Numerical Modeling and Experimental Investigation for Optimization in Quenching Processes of Aluminum and Steel Parts

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Numerical Modeling and Experimental Investigation for Optimization in Quenching Processes of Aluminum and Steel Parts

by

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ABSTRACT

Aluminum and steel components are usually quenched in forced gas, oil or water flow to improve mechanical properties and improve product life. During the quenching process, heat is transferred rapidly from the hot metal component to the quenchant and the rapid temperature drop introduces phase transformation and deformation in the hot metal component. As a result, quenching problems arise such as distortion, cracking and high tensile residual stresses. To avoid or minimize these problems while improving mechanical properties, process optimization is needed for both part geometry and quenching process design.

A series of methods, including four existing methods and two new methods developed in this dissertation, were applied to obtain accurate thermal boundary conditions, i.e., the heat transfer coefficient (HTC) distribution. The commercially available material model DANTE was applied with finite element software ABAQUS to model the phase transformations and constitutive behavior of steel parts during quenching. A user material subroutine was developed for aluminum alloys based on a constitute model and tensile test data. The predicted residual stresses in the quenched parts agreed with those measured using the improved resistance strain gauge hole-drilling method and other methods, which validates the numerical models.
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1 Introduction

Heat treatment is a method mainly used to alter the physical properties such as microstructure and mechanical behavior, and sometimes chemical properties such as carbon concentration, of a material or a part. Unlike grinding and machining, there is usually no material removal in heat treatment processes. Typical heat treatment processes include those altering physical properties such as quenching, tempering, aging, annealing, normalizing, etc. and those involving chemical property changes such as carburizing, nitriding, etc.

This work studies heat transfer, stress, strain, distortion and material property evolution of steel and aluminum alloy components in liquid quenching such as water quenching and oil quenching, and air/gas quenching.

1.1 Background

To improve mechanical properties, aluminum alloy and steel components are usually subject to a heat treatment including quenching. Quenching is a rapid cooling, which prevents low-temperature processes such as phase transformations from occurring. The two cooling curves A and B in Figure 1-1 demonstrate that in a rapid quenching, there is no time for low temperature phase transformation. Figure 1-2 illustrates some phases for steel components at different cooling rates and shows that steel can be hardened in a rapid quenching by introducing martensite. For an aluminum alloy, a rapid quenching will prevent all phase transformation and generate a supersaturated single phase for the followed aging process, which further improves its mechanical properties.
In this rapid cooling process, heat is transferred out from the hot components to the surrounded cool quenching media. As a result, temperature is not uniform as
demonstrated in Figure 1-3 anymore during the cooling process, especially when the cooling rate is very high, which in returns causes unacceptable tolerance, distortion, or even cracking as demonstrated in Figure 1-4 due to the shrinking rate differences at different locations of the component. A significant amount of residual stresses can be also developed in the component when quenched particularly in water [2-7]. The existence of residual stresses, in particular tensile residual stresses, can have a significant detrimental influence on the performance of a structural component. In many cases, the high tensile residual stresses can also result in a severe distortion of the component, and they can even cause cracking during quenching or subsequent manufacturing processes [4, 8, 9].

Figure 1-3. A sample temperature gradient during quenching
1.2 Challenges in optimization of quenching processes

In order to prevent the harmful effects of distortion, residual stress and cracking while improve the mechanical properties of steel and aluminum alloy components, it is highly necessary for heat treaters to optimize component designs and heat treating processes. Experimental trials were used to determine better component designs and process setups, but more and more attentions are being paid to numerical modeling using finite element packages and computational fluid dynamic packages for the benefits on money and time saving.

Numerical simulations of quenching of metal parts are usually carried out by finite element analysis packages such as ABAQUS [10], Ansys [11], etc. As shown in Figure 1-5, a CAD model of the part were first created in 2-D or 3-D form, then the model is meshed with suitable elements. For quenching simulations, the temperature-displacement
simulation is usually decoupled to thermal simulation and structure simulation in industrial practice for two reasons. First, decoupled simulation scheme requires less memory and converges faster than the coupled one. Second, the results from these two schemes are similar since in heat treating processes the heat generated by deformation is usually negligible compared to the heat transferred from hot solid to environmental media. Thus, thermal simulation is first carried out to obtain temperature-time profile of the part. The followed structural simulation reads the temperature-time profile and predicts quenching results such as distortion and residual stresses. In order to obtain high accurate simulation results, the finite element modeling must be validated by experimental measurements of residual stresses, distortion, etc.

Figure 1-5. Flow chart of numerical modeling
The thermal simulation of a heat treating process is usually a transient temperature analysis, in which the hot part temperature changes with respect to time from an initial state to a final state. In the simulation, initial temperature of the hot part and temperature of quenchant are usually easy to obtain and can be assigned with reasonably accurate values. So are the thermophysical properties of the part material. The biggest uncertainty is the heat transfer coefficient (HTC) between the hot part and quenchant. It has been reported that HTC affects the quenching result significantly [3, 12]. In liquid quenching, the heat transfer between hot metal parts and water is very complicated and it is difficult to determine the HTC. When a hot part is quenched in a fluid like oil or water, there are usually 3 stages: vapor stage, boiling stage and convection stage [13, 14]. The complicated interactions between solid and fluid lead to very complicated HTC data [14], which are not uniform in both time and space. Because of the importance of HTC and the determination difficulty, efforts must be made to acquire HTC distribution for a specific part as real as possible. Classical empirical equations from heat transfer textbooks are usually not suitable for real parts because of the complicated interaction and geometry [13]. Current CFD packages are also facing difficulties on this issue.

In the structural simulation, the temperature-time profile from the thermal simulation is read in and the part is shrunk due to the temperature drop. The non-uniform thermal shrinkage is constrained by the geometric structure and material strength that is varying with respect to temperature, strain, strain rate, etc. [4, 15-17] In other words, some portions of the part may not be able to move freely and therefore experience yielding. Thus, how the material behavior during quenching is governed is extremely important to the simulation accuracy.
Quenching results such as temperature-time profile, residual stress and distortion can be predicted by numerical simulations and can be evaluated by experimental measurements. Temperature-time curves acquired from experiments can be used to evaluate the accuracy of thermal model, especially boundary conditions like HTC data. Comparison between predicted distortion and measured one is a good choice to evaluate the accuracy of finite element models, especially the material models in the structural analysis. In this work, residual stresses at some certain locations of the quenched parts were measured and used to validate the numerical models, because of the importance of residual stress [4, 8]. There are many different methods to measure residual stresses such as X-ray diffraction, neutron diffraction, interference strain\slope rosette (ISSR), resistance strain gauge center hole-drilling method, curvature and layer removal methods, magnetic method and ultrasonic method [18]. In this work, residual stresses were measured using the most widely applied method [19], the resistance strain gauges center hole-drilling method described in the ASTM standard E837 [20], because this method can provide residual stress distribution in the depth direction and thus that comparisons of residual stress distributions can be made between predictions and measurements. Unlike other methods, this method requires relatively very cheap equipment. The easy application and high accuracy are other pluses for choosing this method.

### 1.3 Research objectives

This work is dedicated to study the challenges in numerical modeling of quenching processes of aluminum alloy and steel parts and therefore to optimize part geometrical design and production condition parameters using the validated numerical models that are
developed in this work. In addition, these numerical models and simulation procedure can be applied to other temperature and stress related situations such as other heat treating processes, reliability prediction of critical parts under thermal cycling loads, etc.

Specifically, the objectives of this work are:

1) **Heat transfer modeling**
   
The major challenge in thermal analysis of quenching processes is to obtain accurate HTC distribution for the target part. Developing widely applicable methods to determine accurate HTC distribution and constructing an HTC database for various quenchants based on experiments and simulations are the goals of the thermal modeling.

2) **Material property evolution modeling**
   
The key challenge in structural analysis of quenching process is to accurately govern material constitutive behavior at various temperatures, strains, strain rates, microstructure, etc. The goals of the material property evolution modeling are to analyze the evolution of material properties of steels and aluminum alloys and develop corresponding user material constitutive subroutines for FEA packages such as ABAQUS to accurately govern evolution of material microstructure and mechanical properties.

3) **Prediction and optimization of quenching results**
   
Another objective of this work is to predict quenching results such as distortion and residual stresses of a specific part. Optimization of part geometric design and quenching production setup can therefore be conducted using the developed numerical models at
low cost of money and time. For accuracy, these numerical models must be validated by comparing the predictions to experimental measurements.

1.4 Dissertation organization

In correspondence to the research objectives, this work includes chapters to address the challenges in numerical modeling.

Chapter 2 applies four existing methods and two developed methods to various quenching processes (water quenching, air quenching and high pressure hydrogen quenching) to determine HTC data. Specifically, these existing methods include empirical equation method, lumped heat capacity method, iterative modification method and CFD simulation method. The newly developed methods include semi-empirical equation method and the integration method. An HTC database for various quenchants is also constructed and presented.

Chapter 3 presents analyses of material property evolution of aluminum alloy and steel parts and development of a user material constitutive subroutine for quenching of aluminum alloy castings. A framework of governing material mechanical property evolution of aluminum alloy casting in both quenching and aging processes is presented as well. The commercially available user subroutine sets DANTE [21] for steels is also introduced in this chapter.

Chapter 4 presents prediction and measurement of residual stresses in as-quenched aluminum alloy castings. In the prediction of residual stresses, thermal models and material property evolution models are applied. As for measurement of residual stresses,
the widely used resistance strain gauge center hole-drilling method is improved and applied. Good agreements between prediction and measurement of residual stresses in these parts validate the numerical models developed in this work.

Chapter 5 presents numerical comparisons between high pressure hydrogen quenching and oil quenching by applying the thermal models and commercially available user material subroutine sets, DANTE. This chapter compares the quench severities of high pressure hydrogen quenching (HPHQ) and typical oil quenching from the points of view of microstructure and hardness. The quenching conditions for HPHQ that produce similar microstructure as typical oil quenching are also inversely determined. This chapter also illustrates the possibility of minimizing distortion of a part by properly setting up the quenching condition.

Chapter 6 concludes the numerical modeling and experimental investigation in this work. It also demonstrates the potential application of the numerical models and simulation procedure in other temperature and stress related situations such as other heat treating processes, welding processes, reliability prediction of critical parts under thermal cycling loads in PowerTrain systems and energy systems, etc.
2 Heat transfer modeling

During quenching, heat is transferred from hot solid components to the surrounded quenchants. The temperature variations of the hot components are the driving force of wanted and unwanted material property evolution, deformation and residual stress. Well control of the quenching results begins with the temperature control of the components.

This chapter analyzes the heat transfer in various quenching processes, develops and applies methods to determine accurate heat transfer coefficient (HTC) distribution, which is key to accurate thermal modeling and simulation.

2.1 Introduction

Whenever a temperature gradient exists in a body or a system, there will be an energy transfer from the high-temperature region to the low-temperature region. This transition of thermal energy is defined as heat transfer, consisting of convection, radiation and conduction.

Figure 2-1. A schematic illustration of heat transfer in quenching
Particular for a quenching process as shown schematically in Figure 2-1, the heat is transferred from the hot solid to the surrounded quenchant via convection and radiation while at the same time conduction occurs in the hot solid and quenchants respectively.

1) Conduction

Conduction occurs when there is a temperature difference within a body. The heat transfer rate is governed by Equation 1 [13].

$$\dot{Q}_{\text{cond}} = -KA \frac{\partial T}{\partial x}$$  \hspace{1cm} (1)

where:

- $\dot{Q}_{\text{cond}}$ = heat transfer rate via conduction
- $K$ = thermal conductivity of a material, W/m°C
- $A$ = cross section area, m²
- $\partial T / \partial x$ = thermal gradient in the direction of the heat flow, °C/m

2) Convection

When a heated component is exposed to ambient quenchant, natural or free convection occurs when the quenchant is still, or forced convection occurs in the case of the quenchant in motion. The heat transfer rate is governed by Equation 2 [13].

$$\dot{Q}_{\text{conv}} = h_c A(T - T_\infty)$$  \hspace{1cm} (2)

where:

- $\dot{Q}_{\text{conv}}$ = heat transfer rate via convection
- $h_c$ = convection heat transfer coefficient, W/m²°C
\[ A = \text{surface area, m}^2 \]
\[ T = \text{component temperature, } ^\circ\text{C} \]
\[ T_\infty = \text{quenchant temperature, } ^\circ\text{C} \]

3) Radiation

In contrast to the mechanisms of conduction and convection, heat can transfer in perfect vacuum. This mechanism is called thermal radiation caused by the temperature difference. Equation 3 expresses the heat transfer rate for a simple radiation problem when the heat transfer surface enclosed by a much larger surface [13].

\[
\dot{Q}_{\text{rad}} = \varepsilon\sigma A \cdot (T^4 - T_{\infty}^4) \approx \varepsilon\sigma A \cdot (4T_o^3 \cdot (T - T_{\infty})) \tag{3}
\]

where:

\[ \dot{Q}_{\text{rad}} = \text{heat transfer rate via radiation} \]
\[ \sigma = \text{universal Stefan Boltzman constant, } 5.6704 \times 10^{-8} \text{ W/m}^2\text{K}^4 \]
\[ \varepsilon = \text{emissivity of the body} \]
\[ T = \text{component temperature, } ^\circ\text{C} \]
\[ T_\infty = \text{quenchant temperature, } ^\circ\text{C} \]
\[ T_o = \text{a temperature depending on } T \text{ and } T_\infty, ^\circ\text{C} \]

4) Generalized HTC

As seen from Figure 2-1, the heat in quenching process is transferred via both convection and radiation, which is expressed in Equation 4 if the two mechanisms are added together. Since the heat transferred via radiation is much smaller than that via convection in quenching processes, adding the heat transferred via radiation to convection is reasonable,
especially if the predicted temperature-time curves are agreeable to the experimentally measured ones, as illustrated in Figure 2-2, which is the goal of the thermal modeling.

Thus, when we talk about HTC in the following sections, the small fraction of heat transferred via radiation is also included, if not specified.

\[
\dot{Q}_{\text{alt}} = (h_c + \sigma \varepsilon A T^3) \cdot A \cdot (T - T_\infty) = \overbrace{HTC}^{\text{generalized}} \cdot A \cdot (T - T_\infty)
\]  \quad (4)

![Figure 2-2. The goal of heat transfer modeling](image)

### 2.2 Challenges in heat transfer modeling

The amount of residual stresses and distortion generated in a component during quenching significantly depends on the cooling rate and the extent of non-uniformity of the temperature distribution in the component. Experimental investigation and numerical simulation results have shown that HTC between the component and the quenching media plays an important role in resultant distortion, residual stress and hardness.
distribution of the quenched object [3, 12, 22], therefore HTC distribution data are very important to the accuracy of numerical prediction of quenching results.

However, determination of HTC for a part in a specific quenching process is full of challenges. First of all, HTC data for a specific part are usually not available in literatures or handbooks. Second of all, determination of HTC distribution for a specific part in a particular quenching process is not an easy job, especially for liquid quenching where the heat transfer between hot metal parts and liquid quenchants is very complicated. When a hot part is quenched in fluid like oil or water, there are usually 3 stages: vapor stage, boiling stage and convection stage [13, 14]. The big difference of interactions in the 3 stages between solid and fluid leads to very complicated HTC data [14]. As a result, the HTC data vary in both time and space. The third, current practice of determining HTC cannot provide accurate HTC data. Classical empirical equations from heat transfer textbooks [13] are usually not suitable for real parts because of the complicated interaction and geometry. Current CFD packages are also facing difficulties to generate accurate HTC distribution, especially for liquid quenching.

Thus, reliable methods must be developed to determine HTC distribution for a specific part in a quenching process, because of its importance and the difficulties encountered in current practice.

