COMPUTER SIMULATION OF THE THERMAL-MECHANICS OF STEEL QUENCHING

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ABSTRACT

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Thermal stresses and associated component distortion remains one of the major problems that perplex heat treaters. It may become more significant when dealing with quenching processes, a dominant method of hardening materials in heat treatment. Excessive distortion or even fracture is one of the biggest problems associated with quenching processes, which not only increases the cost of the production but may also directly impair the quality of the heat treated components. Past work focusing on steel quenching has been experimental in nature with emphasis on experimental tests, material selection, cycle design, quenchant selection and quenching equipment design. This traditional methodology has some limitations including significant expense and difficulty of extending accumulated experience to applications other than those from which the data was derived. Mathematical modeling and computer simulation has developed rapidly in recent history, especially with the evolution of high-speed digital computers. Thanks to the rapid development of various numerical analysis software and the speed of computer hardware, large scale and sophisticated models can now be analyzed routinely. Nevertheless, difficulties still exist which stem from uncertainties in the theories and processes, limited availability of representative physical and mechanical property data, complexities of boundary conditions and excessive cost and time required for modeling procedures.

Mathematical modeling and computer simulation forms a virtual laboratory platform for quenching analysis. Important issues on process modeling in quenching practice, including the quenching model and its implementation will be discussed and presented. Work in this study focused on liquid quenching involving oil, polymer and water quenching. The challenges and limitations of process modeling of steel quenching will be discussed from both theoretical and practical perspectives. Standardized methodology of studying heat transfer behavior between the quenchant and quenched component, specifically, the quenching probe, were studied, especially the method involving lumped capacitance analysis for deriving heat transfer coefficients. Α numerical validation procedure was proposed and implemented. Limitations of the standard lumped capacitance model were analyzed quantitatively. A modified lumped capacitance method was developed and implemented in a numerical analysis procedure and validated against experimentally derived results. Significant improvement was achieved especially for low-to-moderate sensitivity quenching probes.

A weakly coupled numerical modeling procedure was proposed to predict the effectiveness of a new quenching cycle for a practical application. Temperature fields of the quenching process were simulated and results were in good agreement with those derived experimentally. Phase transformation products and residual stresses were predicted and their implications discussed with respect to the quenching conditions. The validity of the quenching cycle was examined critically and deemed acceptable with the aid of computer simulations and predictions. The role of the computer in process modeling was examined and discussed. Two application tools for facilitating heat treatment process modeling practice were developed and tested against well-established experimental standards. Development and use of relational database and object-oriented database procedures in process modeling practice was explored. The objective of incorporating database applications in this study was to initiate an efficient and systematic method for modeling practice so that process related data and results could be stored and/or retrieved efficiently.

CHAPTER 1

RESEARCH BACKGROUND AND LITERATURE REVIEW

The significance of computer simulation of practical problems such as heat treating is quite far reaching. The benefits of this are directly implicit in production qualities and costs. With simplification, a real world problem is mapped into a mini world - a model, which can be solved with the assistance of mathematics, numerical methods and computer simulation. As a result, sophisticated modeling and simulation could turn to be a powerful "virtual laboratory", where real world problems can be studied, valuable "experiments" such as cycle prediction, optimization and validation can be carried out. In specific terms, as presented in this dissertation, it may be used as a design tool to study the quenching processes. Valuable information and suggestions could be drawn from the simulations with the goal of producing components with little or no post production distortion.

1.1 Introduction

Quenching is the major method used to harden components in heat treatment.^[1] It is a process of rapid cooling of metal components from the austenization or solution treating temperature range from 780°C for low carbon steels to as high as 1250°C for high alloy tool steels. The purpose of quenching processes, for most carbon, low alloy and tool steels, is to produce desired amounts of martensite, a high strength phase, in the microstructure. Other purposes of quenching also include minimizing the presence of grain boundary carbides, improving the ferrite distribution, or acting as the pre-treatment for solution hardening.

