often applied to steel elements in order to increase their strength and durability. In order to minimize these distortions, the Vacuum UCM furnace manufactured by SECO/WARWICK conducted by single piece flow method is proposed. A refined simulation that describes the quenching phenomena with enough accuracy can reduce the project and optimization costs as it replaces the trial and error method. The goal of this study was to create a computer model that can predict the behaviour of the phase transformations that occurs at 4D quenching chamber after low pressure carburizing in single piece flow technology. First, an investigation about the simulations that has been developed in this area was done. Based on physical phenomena involved in this process, a numerical scheme was created; The numerical scheme was applied to the real steel element that was submitted to the single piece flow technology process; The numerical simulation was compared with the experimental data. As a result, a numerical model able to simulate phase transformation after complex chemical-heat treatment in the single piece flow technology was obtained.

1. Introduction

Thermal surface treatments as low pressure carburizing (LPC) followed by high pressure gas quenching (HPGQ) are often applied to steel elements in order to increase their strength and durability. LPC started being applied in industries two decades ago, since it gives better results in terms of carburizing precision and evenness in comparison to the traditional carburizing in atmospheres [1], [2], [3]. The HPGQ improved significantly the result of the quenching process by decreasing the deformation rate when compared with the traditional oil quenching [2], [4], [5], [6]. The goal of these treatments is to provide carbon diffusion into the material and then the phase transformation from austenite to martensite. As a result, the hardness in the surface of the material are improved, promoting greater durability [7].

Undesirable distortions are caused in the steel during these processes. They are mainly formed by the change of the steel structure volume that occurs due the phase transformation and non-uniform parameters during the quenching [6]. The correction of these distortions is one of the most expensive processes [4]. For this reason, despite they are inevitable [3], the distortions need to be avoided as much as possible.

The Vacuum UCM furnace manufactured by SECO/WARWICK (Figure 1) proposes a thermochemical treatment being conducted by single piece flow technology that comes to replace the traditional batch method for LPC/HPGC in order to minimize distortions. As in the batch method more than one element is submitted to the chamber, the physical and metallurgical proprieties varies over the
placement which the element occupies [8], [2]. On the other hand, the single piece flow model proposes that every single piece goes through the exact same position and process conditions as every other piece, furthermore the carburization in this method produces a favourable, i.e. compressible distribution of residual stress in the technological surface layer [4], [9]. In the 4D quenching chamber, the device provides the inflow of cooling gas from all sides and the rotation of parts to support uniform cooling effect [10]. Through becoming more uniform the parameters, especially during the quenching, it is possible to obtain better outcomes.

![Figure 1. Vacuum UCM furnace SECO/WARWICK](image)

A refined simulation that describes the quenching phenomena with enough accuracy can reduce the project and optimization costs. The computer model allows better comprehension about the process, the device and how the design influences the results [11]. Understanding the parameters that affect the intensity of the process is crucial to accomplish the desired performance [2]. Therefore, a computer model replaces the trial and error method that is costly in terms of time and resources, affording the process optimization.

However, currently, there is no commercial software that simulates the influence of the complex fluid flow field in the phase transformation that occurs in high pressure gas quenching (HPGQ). In recent researches, including the works developed by Ferguson et al. [12], Li [3] and Sims et al. [6], [11], [13], phase transformation simulations were done at DANTE modelling software in order to predict the stress formation during HPGQ. In all these cases, the heat transfer coefficient was considered constant and the combination of more than one modelling program was required. The heat transfer coefficient has significant influence on the quenching results, including distortion, residual stresses and hardness distribution [2]. Hence, an algorithm scheme that takes in account the complex fluid flow and the heat transfer coefficient as function of the space and time is needed.

2. Numerical Algorithm Scheme

The numerical simulation of phase transformation that occurs in the steel element in 4D quenching chamber in the single piece flow technology is based on a Multiphysics Field. It takes into account the carbon diffusion, heat and mass balances, heat transport and the kinetics of phase transformation.

The goal of the algorithm scheme is to obtain the carbon concentration, cooling speed and temperature field which are parameters that determine the transformation to martensite at the steel. These solved variables are used to evaluate the phase transformation based on data generated in JMatPro.

The system consists of the fluid domain in the quenching chamber and the solid steel element. The computer model was simulated in Ansys CFX solver for computational fluid dynamics. Hexagonal elements of the grid was created, whose regular shapes assist in obtaining more accurate results in numerical simulation [14].