### 2.3 Determining HTC using empirical equations

In current practice, classic empirical equations are used to calculate HTC in convection. This method is applied and analyzed in this section.
2.3.1 Principle

There are many classical empirical equations reported in literatures for calculating convection HTC data [13]. With the classical heat transfer theory, the dimensionless Reynolds number, Prandtl number and Nusselt number are defined in Equation 5-7, respectively.

\[
Re = \frac{\rho v L}{\mu} \quad (5)
\]

\[
Pr = \frac{C_p \mu}{K} \quad (6)
\]

\[
Nu = \frac{h_c L}{K} \quad (7)
\]

where:

- \( v \) = quenchant flow velocity, \( m/s \)
- \( \rho \) = quenchant density, \( kg/m^3 \)
- \( L \) = characteristic length of the work piece, \( m \)
- \( C_p \) = quenchant specific heat, \( J/kg\,°C \)
- \( \mu \) = quenchant dynamic (absolute) viscosity, \( kg/ms \)
- \( K \) = quenchant thermal conductivity, \( W/m\,°C \)
- \( h_c \) = quenchant heat transfer coefficient, \( W/m^2\,°C \)

The Nusselt number can be calculated from Reynolds number and Prandtl number using empirical equations. For instance, for the case of flow across a cylinder as shown in Figure 2-3, the equation expressed in Equation 8 can be used to calculate the Nusselt number [23]. After the Nusselt number is calculated, HTC can be determined from
Equation 7. The corresponding calculation of HTC is expressed in Equation 9. Another equation used to calculate HTC of gases [24] is expressed in Equation 10. Equations 9 and 10 show clearly that the HTC is a function of gas thermophysical properties, gas pressure (density) and velocity. Equation 11 [25] has a wide application range of Reynolds numbers and relatively higher accuracy and therefore is recommended by the textbook [13].

\[
Nu = 0.023 \cdot Re^{0.8} \cdot Pr^{1/3} 
\]

\[
\dot{h}_c = C_1 \cdot (\rho u)^{0.8} \cdot u^{-0.47} \cdot C_p^{0.33} \cdot K^{0.67} \cdot L^{-0.2} 
\]

\[
\dot{h}_c = C_2 \cdot (\rho u)^{0.8} \cdot u^{-0.4} \cdot C_p^{0.4} \cdot K^{0.6} \cdot L^{-0.2} 
\]

Where \(C_1\) and \(C_2\) are constants.

\[
Nu = 0.3 + \frac{0.62 \cdot Re^{2} \cdot Pr^{3}}{[1 + (0.4 \cdot \frac{Pr}{Re})^{3/4}]} \cdot \left[ 1 + \left( \frac{Re}{282000} \right)^{5/8} \right]^{4/5} 
\]
2.3.2 Applications

This method was applied to study the variation of HTC with respect to gas pressure and velocity in high pressure hydrogen quenching (HPHQ). The hydrogen thermophysical properties at different pressures and temperatures are gathered from two websites: Innovative Nuclear Space Power and Propulsion Institute (INSPI) [27] and the National Institute of Standards and Technology (NIST) [28]. Thermal conductivity, specific heat and viscosity of hydrogen vary slightly with respect to pressure for the range from 1 bar to 30 bar, and the density increases proportionally to pressure, in agreement with ideal gas law [28]. For simplicity, it is assumed in the HTC calculation that thermal conductivity, specific heat and viscosity are independent of gas pressure and velocity and the density variation is computed by the ideal gas flow. It is also assumed that the hydrogen temperature remains constant because the hydrogen is circulated and heat absorbed from the hot cylinder is taken away by the cooling system of the HPHQ equipment.

Table 1. Gas thermophysical properties at 1 bar and room temperature [27-29]

<table>
<thead>
<tr>
<th>Properties</th>
<th>Hydrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular Weight</td>
<td>2.016</td>
</tr>
<tr>
<td>Density at atmospheric pressure (kg/m³)</td>
<td>0.082644628</td>
</tr>
<tr>
<td>Absolute (Dynamic) Viscosity (kg/ms)</td>
<td>0.000009</td>
</tr>
<tr>
<td>Specific Heat (J/kgK)</td>
<td>14310</td>
</tr>
<tr>
<td>Thermal Conductivity (W/m²°C)</td>
<td>0.182</td>
</tr>
<tr>
<td>Flammable</td>
<td>yes</td>
</tr>
</tbody>
</table>

With the physical properties of hydrogen in Table 1, the HTC data at different pressures and velocities are calculated using Equation 11 and shown in Figure 2-4 and Figure 2-5. These figures and Equations 9 and 10 show clearly that HTC is an increasing function of
pressure (density), velocity, specific heat, thermal conductivity, and a decreasing function of viscosity and characteristic length. In Figure 2-4 and Figure 2-5, it is seen that HTC for HPHQ at 20 bar and 20 m/s can be as high as $1900 \text{W} / \text{m}^2 \cdot ^\circ \text{C}$. Other than the significant effects of gas pressure and velocity, it has been pointed out and verified by experiments that HTC of two-component gas mixture might be higher than that of the pure gases [24, 26, 30, 31]. It is further reported that the hydrogen-nitrogen mixture produces a peak HTC which is about 35% higher than that of pure hydrogen when the volume fraction of hydrogen ranges from 75% to 85% [30].

![HTC variation with respect to hydrogen pressure and velocity](image)

Figure 2-4. HTC variation with respect to hydrogen pressure and velocity
Figure 2-5. A contour of HTC variation

### 2.3.3 Advantages and disadvantages

It is pretty easy to apply this method and there is no need of experiments and simulations. However, the applications are very limited since almost all of them are calibrated under some specific experimental conditions which are significantly different from actual production situations. In addition, no HTC distribution can be calculated from this method.

### 2.4 Determining HTC using lumped heat capacity method

Experimental approach with a small probe can be utilized to determine the HTC. The method, called lumped heat capacity method [14, 32] is applied in this work.
2.4.1 Principle

The principle of this method to determine HTC is simply based on the energy (heat) conservation and the assumption that all the heat lost of the probe during quenching is transferred to the quenchant flow via convection. An experimental system shown in Figure 2-6 is used to collect temperature-time curves of a probe shown in Figure 2-7. These temperature-time curves of the probe are acquired and used to inversely calculate HTC in terms of probe surface temperature [13, 23, 32-35]. Because of its small size and in particular high thermal conductivity of probe material like silver and aluminum alloy, the Biot number calculated by Equation 12 is less than 0.1 and thus the temperature field in the probe can be considered uniform during quenching [36]. The average HTC of the probe can then be determined simply from the temperature-time curve at the center of the probe using Equation 13.

\[
Biot = \frac{h_c L}{K_s}
\]

(12)

\[
h_c = -\frac{m \cdot C_p(T)}{A(T - T_\infty)} \frac{dT}{dt}
\]

(13)

where:

- \( h_c \) = HTC averaged over the surface area, W/m\(^2\)C
- \( L \) = characteristic length, m
- \( K_s \) = solid thermal conductivity, W/m\(^o\)C
- \( m \) = probe mass, kg
- \( A \) = probe surface area, m\(^2\)
- \( T \) = temperature of the probe, \(^o\)C
$T_\infty$ = temperature of the quenchant, °C

$C_p$ = specific heat of the probe material, J/kg°C

Figure 2-6. An experimental system for forced air quenching

In the calculation of cooling rate, background noise in the measured probe cooling curve can introduce a significant error because any oscillation in the cooling curve will be magnified during differentiating. To eliminate any possible background noise in the cooling curves, a curve fitting scheme was used in this work. The 4th order polynomial function provided by Matlab [37] was employed to smooth the cooling curves. With the smoothed cooling curve, a reliable cooling rate and accurate HTC data can be calculated.
using Equation 13. The specific heat of probe, which influences the HTC calculation significantly, was also treated as a function of probe temperature in the Matlab calculation routine. Figure 2-8 shows one example HTC as a function of probe temperature in air quenching.

Figure 2-7. A schematic draw of the cast aluminum alloy probe

Figure 2-8. The calculated HTC as a function of probe surface temperature

2.4.2 Applications

This method was applied in air quenching process using an aluminum alloy probe. The experimental test conditions are tabulated in Table 2. The velocities of the air flow in the
quenching area were adjusted by varying the input voltage of the blower using a variac, and calibrated using an anemometer. Air humidity and air temperature in the quenching room were also controlled and measured every time when carrying out experiments. The probe was placed in the air flow at different orientations, the degrees of which are defined and shown in Figure 2-9.

Table 2. Experimental test matrix

<table>
<thead>
<tr>
<th>Air temperature (°C)</th>
<th>Air relative humidity</th>
<th>Air velocity (m/s)</th>
<th>Probe orientation (degree)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>30%</td>
<td>4.8</td>
<td>90, Vertical</td>
</tr>
<tr>
<td>25</td>
<td>50%</td>
<td>7.5</td>
<td>70</td>
</tr>
<tr>
<td></td>
<td></td>
<td>10.5</td>
<td>45</td>
</tr>
<tr>
<td></td>
<td></td>
<td>13.7</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td></td>
<td>18</td>
<td>0, Horizontal</td>
</tr>
</tbody>
</table>

Figure 2-9. A schematic illustration of three quenching orientations

HTC data at various conditions were inversely determined and tabulated in Table 3. For high accuracy, the experiment at each condition was repeated once and the average was calculated.
Table 3. Experimental results of HTC in air quenching (first phase)

<table>
<thead>
<tr>
<th>Velocity (m/s)</th>
<th>Air temperature (°C)</th>
<th>Relative humidity</th>
<th>Orientation</th>
<th>HTC experiment1 (W/m²°C)</th>
<th>HTC experiment2 (W/m²°C)</th>
<th>Average HTC (W/m²°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>15</td>
<td>31~33%</td>
<td>Vertical</td>
<td>147.97</td>
<td>146.40</td>
<td>147.19</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>45 degree</td>
<td>153.80</td>
<td>155.99</td>
<td>154.89</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Horizontal</td>
<td>139.43</td>
<td>139.32</td>
<td>139.37</td>
</tr>
<tr>
<td></td>
<td></td>
<td>46~50%</td>
<td>Vertical</td>
<td>148.71</td>
<td>148.18</td>
<td>148.45</td>
</tr>
<tr>
<td>25</td>
<td>31~33%</td>
<td></td>
<td>Vertical</td>
<td>146.48</td>
<td>148.70</td>
<td>147.59</td>
</tr>
<tr>
<td>10.5</td>
<td>15</td>
<td>31~33%</td>
<td>Vertical</td>
<td>98.66</td>
<td>102.49</td>
<td>100.58</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>45 degree</td>
<td>108.48</td>
<td>107.99</td>
<td>108.24</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Horizontal</td>
<td>93.32</td>
<td>96.32</td>
<td>94.82</td>
</tr>
<tr>
<td></td>
<td></td>
<td>46~50%</td>
<td>Vertical</td>
<td>106.04</td>
<td>106.00</td>
<td>106.02</td>
</tr>
<tr>
<td>25</td>
<td>31~33%</td>
<td></td>
<td>Vertical</td>
<td>106.29</td>
<td>107.32</td>
<td>106.81</td>
</tr>
<tr>
<td>4.8</td>
<td>15</td>
<td>31~33%</td>
<td>Vertical</td>
<td>66.90</td>
<td>65.83</td>
<td>66.37</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>45 degree</td>
<td>69.68</td>
<td>71.37</td>
<td>70.52</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Horizontal</td>
<td>58.58</td>
<td>59.32</td>
<td>58.95</td>
</tr>
<tr>
<td></td>
<td></td>
<td>46~50%</td>
<td>Vertical</td>
<td>61.90</td>
<td>65.89</td>
<td>63.90</td>
</tr>
<tr>
<td>25</td>
<td>31~33%</td>
<td></td>
<td>Vertical</td>
<td>70.50</td>
<td>70.55</td>
<td>70.53</td>
</tr>
</tbody>
</table>

It is apparent from Table 3 that air relative humidity and air temperature affect the HTC slightly. If the HTC data are divided by the HTC value (denoted as HTC₀) at a standard condition (1 bar, 10.5 m/s, 25 °C and the vertical orientation), it is seen in Figure 2-10 that HTC varies linearly with respect to air velocity in the velocity range from 5 m/s to 18 m/s and this linear relationship can be expressed as in Equation 14.
To further explore the effect of probe orientation, some more experiments at other orientations were performed in phase 2. Please note that the air velocities in phase 2 were slightly different from those in phase 1. For each velocity level, the HTC data at different orientations were divided by the HTC at the vertical orientation and the ratios were plotted in Figure 2-11. The effect of probe orientation was regressed by a second order polynomial as shown in Equation 15.

$$K_{velocity} = \frac{HTC}{HTC_o} = 0.57 \times \frac{Vel}{Vel_o} + 0.41$$  \hspace{1cm} (14)
Figure 2-11. The factor for orientation

$$y = -0.6933x^2 + 0.7882x + 0.906$$
$$R^2 = 0.9649$$

2.4.3 Advantages and disadvantages

This lumped heat capacity method assumes that the thermal resistance of the probe (body) is negligible in comparison with the resistance of the surrounding environment and therefore its temperature distribution is uniform during the cooling process. Accordingly, it is usually required to make the probe very small, or in some cases, the probe is made of material with high thermal conductivity like silver [32] so that the temperature of the probe is uniform during quenching in order to calculate HTC inversely [14]. Because of
the constraints, it is very difficult to apply this method to real part. In other words, it is not suitable for obtaining HTC distribution of a complicated part.

2.5 Determining HTC using semi-empirical equations

The semi-empirical equations were developed in this work for the purpose of determining HTC data at new conditions based on known HTC data at the baseline condition to save money and time for new experiments.

2.5.1 Principle

With this method, a specified standard condition (where the HTC is denoted as $HTC_o$) is first chosen as a standard value, and the HTC values at other conditions can be scaled up or down by some factors governing their influences. Equation 15 expresses the main idea of the semi-empirical equation system.

$$HTC = K_1 K_2 K_3 \cdots K_n \cdot HTC_o$$  \hspace{1cm} (16)

where,

$HTC_o$ = the standard HTC at a baseline condition, $W/m^2\cdot^\circ C$

$K_1, K_2, K_3, \cdots, K_n$ = modification factors

These modification factors are governing the effects of various influencing factors such as quenchant velocity, quenchant flow direction, quenchant temperature, work piece surface quality and material and can be constant, linear or nonlinear functions. For air quenching, the modification factor for air velocity is expressed in Equation 14 and the
one for probe orientation, in Equation 15. Factors for relative humidity, air temperature, etc. are taken as constant, one.

### 2.5.2 Applications

This method is further integrated in the method described in section 2.8.

### 2.5.3 Advantages and disadvantages

Once the semi-empirical equation system is established and the factors are calibrated, time and money for new experiments and simulations can be saved, especially when no high accuracy is required. The negative sides of this method include the efforts to establish the equation system and calibrate factors and relatively lower accuracy.

### 2.6 Determining HTC using iterative modification method

The iterative modification method was recently applied to determine accurate HTC distribution for complicated components. Automatic routines coded in Python [38] for ABAQUS [10] were developed and applied to several quenching cases in this section.

#### 2.6.1 Principle

First some thermocouples were embedded into a component and quenching experiments were carried out to acquire cooling curves at various locations of the component. Then surfaces of the component were grouped to several sub-zones and it was assumed that the HTC of each zone was uniform over the whole zone surface. The HTC of each zone was associated with a few cooling curves at nearby locations. Figure 2-12 illustrates the
surface grouping of the frame shape casting during water quenching at the orientation named thin leg down.

Next, as shown in Figure 2-13, an initial set of HTC data for surface zones were guessed and used in the thermal analysis. Then the HTC data were modified iteratively based on the differences between the predicted temperatures from finite element package and the experimentally measured temperatures at various locations of the thermocouples using Equation 17 and 18. For a given quenching condition, the optimal heat transfer coefficients for different surface zones were obtained till the temperature differences
between the predictions and the measurements were reduced to an acceptable tolerance such as 5 °C or the iteration numbers exceed a preset number. Finally the routine stops and outputs optimized HTC data.

\[ \Delta T = 5 \, ^\circ\text{C} \]
\[ \text{Iteration } \# \leq 50 \]

\[ HTC_{\text{new}} = HTC_{\text{old}} + \Delta HTC \]  \hspace{1cm} (17)
\[ \Delta HTC = k \cdot \Delta T \]  \hspace{1cm} (18)

where \( k \) is a constant number that is picked by experience. It does not affect the results other than the convergence rate.