Controlling the volumetric fraction of desired phases such as bainite or mostly martensite, morphology of the microstructure, and distortion of the components, is the ultimate goal of the heat treaters in quenching practice. However, the target is rather hard to achieve, due to the complexity of the process and the mechanisms of heat transfer, mechanics and microstructural evolution associated with the process. Various approaches at different levels of emphasis have been carried out, including quenchants, equipment design, quenching cycle optimization and even the selection of materials of the quenched components.^[2] In the past, residual stresses and distortions were studied principally on an experimental basis. The experimental approaches require considerable time, cost and labor. Furthermore it is difficult to extend the results to predict the effects caused by changes in constituent materials, dimensions, cooling rate, etc. This stems from the nature of complexity of the problem, high cost and even the uncertainties of the process itself.

Computerized prediction and technology planning have become increasingly popular in the past decade.^[3-15] Modeling and simulation forms a virtual experimental platform or a virtual laboratory, which is so versatile that many unknowns or results of the quenching process can be predicted and tested in advance of final part production.^[11,16-29] It has the potential to overcome the limitation of physical experiments so that the study of the quenching process could be carried out more efficiently.

1.1.1 Characteristics of Quenching Processes

Varieties of quenching techniques have been introduced in order to have some control over the cooling rate and the heat transfer from the surface of the component being quenched. In view of quenching cycle itself, the major techniques are categorized as follows:^[2]

- *Direct quenching* quenches components directly from austenization temperature. This is the most commonly used in quenching practice.
- *Time quenching* has abrupt change of cooling rate in the cycle, which may use multiple quenchants in different stages of the quenching process. The objective of this technique is to have significant control of the cooling rate during the process so that desired results can be achieved. The design of such a process is based mostly on the transformation curves, such as time-temperature-transformation (TTT) or continuous-cooling-transformation (CCT).
- Selective quenching uses non-uniform quenching of a component, for example, quenching of only certain regions of the part so as to achieve a significant difference in the range of properties of the quenched component.
- Spray quenching scatters a high-pressure steam of quenchant onto the surface of the component, usually on the desired portion only. Generally a very rapid cooling rate can be achieved because of the efficient removal of heat by the high intensity quenchant droplets sprayed onto the surface of the component.
- Interrupted quenching rapidly cools components from austenization temperature to a point before martensitic transformation takes place, i.e. above the *Ms* temperature. The components are held at that temperature for a specific period of time, followed by cooling, mostly in air. Three typical processes belong to this category: austempering, marquenching and isothermal quenching. The distinction between the processes lies in their behavior at the holding temperature. In a broader sense, interrupted quenching may also refer to those processes using more than one holding temperature so as to reduce the risk of excessive distortion, cracking or even fracture.

The quenching medium is one of the most critical factors in quenching practice.^[30-34] One quenchant may behave considerably differently from another due to its chemistry. Consequently the chemistry and associated heat transfer mechanism of quenchants have drawn wide and intensive attention from chemists and heat treaters. The

commonly used quenching media include oil, water, polymer solution, gases (air, nitrogen, helium, etc.), fluidized bed, etc. Liquid quenchants form the core interest of the work presented in this dissertation, and are discussed in much detail as follows:

Liquid quenchants, for example water, oil or polymer solution, are most widely used in quenching practice. Cooling curve analysis, commonly carried out by a quenching probe, becomes increasingly popular and perhaps the most informative method of characterizing a quenching medium.^[33,35-41] Generally, three stages of heat removal are associated with the cooling process in a liquid quenchant, namely vapor blanket cooling, nucleate boiling and liquid cooling stage,^[2,42] as illustrated in Figures 1.1.

The first stage is characterized by a blanket of vapor formed uniformly around the surface of the component. The vapor blanket takes place in the early stage of the cooling process, due to the heat supply from the interior of the component to the surface exceeding the amount of heat needed to vaporize the quenchant and maintain the vapor phase. This vapor film serves as an insulator and significantly reduces the cooling rate in this stage. The significance of this phenomenon leads to the definition of a characteristic temperature above which the vapor blanket is fully maintained. Past studies have revealed that the characteristic temperature of the quenchant is independent of the initial temperature of the component quenched.^[2] However, it shows significant dependence on the chemistry of the quenchant as well as the degree of agitation of the quenchant. The vapor blanket stage is usually not present in aqueous solutions containing more that 5 weight percent ionic material, such as potassium chloride, lithium chloride, sodium hydroxide or sulfuric acid. It does not exist in nonvolatile quenchants at all, such as molten salt baths.

The second stage, nucleate boiling involves the highest cooling rates of the whole cooling process. When the heat supply from the interior of the component can not maintain the vapor blanket, the vapor film collapses and a tremendous amount of heat is removed from the component by nucleate boiling of the quenchant on the surface of the component.