Numerical Algorithm Scheme is illustrated in Figure 2. With the results obtained, it is possible to analyse if some change in geometry or input data would be profitable in view of optimization. If so, the simulation process restarts.
2.1. Diffusion module
In the Low Pressure Carburizing chamber, the steel is submitted to the boost and diffusion sequence procedure, where the surface is saturated with carbon. After it is transferred and indexed through the chamber where the diffusion occurs [1]. The carbon diffusion is governed by Fick’s Laws.

- Fick’s Law:

\[ J = -D \nabla \phi \]  
\[ \frac{\partial \phi}{\partial t} = -D \nabla^2 \phi \]  

Where \( J \) is the flux, \( D \) the diffusion coefficient, \( \phi \) the carbon concentration, \( t \) the time. The equation (1) is used as boundary condition and the equation (2) describes the carbon concentration distribution in the element.

2.2. Fluid module
The flow field is described by momentum equation, continuity equation and energy equation [15].

- Momentum:

\[ \frac{DU}{Dt} \rho = \rho g - \nabla P + \mu \nabla^2 U \]  

- Continuity:

\[ \frac{\partial \rho}{\partial t} + \text{div} \rho U = 0 \]  

- Energy:

\[ \frac{\partial (\rho h)}{\partial t} + \nabla (\rho Uh) = \nabla (\lambda \nabla T) + \tau : \nabla U + S_E \]  

Where \( \rho \) is the specific mass, \( h \) is the enthalpy, \( U \) is the velocity, \( T \) is the temperature, \( \lambda \) is the conduction coefficient, \( \tau : \nabla U \) is the viscous dissipation and \( S_E \) the source term.

2.2.1. Turbulence Model. The turbulence model is done according to k-\( \omega \) based SST (Shear Stress Transport) models available in Ansys CFX, that is a combination of k-\( \omega \) and k-\( \epsilon \) models. In the boundary layer, k-\( \omega \) model is applied. As k-\( \omega \) model is replaced by k-\( \epsilon \) in the layers located further away from the wall because it models turbulence in free flow very well and it is less sensitive to inlet conditions for values that describe the turbulence. The desired characteristics of both models are joined into one due the fact that the standard k-\( \epsilon \) model can be transformed into equations on k and \( \omega \), as the
The dissipation of the turbulence kinetic energy, therefore, $\omega = \frac{\varepsilon}{k}$. The equations of this model are then multiplied by the function whose value is 1 in the free flow and 0 by the wall, and the standard $k$-$\omega$ model equations are multiplied by $F_1$ function [14]. These two-equation models are the most prominent in this area, supported by a large number of validation studies [16]. The SST model is proposed for accurate boundary layer simulation [15].

The applied model equation are as follows:

- **Turbulent Kinetic energy:**
  \[
  \frac{\partial (p k)}{\partial t} + \frac{\partial (\rho u_j k)}{\partial x_j} = - \nabla \cdot P - \beta^* \rho \omega k + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} \right] \quad (6)
  \]

- **Dissipation of the turbulent kinetic energy:**
  \[
  \frac{\partial (\rho \omega)}{\partial t} + \frac{\partial (\rho u_j \omega)}{\partial x_j} = - \nabla \cdot P - \beta^* \rho \omega^2 + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_\omega \mu_t) \frac{\partial \omega}{\partial x_j} \right] + 2(1 - F_1) \rho \sigma_{\omega 2} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \quad (7)
  \]

Where:

- **Turbulent viscosity:**
  \[
  \nu_t = \frac{a_{1k}}{\max(a_1 \omega, SF_2)} \quad (8)
  \]

- **Production term:**
  \[
  P = \mu_t SS \quad (9)
  \]

Where:

\[
S = \left( \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2 \right)^{\frac{1}{2}} \quad (10)
\]

- **Functions $F_1$ and $F_2$:**
  \[
  F_1 = \tanh(arg_1^4), \quad arg_1 = \min(\max\left(\frac{k^2}{0.09 \omega y'}, \frac{500 \nu}{C D k \omega y^2}\right), \frac{A_p \sigma \omega^2 k}{C D k \omega y^2}) \quad (11)
  \]
  \[
  F_2 = \tanh(arg_2^2), \quad arg_2 = \max\left(2 \frac{k^2}{0.09 \omega y'}, \frac{500 \nu}{C D k \omega y^2}\right) \quad (12)
  \]