The above describes my development of the script code in Python [38] for finite element package ABAQUS [10]. The optimization process using CFD package Wraft [39] was
also used in this dissertation work. Recently, some work has been done with such an approach using finite element packages such as ABAQUS and Deform [40] and optimization software such as Isight [41] to determine HTC iteratively [6, 32].

2.6.2 Applications

This method was applied to a few cases: water quenching of aluminum alloy frame-shape casting, water quenching of cylinder head and air quenching of engine block.

♦ Application case 1: water quenching of aluminum alloy casting frame

Figure 2-14. A frame shape casting with 11 thermocouples
An aluminum alloy frame-shape casting with thermocouples instrumented at different locations was shown in Figure 2-14. Dots on thermocouple lines indicate where they went into the casting and lengths of the dash lines indicate how deep they went. The thermocouples were cast-in-place in the casting to ensure the tight and firm connections with the casting and a no-water environment in the connections. During quenching, the thermocouples recorded the temperature changes and distributions in the casting.

Figure 2-15 and Figure 2-16 show the schematic design and a picture of the water quenching setup, respectively. The quenching setup was constructed in the residual stress lab at Oakland University. In quenching experiment, the casting was first heated up and held at a specific temperature for at least 30 minutes in a furnace and then placed on the pneumatic lifting system that immersed the casting into water at a constant speed. To simulate actual production condition, the water was heated up and hold at 75°C. For experiments with agitation, the water was pumped and circulated using an electric pump, as shown in Figure 2-15 and Figure 2-16. The water flow velocity at the location where the test casting was quenched was controlled at about 0.08m/s, which was similar to the production condition. After cooled down to water temperature, the casting was then taken out by the pneumatic lifting system.
Figure 2-15. A schematic illustration of experimental setup for water quenching

Figure 2-16. A photo of the water quenching bed
In the quenching experiments, the temperatures at different locations of the casting were acquired using a data acquisition system. Figure 2-17 shows the cooling curves at the places where thermocouples are embedded at the thin leg down orientation.

![Temperature - time curves](image)

**Figure 2-17.** The measured cooling curves for thin leg down quench orientation

Because bubbles form on the casting surfaces during water quenching, HTC can vary significantly from surface to surface in different quenching orientations [13, 14]. To simplify the calculations in HTC optimization, the surfaces with similar orientation during quenching were grouped together although the heat transfer can be different from point to point even on the same surface. Figure 2-12 shows how the three different kinds of surfaces were grouped for the thin leg down orientation.
It is generally accepted that the heat transfer of a hot object undergoes three main stages when it is quenched in a fluid like oil or water. The first stage is called film boiling [13], or vapor [14], or vapor blanket [23, 42] in high temperature region. At this stage, there is a rapid local boiling, leading to the formation of a vapor blanket (water steam) around the surface of the hot part. Heat is then transferred to the fluid through this vapor film. The second stage is called nucleate boiling [13, 23, 42], or boiling [14], where fluid comes into direct contact with the hot part surface and a nucleate boiling regime is developed. The heat transfer mechanism in the nucleate boiling stage is very complicated because of the complex physics relating to bubbles nucleation, growth, and departure from the hot metal surface. During the bubble growth and departure, heat is transferred from the hot metal surface to the growing bubbles and the nearby liquid. Usually more heat is transferred out from the hot metal during bubble growth because the bubble growth absorbs a lot of heat from the hot metal and the surrounded liquid which absorbs heat from the hot metal eventually [43]. The final stage is called convective cooling [23, 42], or convection [14] when the part surface temperature is lower than boiling temperature of the fluid. In this stage, heat is transferred directly into the fluid [14].

This three-stage heat transfer processes can be read from the inversely calculated temperature-dependent HTC curves for different surfaces of the water-quenched aluminum casting as shown in Figure 2-18. When the surface temperature of the casting is above about 200 °C, heat transfer is in the vapor blanket stage with relatively low HTC values. It is also noticed that the vapor blanket stage in this experimental study is relatively long because the water is heated to 75 °C and it is believed that the higher quenchant temperature typically produce longer vapor blanket stage [42]. When the
surface temperature of the casting is in the range from about 100 °C to 200 °C, nucleate boiling appears to occur, leading to very high HTC values. When the surface temperature is below 100 °C (boiling point of the quenching liquid [42]), however, heat is transferred mainly by convection. The HTC values are reduced significantly.

The bottom surfaces, facing down during quenching, exhibit lower HTC values in comparison with other surfaces. This is probably due to the fact that the bubbles formed on the bottom surfaces cannot easily escape from the surfaces. While bubbles formed on the side surfaces or top surfaces are easier to escape and therefore the heat transfer coefficients are relatively higher.

Figure 2-18. Iteratively determined HTC data from the cooling curves
Application case 2: water quenching of a cylinder head

This method was applied to the case of water quenching of cylinder head as well. Water quenching experiments with a cylinder head with 20 thermocouples at various locations, as shown in Figure 2-19, were carried out at real production condition and temperature-time curves were acquired by Oakland University research team (Parag Jadhav, Bowang Xiao, Keyu Li, Qigui Wang, etc) for GM water quenching project. Accordingly, the surfaces were divided to 8 subgroups as shown in Figure 2-20.

Figure 2-19. A cylinder head with 20 thermocouples
The acquired cooling curves at these 20 locations were used to determine HTC data iteratively. In this case, the CFD package Wraft was used together with a user defined script. After some iteration, the HTC curves converged to those shown in Figure 2-21.
Application case 3: air quenching of an engine block

This method is also applied to the case of air quenching of an engine block. The temperature-curve data for the engine block in air quenching process were provided by GM Powertrain [44]. In the experiments, thermocouples were placed at symmetric locations and therefore only two temperature curves for the whole engine block were useful. Thus the surfaces were divided to 2 subgroups. One is named ‘bottom engine surface’, which is related to the average of temperature curves from the bottom thermocouples, while the other subgroup consists of ‘top engine surface’ and ‘liner surface’, related to the top thermocouples as shown in Figure 2-22.

![Figure 2-22. Subgroups of engine block surfaces](image-url)
After simulations were iterated for a few times, the HTC for ‘top surface’ reached 0.163 mW/ mm²°C and the other HTC reached 0.158 mW/ mm²°C. In this case, the HTC data did not vary with respect to the engine block temperature that much. Two predicted temperature curves of two points in the engine block were compared to experimental measurements in Figure 2-23. It is seen that they are in very good agreements.

![Comparison of cooling curves between simulation and experiment](image)

Figure 2-23. Comparison of cooling curves of the engine block

### 2.6.3 Advantages and disadvantages

This method iteratively modifies the HTC data in order to make the predicted temperature-time curves agreeable with the experimentally measured ones. This method can generate zone-based HTC at relatively high accuracy, but the fact that the HTC data
are not uniform over a subgroup of surfaces while they are assumed the same can introduce some errors. In other words, the zone-based HTC distribution is too rough.

### 2.7 Determining HTC using CFD simulation method

Commercially available computational fluid dynamics (CFD) packages, such as Fluent [45], CFX [46] and others can solve thermal and fluid problems to certain degrees of accuracy. With CFD simulations, node-based HTC distribution can be obtained.

#### 2.7.1 Principle

Computational fluid dynamics is one of the branches of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. In CFD simulations, three equations of conversation (continuity, momentum and energy) are solved to obtain dynamic results in the fluid field. Heat transfer problems can be also solved in both fluid and solid domains. More specifically, heat is conducted in hot solid and transferred to solid surface, and then taken away by the around fluid. Conjugated heat transfer assumptions are made so that the heat fluxes in the fluid and the work piece are equal at the interface. CFD simulation can provide a node-based HTC distribution for the entire surface of the work piece and is applied to do so in the literature [47].

#### 2.7.2 Applications

This method was applied to a few cases: air quenching of an aluminum alloy frame-shape casting and high pressure hydrogen quenching of a spur gear.
Application case 1: air quenching of an aluminum alloy frame-shape casting

A big air box around the casting was created. Boundary conditions were applied to the air box shown in Figure 2-24. One face was defined as the air velocity inlet where normal air flow at specified air velocity was blown in. K-epsilon turbulence model and P1 radiation model were applied in this CFD simulation. Simulation results show that radiation slightly affects the temperature cooling curve.

Figure 2-24. CFD modeling
The whole model was meshed as shown in Figure 2-25. The casting was meshed with elements at the size of 2 mm, while the element sizes for the air box vary from 2 mm at the closest of the casting to 30 mm at the outmost side. Two layers of prism elements were placed close to the solid surfaces for a higher accuracy and convergence rate. As seen from Figure 2-25, the elements in air domain close to the solid casting surfaces are prism element (quad shape in the view plane in Figure 2-25) because usually quad elements provide higher convergence rates in CFD simulations.

Figure 2-25. Mesh scheme for CFD simulation
The air velocity distribution for this orientation is illustrated in Figure 2-26, and the HTC distribution in Figure 2-27. It is seen that the HTC for the top surface is lower than the side surfaces, which agrees with the fact that the air velocities close to the top surface are lower than those to the side surfaces. It is also noted that the HTC data vary from point to point even for the same surface. CFD simulation provides a perfect HTC distribution around the casting. These HTC data are highly related to the local air velocities and differ from each other from point to point.
- Application case 2: high pressure hydrogen quenching of a spur gear

A spur gear shown in Figure 2-28 was quenched in high pressure hydrogen flow.

Figure 2-28. A schematic drawing of the spur gear (gear width: 50mm)
In the CFD modeling, the initial temperature of this spur gear was set as 850°C, and hydrogen temperature, 25°C. In the model, K-e turbulence model is applied. The pressure and velocity was set as 15 bar and 20 m/s, respectively.

Velocity distribution for this orientation is shown in Figure 2-29. It is seen that the local velocities near the front face are very small and even zero at some locations.

The HTC distribution shown in Figure 2-30 corresponds to the velocity distribution tightly: the HTC data on the front face are very small while the HTC data on the center hole are much higher.
2.7.3 Advantages and disadvantages

With CFD simulations, node-based HTC distributions can be obtained. In general, the distribution results in relatively accurate prediction of temperature-time field in the entire work part, but CFD predictions are somehow different from experimental measurements for various reasons including the difficulties of modeling reality in every detail, the uncertainties of the parameters embedded in CFD packages, etc.

2.8 Determining HTC using integration method

CFD simulations can generate nice node-based HTC distribution, but are somehow different from experimental measurements for various reasons. In this section, the CFD
simulation method and the iterative modification method were integrated and a new method to obtain accurate HTC distribution was developed. This method is being registered as a patent [48].

2.8.1 Principle

Figure 2-31 illustrates the idea of the new method, where an initial set of node-based HTC distribution data are first obtained from the CFD simulation based on the work piece geometry, quenching set up and conditions including, work piece initial temperature and material properties, quenchant flow velocity, direction relative to the work piece, quenchant temperature, quenchant thermophysical properties, etc. The initial HTC distribution data for the entire surface of the work piece calculated from the CFD simulation are assigned to finite element package ABAQUS for the thermal simulation. The differences of predicted and measured temperatures are then calculated and used to modify scale factors to minimize the errors for the given quenching condition. The scale factors are used to adjust the CFD produced HTC distribution. Once the scale factors are adjusted to proper values, the HTC distribution used in finite element simulations, which is the product of CFD predicted HTC distribution and the scale factors, can result minimal temperature differences between prediction and measurement. After certain iterations, the temperature differences can be reduced to an acceptable tolerance such as 5 °C.
Equations 19 and 20 illustrate how the scale factors are modified based on the temperature differences between simulation and measurements. In the optimization process, the scale factors are modified iteratively until either acceptable temperature differences such as 5°C are reached or iteration number reaches the preset maximal iteration number (to prevent endless loop).

\[ \text{ScaleFactor}_{\text{new}} = \text{ScaleFactor}_{\text{old}} + \Delta \text{ScaleFactor} \]  \hspace{1cm} (19)

\[ \Delta \text{ScaleFactor} = k \cdot \Delta T \]  \hspace{1cm} (20)

Figure 2-31. The flow chart of optimizing HTC distribution [48]
where \( k \) is a constant number that is picked by experience. It does not affect the results other than the convergence rate.

Please note that the scale factors can vary with respect to surface temperature or time. If the surfaces of the work piece are grouped to several zones, each zone may have a separate scale factor.

The node-based HTC distribution from CFD simulation and the optimized scale factors are then used in the finite element simulation to predict temperature profile of the work piece, based on which the structural analysis can be conducted to obtain distortions and residual stresses.

![Diagram](image.png)

**Figure 2-32.** The integrated method of determining HTC distribution

When the HTC values are optimized for a baseline quenching condition, a set of semi-empirical equations (or weight functions) in section 2-5 can then be further integrated in this method as shown in Figure 2-32, and used to quickly modify the optimized baseline HTC data for different quenching conditions (i.e., variations of quenching conditions from the baseline) without performing thorough heat transfer and optimization calculations. These modification factors are governing the effects of various influencing
factors such as quenchant velocity, quenchant flow direction, quenchant temperature, work piece surface quality, material, etc.

2.8.2 Applications

This new method was applied in the air quenching of aluminum alloy frame-shape casting as shown in Figure 2-33 [48].

Figure 2-33. A frame shape casting with 14 thermocouples

A CFD simulation was conducted according to the quenching geometric setup and conditions and a node-based HTC distribution was obtained in section 2-7. The node-based HTC distribution data were then mapped into a finite element model for thermal and structural analyses. However, Figure 2-34 shows that temperature-time curves from
finite element prediction using original HTC data from CFD simulation differ from the experimentally measured ones.

Therefore, the node-based HTC distribution was scaled up by multiplying optimized scale factors that vary with surface temperature and were determined using the optimization script. As shown in Figure 2-35, after the optimized scaled factors were reached, the predicted temperature-time curves agreed perfectly with the experimentally measured ones.

Figure 2-34. A comparison of temperature-time curves before optimization
2.8.3 Advantages and disadvantages

In general, commercially available CFD software can solve thermal and fluid problems to a certain degree of accuracy, but there are usually differences between predicted results such as temperature and HTC and real ones in production for various reasons. In addition, these differences vary with respect to the CFD package used as well as user’s experience. These differences cannot be eliminated.

In this work, a new method integrating CFD simulation method and iterative modification method was developed to determine accurate node-based HTC distribution.
for a work piece with complicated geometry. With this method, the accurate HTC distribution data can be obtained. When further integrated with semi-empirical equations, this method can be used to predict new HTC distribution at new production conditions at no cost of experiments and simulations. The idea of modifying CFD simulation results based on experimental measurements can be applied in other situations as well.

This method was initially designed for and validated in quenching processes, but it can also be applied in other heat treating processes like heating, annealing, tempering, etc whenever accurate prediction of temperature profile is required.

### 2.9 Summary

In this chapter, a few different approaches of determining HTC distribution for a complicated part were analyzed and compared below.

#### 2.9.1 Comparisons of these methods to obtain HTC

The methods to obtain HTC distribution are compared in Table 4. Determining HTC data by applying empirical equations is very easy and fast since no experiments and CFD simulations get involved. The lumped heat capacity method using a small probe is especially suitable for studying factors in quenching production, but not suitable for big parts since the HTC distribution cannot be determined with this method. Semi-empirical equations are constructed based on the factor study using lumped heat capacity method or others and are suitable for rough calculation without performing new experiments when production condition changes. The iterative modification method can produce accurate
zone-based HTC distribution based on experimental acquired cooling curves for a part with complicated geometry. CFD method can generate node-based HTC distribution and its main con is that the accuracy is not as high as the iterative modification method. The integration method integrates the semi-empirical equations method, CFD simulation method and iterative modification method and takes good advantage of their pros. With this method, accurate node-based HTC distribution can be obtained for complicated parts, particularly in gas quenching process.