The liquid cooling stage starts when the surface temperature of the component is lower than the boiling point of the quenching liquid. During this stage cooling takes place by conduction and convection into the quenchant. The cooling rates in this stage are dependent on viscosity, agitation and temperature of the quenchant.

1.1.2 Thermal Stress and Distortion during Quenching Processes

Stress and strain generated inside components is an inevitable phenomenon associated with a quenching process. Distortion and cracking during quenching limits the maximum applicable cooling rates to a specific quenched component. Some practical and experimental evidence of such phenomena has been well documented.^[2]

Distortion results from warping, thermally induced deformation and phase transformations taking placed during the cooling process. Warping and thermally induced deformation are caused by temperature differences at the different locations of the component. More specifically, warping refers to the result of non-uniform heating or cooling whereas thermally induced deformation refers to the outcome of thermal gradients.

Phase transformation, such as martensitic transformation, is another major source of deformation. Volumetric change occurs during phase transformation due to the difference between the density of original and the new phases. In addition, the phase transformation induces an abnormal plastic behavior, named transformation plasticity, which causes plastic flow during the phase transformation process, even when stresses were still below yield point. This phenomenon is explained as follows:^[43-47]

- The strength of the materials is temporarily lost during the transformation, resulted from the movement of atoms from the original lattice to those required by the new lattice.
- Local yielding occurs at certain points where stress caused by both load and transformation exceeds the yield stress of the material.
- Shape change may result from the slip at interfaces between the phases.
- Preferred orientation of the resultant phase creates an extremely high strain in certain directions relative to the direction of the applied stress.

• The volume changes produced by the transformation causes the creation of point defects that accelerate the creep rate.

Besides quenchants and cycle parameters of the quenching cycle, distortion is also greatly influenced by the material itself, the size and the shape of the component. Physical and mechanical properties of the material can cause significant differences in the thermal history and the associated mechanical response of the quenched component. Large size or high section size ratio of the component generally increases the susceptibility to distortion or cracking. Complex shapes may lead to non-uniform cooling and generates high stress. For example, the presence of slots, keyholes, blind holes, through thickness holes, grooves or notches in the component result in non-uniform cooling and moreover, they could be the initiation of cracking due to the significant stress concentration associated with them.

The objective of this research study was to establish feasible models for thermal stresses and strains generated in typical quenching processes, simulate and predict the final distortion of the components quenched, study the effects of cycle parameters, and establish a quenching database to serve as the guidance for heat treating practice.

1.2 Mathematical Modeling of Quenching Processes

Modeling and predictions of internal stress in steel during quenching processes have been reported in the literature,^[22,48-60] with regard to either direct application to mechanical components, or the analysis of phenomena in the case of simple geometry. When the origin of the stress in purely thermal, the analysis procedure is fairly easy. However when phase transformations take place during the process, the problem becomes much more complicated due to the need of incorporating the coupled metallurgical and mechanical behaviors. In general, modeling of the quenching process involves coupling of heat transfer, mechanical response and metallurgical effects namely phase transformation. The relationship between those models as well as other concerns including microstructural development is illustrated in Figure 1.2.^[61] The feature related to coupling effects can be categorized as follows:^[62]

- Influence of temperature on the mechanical behavior, through thermal expansion or contraction, temperature dependent mechanical properties, such as Young's modulus, yield stress, stress hardening characteristics, and Poisson's ratio.
- (2) Influence of thermal history on the transformation kinetics. The metallurgical models, namely transformation diagrams achieved from experiments, such as CCT and TTT diagrams summarize the effects.
- (3) Influence of phase transformations on the temperature fields, through latent heats of transformation and phase dependent thermodynamic properties, such as thermal conductivity, specific heat and density.
- (4) Influence of phase transformations on the mechanical behavior, through transformation associated with volumetric and mechanical property changes, as well as the phase transformation induced plastic behavior, better known as the transformation plasticity.
- (5) Influence of mechanical behavior on phase transformation kinetics, notably the effect of hydrostatic pressure and uniaxial stresses on martensitic transformation start point (*Ms*).
- (6) Influence of mechanical behavior on the thermal history, through deformation energy.