- **Fixed coefficients:**
  \[
  a_{k1} = 0.85, \sigma_{\omega 1} = 0.5, \beta_1 = 0.075, \beta^* = 0.09, \kappa = 0.41, \gamma_1 = \frac{\beta_1}{\beta^*} - \sigma_{\omega 1} k^2 (\beta^*)^2, \sigma_{k 2} = 1.0,
  \]
  \[
  \sigma_{\omega 2} = 0.856, \beta_2 = 0.0828, \beta^* = 0.09, \kappa = 0.41, \gamma_2 = \frac{\beta_2}{\beta^*} - \sigma_{\omega 2} k^2 (\beta^*)^2.
  \]

**2.2.2. Modification of the production term.** The SST $k$-$\omega$ model tends to over produce turbulence in the pile-up areas because of the high $S$ values generated in these regions. Kato and Launder proposes to replace the tangential stresses $S$ in the turbulence production equation with rotation $\Omega$, then:

\[
P = \mu_t S \Omega \quad (13)
\]
Where:

\[
\Omega = \left( \frac{1}{2} \left( \frac{\partial \mu_i}{\partial x_j} - \frac{\partial \mu_j}{\partial x_i} \right) \right)^2
\]

Therefore, the model enables to introduce a term that limits over-production of the turbulence kinetic energy in the areas of high-pressure gradients[14].

2.3. Thermal module
Calculation of heat transport based on preset boundary and initial conditions. The equation (15) is dependent of material’s characteristics, as conduction coefficient \(k\), specific heat \(C_p\) and density \(\rho\). But these proprieties varies with temperature, cooling speed and carbon concentration. Therefore an iterative procedure is required.

\[
\rho C_p \dot{T} = \nabla \cdot (k \nabla T)
\] (15)

2.4. Phase transformation module
Due the conditions, during the quenching process occurs an extensive rearrangement of atoms. The phase transformations can be classified as diffusional or martensitic. The diffusional phase transformation involves diffusion of carbon and other solute atoms over the time. The martensitic phase transformation is diffusionless and occurs very rapidly. During the quenching these two phase transformations can occurs simultaneously at different locations [17]. The temperature field, cooling speed and carbon concentration are used to evaluate the phase transformation based on data generated in JMatPro.

3. Results
Based on the numerical scheme described above (Figure 2), computational simulation where carried out. The element which was simulated is a flat ring made of 20MnCr5 steel. The material data varying with temperature, cooling speed and carbon concentration was created and implemented to every module of numerical scheme.

3.1. Diffusion
First, the carbon distribution was obtained after heating to 860°C and low pressure carburizing (Figure 3). The numerical results where compared with experimental data by plotting the value of carbon concentration in the middle of top surface (Figure 4). The carbon concentration in a layer was measured with a glow discharge optical emission spectrometer – LECO GDS850A. The comparison shows a good match between both.

Figure 3. Carbon concentration distribution on a planar section.
3.2. Fluid module

Secondly, the CFD summations where carried out to obtain complex flow of cooling gas (Figure 5 and Figure 6) which has the biggest influence on wall heat transfer distribution on the element surface during high pressure gas cooling (Figure 7).

**Figure 4.** Carbon concentration.

**Figure 5.** Velocity distribution on a plane perpendicular to the top cooling surface.

**Figure 6.** Velocity distribution on a plane perpendicular to the top cooling surface.

**Figure 7.** Heat transfer coefficient distribution in the wall of the element.
3.3. Thermal module
Then, after obtaining the wall heat transfer coefficient distribution over the surface of the element and material data, the cooling process could be simulated. Simulation shows that uneven wall heat transfer coefficient affects the temperature distribution over time (Figure 8).

![Temperature distribution over time on cross section.](image)

**Figure 8.** Temperature distribution over time on cross section.

3.4. Phase transformation module
Finally based on generated material data depended on the calculated cooling speed, transient temperature distribution and carbon concentration the numerical scheme is able to calculate the initiation of martensitic transformation. As the Figure 9 shows the martensitic transformation occurs differently depending on location. This phenomena is due to uneven heat transfer coefficient distribution on the element surfaces which may lead to an increase of undesirable quenching deformations.
4. Conclusion
The phase transformation during the gas quenching is a very critical part of the process in term of deformation generation. Therefore, it is advantageous to invest in simulations that describes properly the phenomena in sense of having a good device that operates with improved parameters. The simulation will provide us optimized process, avoiding unnecessary and costly. The presented numerical algorithm scheme was verified positively by the experiment.

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