Table 4. Comparisons of methods to determine HTC distribution

<table>
<thead>
<tr>
<th>Method</th>
<th>Pros</th>
<th>Cons</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical equations</td>
<td>• Easy to use</td>
<td>• No distribution</td>
<td>• Rough calculation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Low accuracy</td>
<td></td>
</tr>
<tr>
<td>Lumped heat capacity</td>
<td>• Relatively high accuracy</td>
<td>• Time-consuming</td>
<td>• Factor study</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Costly</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>• No distribution</td>
<td></td>
</tr>
<tr>
<td>Iterative modification</td>
<td>• Relatively high accuracy</td>
<td>• Time-consuming</td>
<td>• Rough HTC distribution</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Costly</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Rough distribution</td>
<td></td>
</tr>
<tr>
<td>CFD simulation</td>
<td>• Good distribution</td>
<td>• Medium accuracy</td>
<td>• Node-based HTC distribution</td>
</tr>
<tr>
<td></td>
<td>• No experiments</td>
<td>• Complicated modeling</td>
<td></td>
</tr>
<tr>
<td>Semi-empirical equations</td>
<td>• No experiments</td>
<td>• Relatively low accuracy</td>
<td>• Rough calculation</td>
</tr>
<tr>
<td></td>
<td>• No CFD simulations (after calibration)</td>
<td>• No distribution</td>
<td>• New production condition</td>
</tr>
<tr>
<td>Integration method</td>
<td>• Highest accuracy</td>
<td>• Application of CFD</td>
<td>• Accurate node-based HTC distribution</td>
</tr>
<tr>
<td></td>
<td>• Good distribution</td>
<td>• Experiments required</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Complicated modeling</td>
<td></td>
</tr>
</tbody>
</table>

2.9.2 Assignment of HTC data in finite element packages

The HTC data vary in both space and temperature of the hot component or time. A uniform-in-space HTC can be easily assigned in a finite element modeling. So does the zone-based HTC distribution since the number of zones is a small number. However, it is
not an easy job to map node-based HTC distribution from CFD simulation to a finite element model by hand, especially when there are thousands of nodes on surfaces. This can be done by a mapping script as shown in Figure 2-36. In this work, a python code is developed to map node-based HTC distribution data to the finite element package ABAQUS.

Figure 2-36. A schematical show of HTC mapping

However, it should be pointed out that it is possible to convert temperature history of the solid component of CFD simulation into a format that can be read by an FEA package. The beauty of this method is that FEA package can use temperature history from CFD simulation and therefore the thermal analysis in FEA can be saved. The disadvantage is that the temperature history from CFD simulation cannot be adjusted according experimental measurements. Thus, this approach is not applied in this work.
3 Material property evolution modeling

During quenching, aluminum alloy and steel components experience various temperatures, strain rates, etc. The material evolves in the quenching process, especially for steel when phase transformation takes place. As a result, the material properties, particularly the constitutive behaviors, vary significantly in the quenching process, which are highly related to the quenching results such as distortion and residual stress.

This chapter analyzes the evolutions of material properties and material constitutive models of aluminum alloys and steels. A user material constitutive subroutine was developed for quenching of aluminum alloy 319 components. In addition, a frame work of developing user subroutine incorporating aging effect is also proposed. The user material constitutive subroutine package, DANTE [21], was used in the simulation of quenching steel components.

3.1 Introduction

Aluminum alloy and steel components experience various temperatures, strain rates, etc in the quenching process and as a result, the material properties, particularly the constitutive behaviors, evolve and vary significantly in this process. How steel and aluminum alloy components evolve is introduced in this section. In correspondence to numerical modeling, the variation of material constitutive behavior introduced due to evolution of material affects the accuracy of finite element modeling significantly.
3.1.1 Evolution of steel and aluminum alloy during quenching

How steel and aluminum alloy components respond in quenching processes is introduced in this section.

1) Steel

Steel is an alloy of iron and carbon with the carbon content up to about 2 wt%. Other alloying elements can weight up to about 5 wt% in low-alloy steels or higher in high-alloy steels [42]. Steel components are usually quenched to improve mechanical properties and remove some unwanted stresses introduced from previous processes.

When a treatable steel component is heated to and held at the austenizing temperature, uniform face centered cubic austenite is formed inside the component. When the steel is cooled down, austenite is not stable and phase transformation occurs. Figure 3-1 shows two cooling curves at different rates. If a steel 4140 component is cooled down very rapidly like the cooling curve 1, the austenite is transformed to martensite. If a steel 4140 component is cooled down less rapidly like the cooling curve 2, the austenite is transformed to bainite and martensite. If the component is cooled down slowly, pearlite might be formed. The CCT curves are from Cias’s work in 1977 [49]. Figure 1-2 in chapter 1 illustrates the microstructures of these phases.

Other heat treating processes after quenching such as tempering, annealing, etc will further affect the material evolution. This is not discussed in this work due to the objective limitation.
2) Aluminum alloy

Aluminum alloys are alloys consisting of predominant aluminum and other alloying elements such as silicon, copper, zinc, magnesium, etc. Casting alloys (e.g. Al-Si-Cu-Mg based) and wrought alloys (e.g. Al-Cu-Mg-Zn based) are the two principal classifications of Aluminum alloys. The most important cast aluminum alloy system is Al-Si alloy with silicon up to 13% to give good casting characteristics. Aluminum alloys are widely used in engineering structures and components, especially when light weight or corrosion resistance is required [50].

Figure 3-1. Cooling curves in steel CCT diagram
Aluminum alloy is solution treated at a temperature near the liquidus temperature of the alloy to maximize the concentration of hardening elements including silicon, copper, zinc, magnesium, etc in the solid solution, because the concentration of these elements increase with temperature. During solution treatment, these elements are re-dissolved to produce a solute-rich solid solution.

If the aluminum alloy is quickly cooled from the solutionizing temperature, precipitation and diffusion processes of these hardening elements are retarded. For instance, the Al-Cu alloy, whose phase diagram is shown in Figure 3-2 [51], is heated to a solutionizing temperature and all copper is in solid solution as a stable fcc $\alpha$ phase. In quenching, there is no time for any phase transformation to occur in the alloy so that the solid solution is

![Figure 3-2. A sample Al-Cu phase diagram [51]](image-url)
retained unchanged to room temperature. Therefore the solid solution is supersaturated with Cu and a driving force exists for precipitation of the equilibrium phase [52].

If the aluminum alloy is slowly cooled down from the solutionizing temperature, the hardening elements in the alloy precipitate and diffuse from solid solution to concentrate at the train boundaries, small voids, at dislocations and other imperfections in the aluminum lattice [53].

Therefore, aluminum alloys are quenched sufficiently fast to avoid undesirable concentration of the alloy elements in the defect and grain boundary structure. After quenching, aluminum alloys are aged to obtain a fine dispersion of elements for significantly increased material strengths [53]. Figure 3-3 [54] schematically illustrates the solid diffusion processes in a slowly cooling process and a quenching process.

If an Al-Cu alloy is aged, the microstructure is highly likely to change as following,

\[ \alpha_0 \rightarrow \alpha_1 + GP_{zones} \rightarrow \alpha_2 + \theta' \rightarrow \alpha_3 + \theta' \rightarrow \alpha_4 + \theta \]

For instance, if the Al-Cu alloy is aged by holding at a temperature about 130 °C for a period of time, there will be precipitates in the following precipitation process [52]. Figure 3-4 demonstrates the variation of hardness of the alloy as the phase changes during aging process [55].
Figure 3-3. Schematic Illustration of the solid diffusion process [54]

Figure 3-4. Hardness vs. time for various Al-Cu alloys at 130°C [55]
3.1.2 Material constitutive model in FEM

As shown in Figure 3-5, in the numerical simulation of quenching process of aluminum alloy and steel components, thermal analysis is first performed for temperature-time profile. During the temperature drop, the material shrinks due to thermal expansion, which is the driving force of the structural analysis. At the same time, the material properties evolve, which in return affects the constitutive relationship. The finite element solver integrates the driving force of thermal strain, the material property governing model of user material subroutine and other factors such as boundary conditions and load, and computes the quenching results such as distortion, strain, residual stress, etc.

Figure 3-5. Material property evolution modeling
Constitutive model is relationship between two physical quantities (often tensors). The constitutive equation is specific to a material or substance, but it does not follow directly physical law. The first constitutive equation (constitutive law) was discovered by Robert Hooke and is known as Hooke's law. In the constitutive equations, the linear stress-strain relationship was well governed. Another example of constitutive equation is the Coulomb friction where the relationship between friction and the normal force is connected with a friction coefficient.

In finite element modeling, the displacements and forces of a material point are connected by a stiffness matrix \([K]\). Stiffness matrix describes how the point will move in respond to the force applied. The simplest example of it is a spring, where the elastic coefficient \(K\) is a stiffness matrix for a uniaxial elastic problem. For a 3D problem, the stresses and strains at a point consist of 9 components for an anisotropic problem or 6 components for an isotropic one as shown in Figure 3-6.

![Figure 3-6. Components of stress in three dimensions [56]](image-url)
The displacements $u_1, u_2$ and $u_3$ of a point in x, y and z direction respectively are connected to the strains at that point by the geometry equations as expressed in Equation 21 or in tensor form as in Equation 22 [57].

\[
\varepsilon_{11} = \frac{\partial u_1}{\partial x_1} \tag{21-a}
\]

\[
\varepsilon_{22} = \frac{\partial u_2}{\partial x_2} \tag{21-b}
\]

\[
\varepsilon_{33} = \frac{\partial u_3}{\partial x_3} \tag{21-c}
\]

\[
\varepsilon_{31} = \frac{1}{2} \left( \frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right) = \varepsilon_{13} \tag{21-d}
\]

\[
\varepsilon_{23} = \frac{1}{2} \left( \frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3} \right) = \varepsilon_{32} \tag{21-e}
\]

\[
\varepsilon_{21} = \frac{1}{2} \left( \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) = \varepsilon_{12} \tag{21-f}
\]

\[
\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = \varepsilon_{ji} \tag{22}
\]

The forces $\vec{F}_1, \vec{F}_2$ and $\vec{F}_3$ at a point in x, y and z direction respectively are associated with the stresses at that point by the equilibrium equations as expressed in Equation 23 or in tensor form as in Equation 24 [57].

\[
\frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{21}}{\partial x_2} + \frac{\partial \sigma_{31}}{\partial x_3} + \vec{F}_1 = 0 \tag{23-a}
\]

\[
\frac{\partial \sigma_{12}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} + \frac{\partial \sigma_{32}}{\partial x_3} + \vec{F}_2 = 0 \tag{23-b}
\]
\[
\frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} + \frac{\partial \sigma_{33}}{\partial x_3} + \dot{F}_3 = 0 \tag{23-c}
\]

\[
\sigma_{ij} + \dot{F}_i = 0 \tag{24}
\]

The constitutive equations governing the relationship of stresses and strains are a bridge connecting forces and displacement and the very important components of the stiffness matrix as shown in Figure 3-7 [58]. In the numerical modeling, geometry equations and equilibrium equations are known and constant, while the constitutive equations vary with respect to temperature, strain rate and microstructure, etc. It is the constitutive equations that describe the material behaviors and differences among materials. Therefore having accurate material constitutive models is crucial to the accuracy of finite element simulation.

Figure 3-7. Node stiffness matrix in FEA
3.2 Challenges in material property evolution modeling

The development of user material subroutine to govern material property evolution is full of challenges. These challenges lay on the three processes: development of model governing material evolution, development of material constitutive model and development of user subroutine for finite element package.

In the process of development of model governing material evolution, a mathematical model is constructed to describe how the material evolves (e.g. microstructure evolves) based on experimental investigation. This process is highly related to the next one since the material property will of course significantly influence its behavior. Please note that sometimes this process is skipped when developing material constitutive model from the macro behavior point of view. This happens especially when the material does not evolve much. For instance, in quenching of some metal components, there is no phase transformation or other changes in the material microstructure.

In the process of development of material constitutive model, a mathematical model is constructed to govern the material behavior considering the effects of temperature, strain rate, microstructure, etc. when they are involved. The mathematical model is a separate routine and is to describe how the material will respond at various conditions. The prediction of the model should be validated by experimental measurements. This process is also full of challenges because the material constitutive equations cannot be derived from physical laws and must be well describing the complicated phenomenon of material behavior, which involves knowledge of physics, thermodynamics, mechanics, microstructure, etc.
In the process of development of user subroutine, the user developed or calibrated constitutive equations must be converted to a computer program that can work with finite element packages so that the material behavior can be accurately governed in the finite element simulation. This is not an easy job neither for the reasons: (1) The subroutine must be able to handle 3D problems, i.e., the 9 stress components and 9 strain components (6 components each for isotropic material) must be modeled and well coordinated; (2) The modeling of material property usually involves elastic problem, plastic problem, and sometimes viscoplastic problem; and (3) Many constitutive equations are expressed with differential equations because the lack of analytic solutions. When solving these differential equations simultaneously, the convergence can be a problem especially for a 3D case where they are highly interrelated stress and strain components.

### 3.3 Development of material constitutive models and subroutines

The constitutive models and subroutines for steel and aluminum alloy casting are introduced in this section.

#### 3.3.1 Constitutive model and subroutine for steel

Recently, a user subroutine set, DANTE [21] was developed by Deformation Control Technology (DCT), Inc to model the material evolution and constitutive behavior in heat treating processes including heating, quenching, tempering, etc [21]. In this work, DANTE was used together with ABAQUS to simulating quenching of steel components.
Both diffusive and martensitic transformations are included in the metallurgical transformation models in DANTE [21]. Researchers at Colorado School of Mines have developed phase transformation models in cooling processes for steel alloys in the last 20 years [59-65]. DCT developed the heat up kinetics for slow and rapid formation of austenite and Low temperature tempering model [21]. Temperature, time and stress state information were the inputs of the models, which were passed from ABAQUS. The model calculates material evolution in terms of phase transformation, which is passed to the thermal and mechanical models. Steel chemistry, grain size, and kinetics parameters derived from dilatometry, CCT, TTT and Jominy are used to characterize the transformation kinetics [21].

Sandia National Laboratories developed the multiphase mechanics model based on phase transformation model [66]. In the multiphase mechanics model, mechanical response of the composite structure that changes during heat treatment is calculated based on the inputted mechanical properties of each phase [21, 66]. Temperature, strain rate, time and grain size are important factors in the mechanic models.

Figure 3-8 shows the structure of the subroutine set and procedure to run simulation for heat treating processes of steel components. Because carbon concentration plays an important role in the phase transformation, a carbon diffusion analysis of carburizing is usually performed to obtain the carbon profile of the steel component. After the carbon diffusion analysis, the heat transfer analysis and phase transformation analysis are carried out simultaneously to generate temperature-time profile and phase profile, respectively. These two analyses are carried together because they are tightly interrelated and affect
each other strongly. At the end, the structural analysis is performed to predict the stress profile and distortion. [66]

Other researchers also developed some material constitutive models for steel components, but they are more focusing on the stress-strain relationship and pay less attention to the phase transformation mechanism, although the effects of which on stress-strain relationship are governed in the models [67-71].

Figure 3-8. The multiphase mechanics model for steel in DANTE package [66]
3.3.2 Constitutive model for aluminum alloy casting

During quenching, the aluminum alloy castings experience temperature drop and material shrinkage. The deformation rates at different locations are usually different due to geometrical and other constraints. Because of these facts, the material behaviors are varying with respect to both time and location [4, 15-17]. In order to get accurate simulation results, the material behaviors must be well governed. Current FE package incorporated material models are usually for general materials and therefore special material constitutive model must be developed for a specific material under specific conditions. In this work, quenching of components made of casting Al-Si alloy 319, whose composition is tabulated in Table 5, was studied.

Table 5. Material composition of aluminum alloy 319 in weight percent

<table>
<thead>
<tr>
<th>Element</th>
<th>Si</th>
<th>Cu</th>
<th>Fe</th>
<th>Mg</th>
<th>Mn</th>
<th>Zn</th>
<th>Ti</th>
<th>Cr</th>
<th>Sr</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wt(Pct)</td>
<td>7.43</td>
<td>3.33</td>
<td>0.38</td>
<td>0.26</td>
<td>0.24</td>
<td>&lt;0.25</td>
<td>0.12</td>
<td>&lt;0.05</td>
<td>0.03</td>
<td>balance</td>
</tr>
</tbody>
</table>

Figure 3-9. Stress-strain curves for Al-Si alloy 319 casting [15]
Figure 3-9 shows that material constitutive relationship of aluminum alloy 319 depends strongly on temperature and strain rate [15]. These curves were governed by the material constitutive model for aluminum alloy 319 in Newman’s paper [15]. This model is used in this work for its simplicity and special application for water quenching process. This model does not consider changes in microstructure, but focuses on the macro constitutive behavior. In this model, the flow stress $\sigma$ is the sum of three components: an athermal stress $\sigma_a$, an “intrinsic strength” $\sigma_i$ and a state variable $\sigma_e$. The intrinsic strength $\sigma_i$ models yielding and $\sigma_e$ evolves with the deformation to model hardening. For large grain materials, such as cast 319, $\sigma_a$ is assumed to be 0. Thus, the flow stress is expressed as Equation 25.

$$\frac{\sigma}{\mu(T)} = \frac{\sigma_a}{\mu(T)} + S_i(\dot{\varepsilon}, T) \frac{\dot{\sigma}_i}{\mu_0} + S_e(\dot{\varepsilon}, T) \frac{\dot{\sigma}_e}{\mu_0} = S_i(\dot{\varepsilon}, T) \frac{\dot{\sigma}_i}{\mu_0} + S_e(\dot{\varepsilon}, T) \frac{\dot{\sigma}_e}{\mu_0}$$

(25)

Here, $\mu(T)$ is the temperature-dependent shear modulus, given as

$$\mu(T) = \mu_0 - \frac{3440}{\exp\left(\frac{215}{T}\right) - 1}$$

(26)

where $\mu_0$=28.815GPa is the reference value at 0 K and $\dot{\varepsilon} = 10^7$ s$^{-1}$. T is the temperature in Kelvin.

At yielding, $\dot{\sigma}_e = 0$. After yielding, a liner form of the state variable is used in this model as expressed in Equation 27.

$$\dot{\sigma}_e = \dot{\sigma}_e^0 + \frac{\mu(T)}{\mu_0} \theta_0 \left[ 1 - \frac{\dot{\sigma}_e^0}{\dot{\sigma}_{os}} \right] d\varepsilon$$

(27)
where:

\( \theta_0 \) = the slope of the stress-strain curve at yield in the reference state (0 K, \( \dot{\varepsilon} = 10^7 \text{s}^{-1} \))

\( \dot{\sigma}_{ox} \) = a material parameter, MPa

\( \dot{\sigma}_{e}' \) = the previous state variable, MPa

\( d\varepsilon \) = the strain increment during the evolution

Velocity-modified temperatures, \( S_i(\dot{\varepsilon},T) \) and \( S_e(\dot{\varepsilon},T) \), is used to scale the temperature and strain rate as following:

\[
S_i(\dot{\varepsilon},T) = \left[ 1 - \left( \frac{kT}{\mu(T)b^3g_{oi}} \ln(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}) \right)^\frac{1}{p_i} \right]^{\frac{1}{\dot{\varepsilon}}} 
\]

\[
S_e(\dot{\varepsilon},T) = \left[ 1 - \left( \frac{kT}{\mu(T)b^3g_{oe}} \ln(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}) \right)^\frac{1}{p_e} \right]^{\frac{1}{\dot{\varepsilon}}}
\]

where \( g_{oi} \) and \( g_{oe} \) are the activation energy for flow at yield and saturation, respectively. They are normalized by Boltzmann’s constant \( k \), the Burgers vector \( b \), and the shear modules \( \mu(T) \).

The constants \( p_i \), \( q_i \), \( p_e \) and \( q_e \) are related to the interaction of dislocation with precipitates enological constants. Please refer to the literature [15] for value assignments.

Young’s modulus is determined from the stress-strain curves of tensile tests at different temperatures and strain rates and is fitted to a second-order polynomial as shown in Equation 30.
In this material constitutive model, all other parameters are treated as constants, except the four parameters: \( \sigma_{os}, \sigma_{i}, g_{oi} \) and \( g_{os} \), which can be determined from tensile tests at various temperatures and strain rates for a specific material.

### 3.3.3 Development of user constitutive subroutine for aluminum alloy casting

In order to apply the material constitutive model in the finite element simulations, the model must be translated to something that a FE package can use it. In this work, the user material constitutive subroutine, UMAT, was developed in Fortran language based on the isotropic hardening plasticity for FE package ABAQUS [10, 72, 73]. During the simulation, ABAQUS calls UMAT at each integration point.

As shown in the flow chart in Figure 3-10, for each call at every point, UMAT first conducts a trial elastic calculation assuming full elastic deformation governed by Equation 31 with the inputs (previous status, strain increments, temperature, etc) passed in from ABAQUS and generates the new status of stress, strain, etc. The subroutine then by using Equation 32 compares the Von Mises of the trial calculation to the flow stress predicted by the material model to see if there is any plastic flow in this increment. If no, the subroutine updates the status variables and returns the Jacobian matrix as defined in Equation 33 to ABAQUS for global calculation. If yes, the subroutine recalculates the new status including plastic flow as defined in Equation 34 with plastic theory and updates state variables and Jacobian matrix. Jacobian matrix for the constitutive equation governs the evolution of material property. The calculation of new status with plastic
theory usually cannot be done in one step because of the non-linear character and is usually done iteratively.

\[
\sigma_{ij} = \lambda \delta_{ij} \varepsilon_{kk}^{el} + 2 \mu \varepsilon_{ij}^{el}
\]

where:

- \( \sigma_{ij} \) = stress tensor, i,j=1,2,3
- \( \delta_{ij} \) = Kronecker delta, it is 1 if i=j; and 0 otherwise
- \( \mu \) = Shear modulus, \( \mu = G = E/(2(1+\nu)) \), E is Young’s modulus, \( \nu \) is poison’s ratio
- \( \lambda \) = Lame’s constant, \( \lambda = vE/(1+\nu)(1-2\nu) \)
- \( \varepsilon_{ij}^{el} \) = elastic strain tensor, i,j=1,2,3

Figure 3-10. Flow chart of UMAT
\[ \bar{\sigma} = \sqrt{\frac{3}{2}} S_{ij} S_{ij} = \frac{1}{\sqrt{2}} \left( (\sigma_{11} - \sigma_{22})^2 + (\sigma_{11} - \sigma_{33})^2 + (\sigma_{22} - \sigma_{33})^2 + 6\sigma_{12}^2 + 6\sigma_{23}^2 + 6\sigma_{13}^2 \right) \]  

(32)

where:

\( \bar{\sigma} \) = equivalent stress, Von Mises stress

\( S_{ij} \) = deviator stress tensor

\[ J = \frac{\partial \Delta \sigma}{\partial \Delta \varepsilon} = \begin{bmatrix} \frac{\partial (\Delta \sigma_1)}{\partial (\Delta \varepsilon_1)} & \cdots & \frac{\partial (\Delta \sigma_1)}{\partial (\Delta \varepsilon_6)} \\ \frac{\partial (\Delta \varepsilon_1)}{\partial (\Delta \varepsilon_1)} & \cdots & \frac{\partial (\Delta \varepsilon_1)}{\partial (\Delta \varepsilon_6)} \\ \vdots & \ddots & \vdots \\ \frac{\partial (\Delta \sigma_6)}{\partial (\Delta \varepsilon_1)} & \cdots & \frac{\partial (\Delta \sigma_6)}{\partial (\Delta \varepsilon_6)} \end{bmatrix} \]  

(33)

where \( J \) is the Jocabian matrix.

\[ \dot{\varepsilon}_{ij}^{pl} = \frac{3S_{ij}}{2\sigma_y} \dot{\varepsilon}^{pl} \]  

(34)

where:

\( \dot{\varepsilon}_{ij}^{pl} \) = tensor of plastic strain rate, \( i,j=1,2,3 \)

\( \dot{\varepsilon}^{pl} \) = equivalent plastic strain rate

\( \sigma_y \) = yielding stress

### 3.3.4 An extended framework incorporating aging

In the previous section, a user material constitutive subroutine for aluminum alloy 319 without considering aging effect was developed. However, as discussed in the material evolution section, the supersaturated solid solution was obtained in the quenching process,
but it is not a stable phase and there is a driving force for phase transformation, especially when held at an elevated temperature for a period of time.

Other researchers have done some work about the aging effect. The research team of Dr. Sehitoglu had developed a complicated material constitutive model to take account of temperature, strain rate, time and microstructure (represented by SDAS – secondary dendrite arm spacing). That phenomenological constitutive model was developed to govern the stress-strain response of the cast 319 T6/T7 aluminum alloy under thermomechanical loading. [16, 74] and it is potentially possible to be adapted to govern the constitutive behavior in quenching considering aging effect.

CHTE research team at WPI had done some work to study the aging of aluminum alloys in the aging cycle optimization for aluminum alloy project [75]. A model was constructed for yield strength and microstructure prediction of Al-Si-Cu-Mg based cast and Al-Cu-Mg-Zn based wrought aluminum alloys at the degree of accuracy to some certain [76].

Traditional constitutive models, especially phenomenological constitutive model, are designed to predict stress-strain relationship when aluminum alloys experience temperature changes. They can predict constitutive behavior pretty accurately in the designed range of conditions, but are usually unable to predict the material microstructure changes. The one developed by CHTE can predict yielding strength and evolution of some precipitation, but are not designed to describe the constitutive behavior of aluminum alloys.
Therefore, a framework of a constitutive model governing both the evolution of the microstructure and macro constitutive behavior in the quenching was proposed for other researchers who would like to further develop the model. As shown in Figure 3-11, a thermal analysis and phase transformation analysis are performed simultaneously. In this process, the thermal analysis predicts temperature variation with material thermophysical property and thermal boundary condition information. The temperature-time information at each node was passed to the material property evolution model which predicts the evolution of the microstructure due to possible aging effect. The evolution of material property influences the thermal analysis to some certain of degree. In the followed mechanical (structural) analysis, temperature-time profile and microstructure information at each node is passed to the constitutive model which predicts the stress-strain relationship based on the temperature profile, microstructure profile and other factors.
such as strain and strain rate. The stress-strain relationship of each node was used to construct the global stiffness matrix of the whole part as shown in Figure 3-7.

Figure 3-12. Simulation procedure for quenching and aging of aluminum alloy

For some aluminum alloys, the aging effects in quenching processes are negligible. In other words, the evolution of material property analysis can be skipped. But most of aluminum alloys, no matter aging occurs in quenching or not, are further aged for a harder property. In this case, the aging must be numerical modeled as well. Figure 3-12 illustrates the simulation procedure for quenching and aging processes. The simulations
for quenching and aging are carried out sequentially. The temperature profile, microstructure profile and stress, strain profiles generated in quenching process are passed to the models for aging process.

### 3.4 Summary

In this chapter, the material evolutions of aluminum alloy and steel components were analyzed. The material evolutions during quenching processes lead to phase changes and variations of material constitutive behavior. Because of the importance of constitutive models in finite element method, it is extremely important to govern the behavior during quenching processes to accurately predict quenching outcomes such as distortion and residual stress. In finite element practice, the material constitutive models were developed as user material constitutive subroutines, which worked together with finite element packages.

The material evolution of steel components during quenching was analyzed and a commercially available user material subroutine set, DANTE, was conjunctly applied with finite element package ABAQUS for simulation of quenching of steel components.

The material evolution of aluminum alloy components during quenching was also analyzed and a user material constitutive subroutine was developed based on a particular constitutive model that governs the stress-strain behavior during quenching. Considering the big role played by aging particularly in some aluminum alloys, it is necessary to integrate the possible aging effect in the material constitutive model into quenching modeling. A framework of developing a subroutine set incorporating the possible phase
transformation due to aging and variation of constitutive behavior was proposed. This framework covers both the quenching and aging processes.
4 Residual stress prediction and measurement

Residual stresses are the stresses exist in a component without an external load or force (including gravity) or other sources like thermal gradient [18]. The residual stresses may present in engineered components, thin films, surface coatings, composites, multiphase materials, etc. Residual stress in a product will affect its quality mainly in two ways: tensile residual stresses reduce fatigue life significantly and release of residual stress causes unacceptable distortion during usage, especially for big parts.

This chapter presents how to predict residual stresses in as-quenched aluminum alloy and steel components by numerical simulation, based on which optimization of part design and process design can be reached. To improve the accuracy of numerical modeling, the numerical predicted residual stresses are validated by experimental measurements.

4.1 Introduction

The residual stresses may present in engineered components, thin films, surface coatings, composites, multiphase materials, etc. Residual stresses originate from a variety of sources. Macroscopic residual stresses can arise from processes involving plastic deformation including heat treatment, machining, bending, drawing, rolling, forming, pressing, spinning and assembly. Microstructural stresses often result from the CTE (coefficient of thermal expansion) mismatch between phases and constituents or from phase transformations in a grain. It is unlikely that a manufactured component is entirely free from residual stresses.
Residual stress in a product will affect its quality mainly in two ways: tensile residual stresses reduce fatigue life significantly and release of residual stress causes unacceptable distortion during usage, especially for big parts. It is believed that compressive residual stresses are good for the fatigue life, crack propagation and stress corrosion of materials whereas tensile residual stresses reduce their performance capacity because the residual stress is super posed as a mean stress with dynamic stress [8, 18].

Since the residual stresses cannot be eliminated from manufactured components and they have important effects on the performances of components including fatigue, fracture, corrosion, wear and friction, it is highly necessary to control residual stresses in manufactured components by optimizing part design and process setup. In this work, prediction and measurement of residual stresses are addressed for optimization in quenching processes of aluminum alloy and steel components.

As discussed in Chapter 1, optimization of part design and production conditions through numerical modeling are preferred because it saves time and money and provides results in more detail, compared to the experimental method. Numerical models are created to predict residual stresses in as-quenched components, which are validated by experimental measurements.

### 4.2 Challenges in residual stress prediction and measurement

In the numerical prediction of residual stress using finite element packages, challenges lay on the governing of thermal boundary condition (HTC), material constitutive behavior, applied loads and other boundary conditions and using proper mesh scheme. In
simulation of quenching process, the applied loads and constraints are usually not so complicated as the governing of HTC and material constitutive behavior, which have been addressed extensively in the previous chapters. Therefore, the biggest challenge left in numerical prediction is to create and set the computer model properly.

In the measurement of residual stress, accuracy must be ensured in order to validate numerical prediction. Experimental errors and fluctuation must be minimized. In addition, the measurement methods that provide residual stress distribution are preferred for extensive comparisons between prediction and measurement.

### 4.3 Residual stress prediction

As illustrated in Figure 4-1, the quenched components are first meshed with elements before any numerical simulations. The coupled temperature-displacement analysis is decoupled to two steps: heat transfer analysis and stress analysis, because by doing so the stress analysis converges faster and requires less computer memories. Thermal simulation is run first to obtain temperature profiles. Chapter 2 introduced methods to obtain accurate HTC distribution data for the work piece. By using the accurate HTC data, the thermal simulations in ABAQUS can provide very accurate temperature profiles. Structural (stress) simulation is run to obtain residual stresses and distortion generated due to temperature gradients and geometrical constraints. The temperature drop is the driven force of this structural analysis. In the structural analysis, material constitutive behaviors that vary quite different with respect to different temperatures, strain rates, etc. are well governed by using the self-developed user subroutine for aluminum alloy, and
DANTE for steel components. No external forces are applied to the model and constrains are only applied to remove the rigid body movement. In this process, thermal expansion, material constitutive model, external loads and boundary conditions are integrated together by the ABAQUS solver to predict strains, stresses, distortion, etc.

Figure 4-1. Schematic show of structural analysis of quenching process

Table 6. Unit systems for finite element simulation

<table>
<thead>
<tr>
<th>Quantity</th>
<th>SI (engineering)</th>
<th>SI (primary)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>mm</td>
<td>m</td>
</tr>
<tr>
<td>Force</td>
<td>N</td>
<td>N</td>
</tr>
<tr>
<td>Mass</td>
<td>ton, (N/(mm/s²))</td>
<td>kg, (N/(m/s²)) = 10⁻³ ton</td>
</tr>
<tr>
<td>Time</td>
<td>s</td>
<td>s</td>
</tr>
<tr>
<td>Stress</td>
<td>MPa, (N/mm²)</td>
<td>Pa, (N/m²)</td>
</tr>
<tr>
<td>Energy</td>
<td>mJ, (N*mm)</td>
<td>J, (N*m)</td>
</tr>
<tr>
<td>Density</td>
<td>ton/mm³</td>
<td>kg/m³ = 10⁻¹² ton/mm³</td>
</tr>
<tr>
<td>Power</td>
<td>mW, (N*mm/s)</td>
<td>W, (N*m/s)</td>
</tr>
<tr>
<td>Acceleration</td>
<td>mm/s²</td>
<td>m/s²</td>
</tr>
<tr>
<td>Conductivity</td>
<td>mW/(mm*K)</td>
<td>W/(m<em>K) = mW/(mm</em>K)</td>
</tr>
<tr>
<td>Specific heat</td>
<td>mJ/(ton*K)</td>
<td>J/(kg<em>K) = 10⁻⁶ mJ/(ton</em>K)</td>
</tr>
<tr>
<td>HTC</td>
<td>mW/(mm²*K)</td>
<td>W/(m²<em>K) = 10⁻³ mW/(mm²</em>K)</td>
</tr>
</tbody>
</table>
Because there is no specific unit system in the finite element package ABAQUS, the self-consistent unit system using mm, MPa, etc. tabulated in Table 6 is used.

### 4.4 Residual stress measurement

Residual stresses were measured to validate the accuracy of numerical modeling. This section first reviews some common technologies for measuring residual stresses.

#### 4.4.1 Measurement methods

Currently widely applied measurement methods are introduced in this section.

a) **Resistance strain gauge hole-drilling method**

The hole-drilling stress relaxation method is the most widely used modern technique for measuring residual stress [19]. A strain gage rosette shown in Figure 4-2 is mounted onto the surface of a sample, and a small hole is drilled at the center of the three strain gages. A setup of measuring strain relieves in three different directions using three strain indicators during hole-drilling process is illustrated in Figure 4-3.

![A rectangular resistance strain rosette](image)

**Figure 4-2.** A rectangular resistance strain rosette [77]
During the hole-drilling, strains are relieved due to the release of residual stresses. The relieved strains are measured and used to back-calculate residual stresses in that small area. The general expression for the relieved radial strains due to a plane biaxial residual stress state is Equation 35 [19, 20, 77, 78]:

\[
\begin{align*}
\varepsilon_1 &= A(\sigma_x + \sigma_y) + B(\sigma_x - \sigma_y) \cos 2\alpha \\
\varepsilon_2 &= A(\sigma_x + \sigma_y) + B(\sigma_x - \sigma_y) \cos 2\beta \\
\varepsilon_3 &= A(\sigma_x + \sigma_y) + B(\sigma_x - \sigma_y) \cos 2\gamma 
\end{align*}
\]

where:

\( \varepsilon_{1,2,3} \) = measured strain relieved from strain gage 1, 2 and 3, respectively, \( \mu \varepsilon \)

\( \sigma_x \) = stress in x direction, MPa
\( \sigma_y \) = stress in y direction, MPa

A, B = calibration coefficients, MPa/\( \mu \varepsilon \)

\( \alpha \), \( \beta \), \( \gamma \) = angle measured counterclockwise from the x direction to the axis of the strain gage 1, 2 and 3, respectively, degree

For a rectangular strain gage rosette as shown in Figure 4-2, where \( \alpha = 0^\circ \), \( \beta = 45^\circ \), \( \gamma = 90^\circ \), the three strain gages measure the three strains along the gage directions during hole-drilling. The principal stresses and their directions are solved and shown in Equation 36:

\[
\begin{align*}
\sigma_{\text{max}} &= \frac{\varepsilon_1 + \varepsilon_3}{4A} - \frac{1}{4B} \sqrt{(\varepsilon_3 - \varepsilon_1)^2 + (\varepsilon_1 + \varepsilon_3 - 2\varepsilon_2)^2} \\
\sigma_{\text{min}} &= \frac{\varepsilon_1 + \varepsilon_3}{4A} + \frac{1}{4B} \sqrt{(\varepsilon_3 - \varepsilon_1)^2 + (\varepsilon_1 + \varepsilon_3 - 2\varepsilon_2)^2} \\
\tan 2\theta &= \frac{\varepsilon_1 - 2\varepsilon_2 + \varepsilon_3}{\varepsilon_1 - \varepsilon_3}
\end{align*}
\]

where:

\( \sigma_{\text{max}} \) = max principal stress, MPa

\( \sigma_{\text{min}} \) = min principal stress, MPa

\( \theta \) = principal angle from strain gauge 1, degree

Since the coefficients A and B for blind hole-drilling cannot be calculated directly from theoretical considerations, they must be obtained by empirical means, e.g. experimental calibration or numerical procedures such as finite-element analysis [77]. The procedure of determining calibration coefficient by interpolating nondimensional coefficient tables,
a sample of which is shown in Table 7, was proposed to save the calibration process [78].

The nondimensionized coefficients were defined in Equation 37 with respect to variables such as nondimensional hole depth, \( h = z / r_m \), nondimensional depth measured from surface, \( H = Z / r_m \), and the ratio of hole radius to strain gage radius [78]. The definitions of the hole depths, \( z \) and \( Z \), and the mean radius are shown in Figure 4-4.

\[
\frac{a}{1 + \nu} = \frac{2E}{A} \quad b = 2E \cdot B
\]  

**Figure 4-4.** Depths of layers of the drilled hole

<table>
<thead>
<tr>
<th>( h ) | ( H )</th>
<th>.00</th>
<th>.05</th>
<th>.10</th>
<th>.15</th>
<th>.20</th>
<th>.25</th>
</tr>
</thead>
<tbody>
<tr>
<td>.00</td>
<td>.0000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>.05</td>
<td>.0000</td>
<td>-0.0332</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>.10</td>
<td>.0000</td>
<td>-0.0466</td>
<td>-0.0811</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>.15</td>
<td>.0000</td>
<td>-0.0561</td>
<td>-0.1013</td>
<td>-0.1317</td>
<td></td>
<td></td>
</tr>
<tr>
<td>.20</td>
<td>.0000</td>
<td>-0.0622</td>
<td>-0.1147</td>
<td>-0.1522</td>
<td>-0.1747</td>
<td></td>
</tr>
<tr>
<td>.25</td>
<td>.0000</td>
<td>-0.0665</td>
<td>-0.1229</td>
<td>-0.1650</td>
<td>-0.1937</td>
<td>-0.2095</td>
</tr>
</tbody>
</table>

In this procedure, the calibration coefficient for a specific measurement can be interpolated or extrapolated using a quadratic triangular interpolation scheme [78]. For instance, with this scheme, the values at (\( h=0.05, \ H=0.05 \)), (0.10, 0.05), (0.10, 0.10), (0.15, 0.05), (0.15, 0.10), (0.15, 0.15) will be used when interpolating the coefficients for...
a case where $0.10 \leq h \leq 0.15$ and $0.05 \leq H \leq 0.10$. In such a case, this interpolation scheme gives pretty accurate data.

b) **Interferometric Strain/Slope Rosette hole-drilling/ring-core method**

A new optical method to measure strains and residual stresses was developed recently by Dr. Keyu Li at Oakland University. ISSR (Interferometric Strain/Slope Rosette) consists of three micro-indentations and has the configuration of delta or rectangular rosette [79]. A delta rosette, also called 60-deg ISSR, contains three six-faced indentations and the three indentations form an equilateral triangle. Under illumination by an incident laser beam, the six facets of each indentation in a delta rosette reflect and diffract the light in six directions which are at 60° apart from each other and the diffraction patterns from three indentations superpose in six directions. The motion of the fringes is related to the displacements among the indentations and hence to the strains and slopes. The strains and slopes are determined through tracing the shifts of fringe patterns.

The ISSR was combined with hole-drilling method [80] and ring-core cutting method [81] to measure residual stresses. The principles are similar to the resistance strain gauge hole-drilling method: residual stresses are relieved by removing some material of the sample and strain changes are measured and used to back calculate residuals stresses using some coefficients that are calibrated in advance. Figure 4-5 shows the relative positions of the ring-core center and the ISSR.
c) **X-ray, neutron diffraction and other methods**

X-ray and neutron diffraction methods attract a lot of attentions because they enable a nondestructive measurement of stresses. This is very useful when estimating the fatigue life of mechanical components. Compared with conventional techniques, X-ray and neutron diffraction methods enable local measurements and real-time analysis of stress [18].

When a monochromatic X-ray or a moving neutron beam irradiates a solid material, the beam is scattered by the atoms composing the material, as shown in Figure 4-6 [82]. Atoms are packed regularly intro a three-dimensional periodic lattice for a perfect crystalline material. When the X-ray or moving neutron beam incidences at a certain angle that meets the condition expressed in Equation 34, the intensities of scattered waves sum up into a constructive interference and the diffraction pattern can be observed. [18, 82]
where \( d \) is the spacing between the planes in the atomic lattice, \( n \) is an integer, \( \lambda \) is the wavelength of the X-rays or moving neutrons (or moving electrons or protons), and \( \theta \) is the angle between the incident X-ray or moving neutrons and the scattering planes [82, 83].

When an X-ray beam or moving neutron beam irradiates the surface of a crystalline material, the beam is scattered constructively only if the lattice planes orient and fulfill the Bragg’s law. There will be always some grains meet the diffraction condition, if the material is composed of many grains (crystallites) randomly oriented. If the grain size is big, fewer grains will be irradiated and therefore there will be fewer suitably oriented lattice planes fulfilling Bragg’s Law. In this case, the local crystal defect such as dislocations, vacancies, stacking faults will lead to a local fluctuation of the lattice spacing, resulting in a peak broadening [18]. This will reduce the accuracy of the X-ray and neutron diffraction methods.
4.4.2 Reasons for choosing hole-drilling relaxation method

X-ray diffraction method is getting more and more popular for its characteristics such as non-destructiveness and real time measurement. But resistance strain gauge hole-drilling method was mainly applied in this work to measure residual stresses in quenched aluminum alloy castings because the relative big grain size lead to fluctuations in X-ray measurement. Neutron diffraction method has the similar problem. In addition, resistance strain gauge hole-drilling method provides residual stress distribution at various depths easily and accurately. A few ISSR/ring-core and ISSR/hole-drilling residual stress measurements were also made.

Other methods such as layer remove method and sectioning method involve completely destructive processes of the samples, so the costs are high. Magnetic method and ultrasonic method are developed to measure residual stresses recently, but they have relative narrow application range and their accuracies are relatively low. For these reasons, these methods are not as popular as resistance strain gauge hole-drilling method and not chosen for residual stress measurement in this work.

4.4.3 Improvement on hole-drilling relaxation method [84]

As introduced in the section 4.4.1, in the case where $h=0.05$ and $H=0.05$, this interpolation scheme gives pretty accurate data, but it is not applicable for a case where $h = 0.13$ and $H = 0.13$ because it is not possible to find seven reference data in the tables due to their discontinuities. Linear triangular interpolation can be applied to such a case, but the interpolation results are poor. And note that if the $r_o / r_m$ is among 0.3, 0.4 and 0.5,
the interpolation errors are bigger because another interpolation must be done following this one. Introducing interpolation error not only lowers the accuracy of calculation of residual stress, but also leads to a higher possibility of yielding ill-conditioned matrix which will restrict the reliability of this technique considerably [85].

Neither interpolation nor extrapolation of calibration coefficients for integral method is reliable, when the drilling parameters in a real test are not close to nodes in the tables. More accurate residual stresses can be calculated if the errors of interpolation of calibration coefficients can be avoided, for instance, by determining the calibration coefficients directly from experiments or FEA for a specific measurement.

Therefore, an automatic routine coded in Python language [38] for finite element package ABAQUS [10] was developed based on the study of factors of element size, sample geometry dimensions, radius, offset and incline of the drilled hole, and material properties [84]. As shown in Figure 4-7, a technician conducts the residual stress measurement as usual and then inputs the relieved strains and measurement conditions to the Python routines, which call ABAQUS to generate a 3-D FE model based on user specified thickness, width and length, material properties, depth of cutting hole, loads, boundary conditions, etc. and run simulations automatically. The simulation results are fetched by Python code through ABAQUS API so that coefficients can be determined automatically. Therefore, residual stresses can be calculated based on relieved strains and the determined calibration coefficients by the Python code. In this procedure, the technician conducts the measurement as usual, simply inputs experimental conditions to the Python code and lets the automatic script do all the rest. He or she does not
necessarily know how to run Finite Element software like ABAQUS. The troubles of interpolating calibration coefficients are saved as well.

Figure 4-7. Automatic determination of calibration coefficients and residual stresses

A beam experiment demonstrates the application procedure of the new approach and shows that the Python routines do provide more accurate residual stress results than the conventional method of interpolating coefficient tables [84], as shown in Figure 4-8. With these routines, the calculation can be done automatically with great convenience and efficiency.
4.5 Comparisons of residual stresses between prediction and measurement

Residual stresses in aluminum alloy components after various quenching process were predicted by using the previously developed numerical models including thermal analysis and structural analysis. Comparisons of residual stresses in as-quenched components were made between prediction and measurement.
4.5.1 Water quenching of aluminum alloy frame-shape casting

The quenched components were first meshed with elements before any numerical simulations. Figure 4-9 shows the meshed aluminum alloy casting. The elements in measurement areas (dark areas in Figure 4-9) are 0.5 mm in size, the rest are 2 mm in size. There are total 432,714 second order tetrahedral elements and 611,088 nodes. Thermal analysis is first done to obtain the temperature history of each node, while the structural simulation is then conducted to predict the residual stress and distortion based on the temperature history of each node from the thermal analysis. In the ABAQUS structural model, no external forces or constrains are applied to the casting except for those eliminating free body movements so that the casting can deform freely during water quenching simulation.

Figure 4-9. The mesh scheme for the frame-shape casting
Simulation results at thick leg and thin leg are outputted for comparison with residual stress measurements. Figure 4-10 shows the predicted residual stresses at the measurement area on the thick leg. Table 8 tabulates the three nodes chosen at different depths in the measurement point and residual stresses in the YOZ plane.

![Figure 4-10. Residual stresses on thick leg](image)

**Table 8. Nodes on thick leg of the frame-shape casting**

<table>
<thead>
<tr>
<th>Node ID</th>
<th>x (mm)</th>
<th>y (mm)</th>
<th>z (mm)</th>
<th>σyy (MPa)</th>
<th>σyz (MPa)</th>
<th>σzz (MPa)</th>
<th>Depth from surface (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>534198</td>
<td>0.8041</td>
<td>99.571</td>
<td>12.217</td>
<td>-47.198</td>
<td>-0.16046</td>
<td>-69.067</td>
<td>0</td>
</tr>
<tr>
<td>498904</td>
<td>1.3015</td>
<td>99.571</td>
<td>12.468</td>
<td>-28.569</td>
<td>-0.01405</td>
<td>-43.775</td>
<td>0.5</td>
</tr>
<tr>
<td>497259</td>
<td>1.8063</td>
<td>99.896</td>
<td>12.656</td>
<td>-14.433</td>
<td>-0.07116</td>
<td>-25.342</td>
<td>1</td>
</tr>
</tbody>
</table>
Figure 4-11 shows the predicted residual stresses at the measurement area on the thin leg and Table 9 tabulates the three nodes chosen at different depths in the measurement point and residual stresses in the XOZ plane.

Table 9. Nodes on thin leg of the frame-shape casting

<table>
<thead>
<tr>
<th>Node ID</th>
<th>x (mm)</th>
<th>y (mm)</th>
<th>z (mm)</th>
<th>σxx (MPa)</th>
<th>σxz (MPa)</th>
<th>σzz (MPa)</th>
<th>Depth from surface (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>293411</td>
<td>86.4497</td>
<td>0.57418</td>
<td>12.5001</td>
<td>34.30</td>
<td>-1.52</td>
<td>-22.93</td>
<td>0</td>
</tr>
<tr>
<td>254109</td>
<td>86.3487</td>
<td>1.09666</td>
<td>12.5486</td>
<td>32.70</td>
<td>-1.32</td>
<td>-13.08</td>
<td>0.5</td>
</tr>
<tr>
<td>218700</td>
<td>86.4475</td>
<td>1.56043</td>
<td>12.4033</td>
<td>31.42</td>
<td>-1.02</td>
<td>-6.70</td>
<td>1</td>
</tr>
</tbody>
</table>

Figure 4-12 shows some aluminum alloy frame-shape castings with residual stress measurements on it using resistance strain gauge rosette hole-drilling method. The areas
with finer elements in the mesh scheme shown in Figure 4-9 are corresponding to the measurement areas.

Figure 4-12. Residual stress measurements on frame-shape castings

It is seen from Figures 4-13 and 4-14 that on the thick leg normal stresses are negative (compressed) in both Y and Z directions and the shear stresses are negligible compared to the normal stresses.
Figures 4-13 and 4-14 show that on the thin leg, normal stresses in Z direction are negative and those in X direction are positive (tensile).
Compressed residual stresses are usually expected at surfaces of quenched parts because inside of the part is cooled down later than the surface, causing a compressed effect on the surface and a tensile effect inside. In this frame-shape casting, the thin leg is cooled faster than the thick leg due to the volume difference. Thus, when the thick leg is cooled...
down to room temperature, the thin leg is already cooled down, producing a tensile effect on the thin legs.

Because of the geometric symmetry, the principle directions of residual stresses in the surface plane at the measurement areas are in the longitudinal and latitude directions. The residual stresses in the depth direction are very small due to the free surface effect. Averages and upper and lower bounds of the experimental measured residual stresses at these two locations were obtained and plotted in Figures 4-13 to 4-16 to evaluate numerical simulation accuracy.

As we can see in Figures 4-13 and 4-14, measured residual stresses in both Y and Z directions confirm the simulation, especially at depth from about 0.5mm to 1 mm. Small residual stresses were measured at the surface because the casting surface is not flat and must be filed to a smooth surface before mounting the resistance strain gauge rosette, during which some residual stresses near surface were relieved. Similar conclusions can be reached for the residual stresses at thin leg from Figures 4-15 and 4-16. It is also noted that the fluctuation of the measured residual stresses at thin leg are bigger than that at thick leg. This might result from the fact that the thickness of thin leg is very small and relative easy to deform during the transportation from quenching place to measurement place, etc.

More comparisons of residual stresses in the water-quenched aluminum alloy castings among measurements using resistance strain gauge hole-drilling method, ISSR/ring-core cutting method, X-ray diffraction method and neutron diffraction method were reported in the article [5].
4.5.2 Water quenching of aluminum alloy cylinder head

The approach and the models were also applied to the simulation of water quenching of an aluminum alloy cylinder head. Multiple thermocouples were imbedded to the cylinder head and experiments were conducted to obtain zone-based HTC distribution as introduced in section 2.6. The material constitutive model was also applied in the simulation. As shown in Figure 4-17, there are 1,089,515 tetrahedral elements and 1,757,074 nodes. The elements range from 5mm to 10 mm in size. The cylinder head was heated to an elevated temperature and then quenched in hot water. Cracking occurs during quenching at the location named ‘high stress area’ shown in Figure 4-18. In order to study the quenching effect and optimize the part design, finite element simulation was performed to predict residual stresses at the location near the high stress area. Residual stresses at the location were also measured as shown in Figure 4-19.

Figure 4-17. The meshed cylinder head
Figure 4-18. High residual stress predicted at the cracking area

Figure 4-19. Residual stress measurements on the cylinder head
Maximal principal stresses predicted by numerical simulation at location 1 and 2 are shown in Figure 4-20 and minimal ones are shown in Figure 4-21. It can be seen from Figures 4-18, 4-20 and 4-21 that the residual stresses at surface are most negative, except these areas are strongly constrained by structure where high tensile stresses are observed. Because it is of difficulty to have elements in about 0.5 mm for this huge part, the predicted residual stresses at the measured areas were compared to the average measured stresses over the depths. These average stresses are tabulated in Table 10. It is seen from the table that in general, the numerical predictions are very close to the measurements. Both the numerical prediction and measurement show high tensile stress at location 2, which is close to the cracking area (high stress area in Figure 4-18). Please note that the measured residual stresses are averaged over only a depth of about 0.5 mm, but the elements in the numerical model at the measurement areas are ranging from about 5 mm to 10 mm, which somehow averages the predicted stresses on the nodes at the surface. Because of that, the predicted stresses are in general lower than measurement in magnitude. Higher residual stresses are expected at the surface nodes if the elements are refined in size, however, in this simulation, the elements are not further refined because of the huge node volume.

Table 10. Comparison of residual stresses on cylinder head

<table>
<thead>
<tr>
<th>Note: approximated data were used.</th>
<th>Location 1</th>
<th>Location 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Max principal stress (MPa)</td>
<td>Min principal stress (MPa)</td>
</tr>
<tr>
<td>Simulation</td>
<td>-10</td>
<td>-30</td>
</tr>
<tr>
<td>Measurement</td>
<td>-20</td>
<td>-35</td>
</tr>
</tbody>
</table>
Figure 4-20. Maximal principal residual stresses in the cylinder head

Max principal residual stresses at location measurement 1 is about -20 MPa.

Max principal residual stress at measurement 2 is greater than 90 MPa.

Figure 4-21. Minimal principal residual stresses in the cylinder head

Minimal principal stress at measurement 2 is about -50 MPa.

Minimal principal stress at measurement 1 is about -35 MPa.
4.5.3 Air quenching of aluminum alloy frame-shape casting

The approach and the models were also applied in the simulation of air quenching of aluminum alloy frame shape castings. The quenched casting was first meshed in the same manner as in the case of water quenching of aluminum alloy frame-shape casting.

Residual stress simulation results are shown in Figure 4-22 and Figure 4-23. It is seen that the residual stresses in the air-quenched casting are in the order of 1 MPa. In particular, the residual stresses in the air-quenched aluminum casting are very uniform across the entire casting although slight compressive stresses on the surfaces and tensile stresses at the central sections are observed. At the thin leg, positive stresses were observed at the outside surface due to the bending effect of this frame, because the thick leg was cooled down to room temperature later than the thin leg. Thus the frame was bent when the thick leg was shrunken.

Figure 4-22. Distribution of simulated residual stresses (MPa) at cross section 1
Figure 4-23. Distribution of simulated residual stresses (MPa) at cross section 2

Figure 4-24. Residual stress measurements on air quenched frame castings
Predicted residual stresses of nodes at different depths at the two measurement areas (identical to the water quenching case) corresponding to the measurement areas as shown in Figure 4-24 are also outputted for comparison purpose.

Figure 4-25 compares the numerically predicted residual stresses near the surface of the thick wall of the air-quenched aluminum casting with the experimental measurements. In general, the predicted residual stresses are very small and uniform from the surface to inside. The measurement results are also small and uniform, although some oscillations present due to the difficulty of measuring small residual stresses. Both the measurement and simulation say the residual stresses increase from surface to inside, which agree with that negative stresses present at surface and positive stresses inside.

![Image](image.png)

a) Measured residual stresses  
b) Predicted residual stresses

Figure 4-25. Residual stresses at thick wall after air quenching

Figure 4-26 compares the numerically predicted residual stresses near the surface of the thin wall [7]. It is seen from both measurement and prediction that the residual stresses are increasing from surface to inside and the stresses in the X direction are positive due to the bending effect. It is noticed that the measured residual stresses are different from
simulations by 4-8 MPa. Considering the relatively high practical errors in measuring residual stresses, the simulation results are in good agreement with measurements.

Figure 4-26. Residual stresses at thin wall after air quenching

![Graph](image)

a) Measured residual stresses  

b) Simulated residual stresses

Figure 4-27 compares the measured residual stress distributions at the thick wall of the air-quenched aluminum casting with the ones measured at the same location of the water-quenched casting [5]. It is seen that the residual stresses in the air-quenched aluminum casting are less than 10 MPa, which are much smaller than those in the water-quenched casting. In the water-quenched aluminum casting, the absolute values of residual stresses vary from 40 MPa to 100 MPa. Small and uniform residual stresses in air-quenched castings are good to the fatigue life and distortion control.
4.5.4 Air quenching of aluminum alloy engine block

The mesh scheme used for the aluminum alloy engine block in the simulation is shown in Figure 4-28. The elements are about 5-8 mm in size. There are 595,034 elements. Please note that the blue part of the elements is for liners that are made of cast iron, and the yellow part is for the engine block made of aluminum alloy 319. The cast iron liners were put in their positions when the engine block was casted, so a very firm contact is between the liners and the block, which is simulated using a tie contact conditions in the modeling. No slip will occur during the quenching process.
Residual stresses produced in the quenching process are plotted in Figure 4-29. It can be seen that the Von Mises stresses are smaller than 40 MPa in the most area of the block except the cylinder area where the stresses are as high as 120 MPa for aluminum alloy casting and 300 MPa for cast iron liners. The reason why the residual stresses in cast iron are much higher than aluminum alloy is that former material poses a higher yielding stress than the latter.
In this project, we are more interested in the stresses in the aluminum alloy castings. In order to compare the numerically predicted stresses to measurement results, simulation results in the measurement area are outputted. The measurement area is presented by the four elements shown in Figure 4-30.

Because of the coarse elements used in this simulation, simulation results at the center of the two cylinders are unable to be obtained directly from a node in the middle. Results at the integration points of these 4 elements are outputted and averaged instead. These results are tabulated in Table 11.
Table 11. Simulation results in the measurement area

<table>
<thead>
<tr>
<th>element #</th>
<th>S11 (Mpa)</th>
<th>S22 (Mpa)</th>
<th>S33 (Mpa)</th>
<th>S12 (Mpa)</th>
<th>S13 (Mpa)</th>
<th>S23 (Mpa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>330538</td>
<td>-61.51</td>
<td>61.92</td>
<td>57.48</td>
<td>-0.50</td>
<td>-0.14</td>
<td>6.99</td>
</tr>
<tr>
<td>543813</td>
<td>-47.26</td>
<td>72.75</td>
<td>73.61</td>
<td>-2.30</td>
<td>2.60</td>
<td>6.24</td>
</tr>
<tr>
<td>222419</td>
<td>-48.34</td>
<td>71.88</td>
<td>72.58</td>
<td>1.71</td>
<td>-1.17</td>
<td>6.78</td>
</tr>
<tr>
<td>132819</td>
<td>-52.13</td>
<td>66.92</td>
<td>71.00</td>
<td>0.49</td>
<td>0.43</td>
<td>7.24</td>
</tr>
<tr>
<td>Average</td>
<td>-52.31</td>
<td>68.37</td>
<td>68.67</td>
<td>-0.15</td>
<td>0.43</td>
<td>6.81</td>
</tr>
</tbody>
</table>

Because residual stress measurements only measure the stresses on the surface which are about in the direction of 45 degree to both Y axis and Z axis in the YZ plane, the predicted results must be transformed to this direction so that comparison between simulation and measurement can be made. A diagram of status of stress in the measurement area is plotted in Figure 4-31. The normal stress in the red arrow direction...
is calculated using the transformation equation expressed in Equation 39. The positive residual stress stands that that area is being tensioned.

\[
\sigma_{45} = \sigma_{zz} \cos^2 \theta + \sigma_{yy} \sin^2 \theta + 2\tau \sin \theta \cos \theta
\]

\[
\sigma_{45} = 75.33\text{MPa}
\]

where:

\(\sigma_{zz}\) = stress in Z direction, 68.67 MPa

\(\sigma_{yy}\) = stress in Y direction, 68.37 MPa

\(\tau\) = shear stress, -6.81 MPa

\(\theta\) = transform angle, 45°

Section cutting method was applied to the measurement of residual stresses on the engine bock. This method involves the procedure of mounting strain gage, cutting the object to
pieces and recording strains relived during the cutting. This method is a destructive method, after which the work piece cannot be used any more.

A strain gage was mounted onto the surface of area, shown in Figure 4-32, and then the engine block was cut into small pieces, so that the residuals stresses at the measurement area can be fully released. The strains relieved during this process are recorded and used to calculate residual stress. Since all the strains relieved are caused by the full release of residual stresses, the residual stresses can be calculated from the relived strains by using Hooke’s law.

Figure 4-32. A strain gage is mounted onto the surface of engine block [86]

The results of the measurements on 5.3 liter engine block are provide by GM R&D technical center [86] and tabulated in Table 12. The measured residual stresses vary from
68.6 MPa to 124.25 MPa, with an average of 90.6 MPa and standard deviation of 17.8 MPa.

Table 12. Residual stress measurements on the 5.3 liter engine block [86]

<table>
<thead>
<tr>
<th>Serial #</th>
<th>Date</th>
<th>Operator</th>
<th>Residual stress (Mpa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4362-1</td>
<td>October, 2004</td>
<td>Mary Cawford</td>
<td>92.29</td>
</tr>
<tr>
<td>4362-2</td>
<td>October, 2004</td>
<td>Mary Cawford</td>
<td>73.66</td>
</tr>
<tr>
<td>4358-1</td>
<td>October, 2004</td>
<td>Mary Cawford</td>
<td>96.66</td>
</tr>
<tr>
<td>4358-2</td>
<td>October, 2004</td>
<td>Mary Cawford</td>
<td>82.39</td>
</tr>
<tr>
<td>4265-1</td>
<td>October, 2004</td>
<td>Mary Cawford</td>
<td>92.58</td>
</tr>
<tr>
<td>4265-2</td>
<td>October, 2004</td>
<td>Mary Cawford</td>
<td>85.20</td>
</tr>
<tr>
<td>3743</td>
<td>January, 2006</td>
<td>Mary Cawford</td>
<td>75.60</td>
</tr>
<tr>
<td>3795</td>
<td>January, 2006</td>
<td>Mary Cawford</td>
<td>68.60</td>
</tr>
<tr>
<td>PS168/J057</td>
<td>January, 2006</td>
<td>Mary Cawford</td>
<td>114.73</td>
</tr>
<tr>
<td>PS168/J046</td>
<td>January, 2006</td>
<td>Mary Cawford</td>
<td>124.25</td>
</tr>
<tr>
<td>Max</td>
<td>124.25</td>
<td>Average:</td>
<td>90.60</td>
</tr>
<tr>
<td>Min</td>
<td>68.60</td>
<td>deviation</td>
<td>17.80</td>
</tr>
</tbody>
</table>

Simulation results show that the stress in the measurement direction is about 75.33 MPa, which is in the range of measurement. The simulation result is lower than the average of measurement results, because of two facts. First of all, the element size in the simulation is a little too big; as it is seen from Figure 4-30 that there is only one element between two cylinders. In this case, the two cylinders are bonded to cast iron liners and high residual stresses are expected in this area because of the big differences between cast iron and aluminum alloy properties. It is expected that the stresses in cast iron and aluminum alloy will go opposite. Too coarse elements average the simulation results. Second of all, the residual stresses in this area are very high, close to yielding stress. It is very likely that plastic deformation occurs during section cutting, as a result of which, the relieved strains measured are greater than the pure elastic strains, which is supposed to be used for
the calculation of residual stresses. In the case of plastic deformation, application of Hooke’s law will introduce some errors and bigger residual stresses will be calculated.

4.6 Summary

In this chapter, numerical models were created and successfully predicted residual stresses in a few quenching cases: water quenching of an aluminum alloy frame-shape casting, water quenching of an aluminum alloy cylinder head, air quenching of an aluminum alloy frame-shape casting and air quenching of an aluminum alloy engine block. In the numerical modeling, accurate HTC distribution data discussed in chapter 2 and material constitutive models discussed in chapter 3 were applied.

This chapter also reviews a few popular methods for measuring residual stresses. The resistance strain gauge rosette hole-drilling method was introduced in detail and some work was conducted to improve the accuracy of this method. This method was applied to measure residual stresses in as-quenched components. The measurements were compared to other measurements using X-ray diffraction, neutron diffraction [5] and sectioning methods.

Comparisons of residual stresses between simulation prediction and experimental measurements were made in this chapter. Good agreements between simulation predictions and experimental measurements validate the numerical models. In addition, successful prediction of some quenching problems like cracking observed from production further validate these numerical models and the simulation procedure, which can be used to help optimize part design and production condition.
5 Numerical comparisons between gas and liquid quenching

This chapter applies the numerical modeling technologies to high pressure hydrogen quenching of steel components. A distortion study is also included in this chapter.

5.1 Introduction

Distortion can be defined as an irreversible dimensional change in the component during processing from temperature variations and loading in service, and from heat treatment. The term dimensional change is used to denote changes in both shape and size. The heat treatment distortion is used by engineers to describe a movement that has occurred in a component in heat treating process [42]. Reversible changes refer to a change of shape or size in elastic field due to external stress or temperature variation. On the other hand, irreversible changes in size and shape of a component are those involving plastic deformation.

Distortion in heat treatment operations can be classified into size distortion and shape distortion or warpage. Size distortion is the net change in specific volume, where phase transformation plays an important role. Shape distortion or warpage is a change in geometrical form or shape [42, 87].

Both size distortion and shape distortion or warpage occur during heat treatment processes. Usually there is a conflict between distortion control and quenching severity. On one hand, in order to have better quenching results, the cooling rates are very high.
On the other hand, very high cooling rates lead to high distortion. Distortion may also occur after heat treating in the relief of residual stresses.

Very high distortion in a component will lead to a requirement of extra machining processes after heat treatment, or even cracking and malfunction. Therefore, it is highly important to optimize part design and production parameters in heat treating processes to minimize distortion. In this work, the study of minimizing distortion was studied by using numerical modeling.

5.2 High pressure hydrogen quenching of steel parts

The previous section 2.3 shows that HTC will increase when the gas velocity and pressure are increased. This section demonstrates how to calculate the equivalent HTC for a given oil HTC curve and inversely determine the quenching conditions for HPHQ. A distortion analysis is also studied in this section.

5.2.1 Hardenability analysis

This section numerically studies hardenability of steel 4140 and demonstrates how to determine quenching conditions for HPHQ in order to have similar quenching results as a typical oil quenching [88, 89].

Figure 5-1 shows an HTC curve for popularly used hot oil [21]. The mean of this curve is calculated as 1995 \( \text{W/m}^2\ \text{°C} \) and plotted as “mean HPHQ” in the figure. The maximal value (5000 \( \text{W/m}^2\ \text{°C} \)) of this HTC curve is chosen as “max HPHQ” for comparison. These three HTC data are used in the followed finite element simulations to see the
hardenabilities. “Mean HPHQ” and “Max HPHQ” in this article are treated as two quenchants like oil.

![Figure 5-1. A typical oil HTC curve and its mean HTC](image)

In this finite element simulation, a section of an infinite long cylinder shown in Figure 5-2 is picked and meshed to analyze the cooling results from surface to the center of the cylinder. The elements are 0.5mm in size, which is fine enough to catch the variation of microstructure. The cylinder is made of 4140 steel with an initial microstructure of 50% of pearlite and 50% of ferrite. The cylinder is first heated in hot furnace at 850°C for 1800 seconds for fully austenizing and cooled down in typical hot oil, “max HPHQ” and “mean HPHQ”. The heating and cooling simulations were performed using finite element
package ABAQUS [10] in conjunction with DANTE [21]. DANTE is a set of user subroutines developed for ABAQUS to govern phase transformation and material constitutive behavior during heat treatment.

A series of simulations with cylinders varying from 25.4 mm (1 inch) to 76.2 mm (3 inch) in diameter are conducted to compare the cooling capacities of the 3 quenchants and find out their critical diameters. The critical diameter was first introduced by Grossmann and was defined as the largest bar diameter that contains 50% martensite at the center after being quenched in a given quenching media [23, 90]. Please be aware that the term critical diameters is different from the term ideal critical diameters, which refers to the largest bar diameter that contains 50% martensite at the center after being given an “infinite” or “ideal” quench. The ideal quench is one that lowers the surface temperature of an austenized steel to the bath temperature instantaneously and therefore ideal critical diameter is a property of a steel other than a quenchant [23].

Some of the simulation results are illustrated in Figures 5-3, 5-4 and 5-5. Figure 5-3(a) plots the cooling curves at surface and center of the 25.4 mm diameter cylinder in a CCT diagram of 4140 from Climax Molybdenum Company [49]. It is seen from Figure 5-3(a)
that the cooling curves do not enter to the bainite transformation zone that much and as a result, the cylinder is through hardened with high fraction of martensite from surface to center as shown in Figure 5-3(b). From both Figure 5-3(a) and 5-3(b), it is seen that “mean HPHQ” can cool down the cylinder as fast as oil quenching.

(a) Cooling curves in CCT diagram  
(b) Variation of martensite

Figure 5.3. Simulation results for 25.4 mm (1 inch) diameter cylinder

Figure 5-4(a) plots the cooling curves at surface and center of the 50.8 mm diameter cylinder in the CCT diagram of 4140. It is seen from Figure 5-4(a) that the cooling curves enter the bainite transformation zone and as a result, high fraction of bainite and less martensite are produced, especially at center as shown in Figure 5-4(b). From both Figure 5-4(a) and Figure 5-4(b), it is seen that “mean HPHQ” can cool down the cylinder as fast as oil quenching.
(a) Cooling curves in CCT diagram

(b) Variation of martensite

Figure 5-4. Simulation results for 50.8 mm (2 inch) diameter cylinder

(a) Cooling curves in CCT diagram

(b) Phase composition of cylinder quenched in oil

(c) Variation of martensite

(d) Variation of hardness

Figure 5-5. Simulation results for 76.2 mm (3 inch) diameter cylinder
Figure 5-5(a) plots the cooling curves at surface and center of the 76.2 mm diameter cylinder in the CCT diagram of 4140. From Figure 5-5(a), it is seen that the cooling curves at surface do not enter the bainite transformation zone that much and as a result, high fraction of martensite is produced at surface, but the cooling curves at center enter the bainite transformation zone and less martensite is produced at center as shown in Figure 5-5(b). Figure 5-5(c) and 5-5(d) show that variation of martensite fraction and hardness from surface to center of the cylinder. From these figures, it is seen that “mean HPHQ” can cool down the cylinder as fast as oil quenching. Please note that magnitude of the hardness might be different from experiments due to the accuracy of coefficients for this steel in the phase transformation model in DANTE, but the relative difference is reasonable [21].

It is seen that martensite fraction at center of the 50.8 mm diameter cylinder is higher than 50% from Figure 5-6 and martensite fraction at center the 76.2 mm diameter cylinder is less than 50% from Figure 5-6, therefore the critical diameters of this steel in these 3 quenchants should be between 50.8 mm and 76.2 mm. Simulations of cooling down a 56 mm (2.2 inch) diameter cylinder were performed. Figure 5-6 shows the variation of the volume fraction of martensite at center of the cylinder with respect to cylinder diameter. It can be seen that “mean HPHQ” can quench deeper than this typical oil.
From the above analysis, it is seen that HPHQ with the mean of an HTC curve of a sort of oil can produce similar results as the oil quenching. The mean HTC is 1995 $W/m^2\cdot^\circ C$ for this typical hot oil.

It is more important to find out the quenching condition (gas pressure and velocity) of HPHQ to generate such a mean HTC. The conditions to generate such a mean HTC are inversely determined from Equation 11. From the definition, Prandtl number is a constant for a given gas and Nusselt number is a constant if HTC is fixed (as 1995 $W/m^2\cdot^\circ C$ in this case), therefore the gas pressure (density) and velocity can be determined by solving the non-linear equation of Reynolds number. Newton iteration method is applied to solve this non-linear equation and therefore the quenching conditions for HPHQ are determined and plotted in Figure 5-7. HPHQ at 20 bar and 20 m/s will meet the requirement. The counterpoints for helium and nitrogen are also determined and plotted in Figure 5-7. It is
seen that hydrogen requires lower pressure or velocity than helium and nitrogen to generate the mean HTC.

![Conditions for given HTC =1950 ( W/m²K )](image)

Figure 5-7. Conditions of HPHQ for the equivalent HTC

5.2.2 Distortion Analysis

Since HTC around a work piece is not uniform and HTC distributions for different orientations are different, it is worthy to study the differences of distortion for different HTC distributions and find out the optimal part orientation when the distortion of a target portion of a part is minimized. This section studies the effect of HTC distribution on distortion of a ring shown in Figure 5-8 and compares the distortion of the inner circle when quenched at different orientations shown in Figure 5-9 [89, 91]. The ring is made of 4140 steel.
In this work, CFD simulations were conducted to obtain hydrogen flow and HTC distribution. Figure 5-9 shows a half ring in the middle of the gas domain since this is a symmetric problem. The environment pressure is set as 15 bar and inlet gas velocity is set as 21 m/s. The inlet hydrogen temperature is 25 °C and the initial ring temperature is 850°C. K-epsilon turbulence model is applied in the CFD simulation. The HTC distribution from CFD simulation ranges from about 900 to 2500 W/m²°C, as illustrated in Figure 5-11. In gas quenching, the HTC data for front faces are usually smaller than
other faces because the local gas velocities near front faces are usually very small or even zero at some locations. The average HTC in this case is about $1950\, W/m^2\, ^\circ C$.

![Diagram showing CFD modeling for distributed HTC]

**Figure 5-10.** CFD modeling for distributed HTC

![Diagram showing HTC distribution for 0 degree gas flow]

**Figure 5-11.** HTC distribution for 0 degree gas flow

The node-based HTC distributions obtained from CFD simulations are mapped to finite element models. Because the distortion of the inner circle is studied, one point of the inner circle is fixed to remove free body movement as shown in Figure 5-12. In this case, the distortion or the shape of the inner circle after quenching can be compared easier. In the finite element simulations using ABAQUS [10], DANTE [21] is applied to model
phase transformation and material constitutive behavior of steel 4140 in the quenching process. In the ABAQUS models, there are 4305 nodes and 3360 elements. The elements are about 3 mm in size.

Figure 5-12. Finite element modeling

Figure 5-13 shows the distortion of the ring after quenching at two different orientations with a scale factor of 100. It shows clearly that distortion at different orientations is different. In other words, the HTC distribution plays a very big important role in generating distortion.

(a) Distortion of the ring for 0 degree flow
The shapes of the inner circle after quenching at different orientations were calculated by adding scaled displacements in the circle plane of nodes of the path (red line in Figure 5-12) by 100 times to the original shape and plotted in Figure 5-14. The solid blue line was the original shape and other shapes after quenching were scaled up 100 times for a clearer view. The out of roundness values of the inner circle were also calculated approximately and illustrated in Figure 5-15. In the approximate calculation, the displacement in the circle plane of each node of the path was treated as the change of radius. The change of radius was assigned positive or negative symbol according to the displacement direction. The out of roundness was determined as the difference between maximum and minimum changes of radius. The figures show clearly that the distortion for each orientation is different and implies that:

(a) For a specific portion of a part, uniform-in-space HTC data do not necessarily produce the best results. In this case, the shapes using uniform-in-space HTC labeled as h2_avg and oil is even worse than the shapes at 0 degree and 90 degree.
(b) For this ring, 0, 30 and 90 degree flows generate the lowest distortion of the inner circle. It should be chosen for production if the distortion of the inner circle must be minimized.

(c) It should be noted that 0, 30 and 90 degree flows might not produce the best results for other portion of the part. The best orientation may be determined after comparing distortions of all critical portions of the part.

Figure 5-14. Comparison of scaled shapes of inner circle

Figure 5-15. Approximation of out of roundness of the inner circle
5.3 Summary

In this work, a few numerical simulations of high pressure hydrogen quenching of steel components using finite element package ABAQUS and a user subroutine set DANTE were conducted. A hardenability analysis of a steel rod was conducted to compare the quenching severity of HPHQ and oil quenching from the points of view of microstructure and hardness. This analysis indicates that HPHQ with an HTC value at the mean level of the HTC curve for a typical oil quenching can produce similar microstructure as the oil quenching. A study was also made on the HTC distribution effect on distortion of a steel ring. This study shows that distortions of the same component at different quenching orientation are different and implies that distortion can be minimized by choosing a proper orientation. It is also illustrated that distortion of the component is lower than oil quenching when similar microstructure is produced in the two quenching processes.
6 Conclusion and potential applications in other areas

This chapter concludes the numerical modeling and experimental investigation of various quenching processes and points out the potential application of the numerical models developed in this work.

6.1 Conclusions

In this work, the problems and challenges in numerical modeling of gas and liquid quenching processes were analyzed and models were developed to solve the key issues in the numerical simulations.

1. In the heat transfer modeling chapter, four existing methods to determine thermal boundary condition, HTC distribution, for solid components in quenchant flow were analyzed and applied in gas and liquid quenching processes. These methods include empirical equation method, lumped heat capacity method, CFD simulation method and iterative modification method. Two new methods were developed to determine the HTC distribution at high accuracy and low cost. The first developed method, called semi-empirical equation method, was established based on experimental investigation. At the end, another new method, integrating CFD simulation method, iterative modification method and semi-empirical equation method together, was developed to determine node-based HTC distributions for complicated components at very high accuracy. A US patent was filled for this new method with General Motors Company. A valuable HTC database for air quenching and water quenching was also built and validated.
2. In the material property evolution modeling chapter, material property evolution of steel and aluminum alloy parts were addressed. The variations of their constitutive behaviors lead to the need of development of user material constitutive subroutines in finite element simulations. The commercially available user material subroutine set, DANTE, was applied with finite element package ABAQUS for simulation of quenching of steel components. The material property evolution of aluminum alloy castings during quenching was also analyzed and a user material constitutive subroutine was developed based on a particular constitutive model that governs the stress-strain behavior during quenching. An extended framework was also proposed in this work to account for the possible aging effect during quenching and to simulate the aging process.

3. In the residual stress prediction and measurement chapter, residual stresses in quenched aluminum alloy and steel components were predicted by applying the heat transfer and material constitutive models, and compared to experimental measurements using mainly resistance strain gauge rosette hole-drilling method. Improvement for this measurement method was proposed for higher accuracy and validated by experimental investigation. Residual stresses were predicted in the quenching cases: water quenching of an aluminum alloy frame-shape casting, water quenching of an aluminum alloy cylinder head, air quenching of an aluminum alloy frame-shape casting and air quenching of an aluminum alloy engine block. Good agreements of residual stresses in the quenched components between predictions and experimental measurements validate the numerical simulation procedure and the numerical models developed in this work.

4. In the numerical comparisons between gas and liquid quenching chapter, a hardenability analysis and a distortion study were conducted for high pressure hydrogen
quenching and typical oil quenching of steel components. The hardenability study shows that high pressure hydrogen quenching with HTC data at the mean level of an HTC curve of oil quenching will produce similar microstructure (martensite volume fraction, etc.) and hardness to what the oil quenching produces. The distortion study indicates that distortion of a steel component in high pressure hydrogen quenching is lower than that in oil quenching when similar microstructures are produced. This study also shows distortions at different quenching orientations are different, which implies that distortion can be minimized by choosing a proper quenching orientation.

6.2 Potential applications in other areas

In this work, the numerical models were developed and applied for quenching processes, but they can also be applied in other situations where temperature, stress and distortion are involved.

A. The numerical models can be applied in other heat treating processes such as annealing, tempering, aging, etc.

For instance, in the steel tempering process, the methods developed in this work to determine HTC distribution for any part can be applied to predict temperature-time profile. The material property evolution model for steel can be applied to govern the phase transformation and constitutive behavior, which in conjunction with finite element package can predict the generation of distortion, stress and strain.

B. The numerical models can be applied in other manufacturing processes such as welding, casting, etc.
For instance, in the welding process, the parts are heated up and then cooled down. The heat transfer modeling and material property evolution modeling can be applied to predict the temperature profile, phase transformation, stress profile, etc.

C. The numerical models can be applied in other industries such as new energy industry, semi-conductor industry, etc.

For instance, in the new energy industry, solar panels and their mounting systems experience temperature variation during usage due to the air temperature change in seasons and the heat from sun. As a result, thermal expansion introduces reliability and deformation problems. The models developed in this work governing thermal and material behavior can be applied in such situations.

Applying the models to the thermal management of electronic systems such as laptop is another example. In this case, the design of the cooling system (fan speed, configuration, etc) strongly depends on heat transfer coefficient, which is well addressed and can be determined with the models in this work.
7 References