The effect of (6) is so small that it has largely been neglected in most of previous modeling work. Both experiments and simulation have shown that the effect of stresses on the temperature is less than that of heat conduction or phase transformation by an order of magnitude. For example if the stresses generated during the quenching process are at the level of 500 MPa, and deformation is about 1%. Thus the deformation energy is about 5×10^6 J/m³. If the heat capacity is about 5×10^6 J/Km³, a typical value for steels, the effect of deformation energy will thus cause about a 2°C temperature change. On the

other hand the temperature change caused by heat conduction or phase transformation is typically more than 50-100°C.

The models for investigating the effects of (1) are well documented and established.^[16,60,63-65] It is the classical thermal stress and strain analysis, which is not only presented in quenching process, but also encountered in many other industry practices. Its theories are fairly mature and well documented. The difficulties of such analysis mainly come from the possibility of finding ways to establish the models so as to obtain the unknowns of interest. Due to the complicated nature of the models, analytical (closed-from) solutions are impossible in most cases. Other methods, principally numerical methods, which involve intensive computations, have to be carried out. With the advent of modern computer software and hardware, numerical modeling is gradually becoming acceptable and affordable.

Influence (2)-(5) consists of the most difficult components hence a significant challenge to modeling. Phase transformation is an important feature associated with a quenching process. The difficulty of handling phase transformation stems from many aspects, including debatable theories, insufficient experimental data, inconsistent results and insufficient functionality of modeling those phenomena in current software.

1.2.1 Modeling of Heat Transfer during the Quenching Process

Thermal history forms the foundation of the whole modeling process. The accuracy of the model is essential not only for thermal analysis itself but also for the calculation of thermal mechanical response and microstructural evolution associated with the process.

A quenching process could involve three modes of heat transfer: conduction taking place across the medium, convection occurring between a surface and a moving fluid and thermal radiation through emitting electromagnetic waves. Figure 1.3 illustrates schematically, the three modes of heat transfer involved in the quenching process. The legitimate and mostly selected analytical domain for purposes of modeling is the heat treated component only. Consequently only heat conduction needs to be considered when dealing with the interior of the component whereas other modes of heat transfer occurring outside of the component such as convection and radiation need to be considered as boundary heat transfer between the component and its surroundings.

The mathematical model for a typical heat conduction problem is discussed as follows:^[66-68]

Governing Equation

In Cartesian coordinates:

$$\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + Q = \rho C p \frac{\partial T}{\partial t}$$
(1.1)

In cylindrical coordinates:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(kr\frac{\partial T}{\partial r}\right) + \frac{1}{r^2}\frac{\partial}{\partial \theta}\left(k\frac{\partial T}{\partial \theta}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) + Q = \rho Cp \frac{\partial T}{\partial t} \quad (1.2)$$

where:

T - temperature	C_p - specific heat
-----------------	-----------------------

k - thermal conductivity ρ - density

Q - heat generation rate per unit volume

Boundary and Initial Conditions

Some of the difficulties associated with modeling heat treatment processes come from the high nonlinearity of the problem resulting from temperature dependent material properties such as k(T), $\rho(T)$, $C_p(T)$, boundary conditions as well as by complex latent heat generation rate. Specifying boundary conditions accurately is quite difficult due to highly nonlinear heat transfer mechanisms occurring at the surfaces of the component, irregularities caused by stacking, or the presence of odd geometric factors like cavities. A simple but efficient way uses a comprehensive boundary heat transfer parameter, generally being the overall heat transfer coefficient. It incorporates all possible heat transfer mechanisms occurring on the boundaries of the component, such as convective and radiative heat transfer. A mixed boundary condition is normally applied in modeling as follows:

$$h_{\Sigma}(T_{surf} - T_f) + k \frac{\partial T}{\partial n}\Big|_{surf} = 0$$
(1.3)

where:

 h_{Σ} - overall heat exchange coefficient

 T_{surf} - surface temperature

 T_f - bulk temperature

Specifying initial conditions is normally straightforward since most heat treating processes start with a uniform temperature such as room temperature. A cooling process may be modeled with a uniform initial temperature too, for instance many quenching processes start from uniform austenization temperatures. Generally the initial condition is expressed as follows:

$$T|_{t=0} = f(x, y, z)$$
 or $T|_{t=0} = f(r, \theta, z)$ (1.4)

in Cartesian and cylindrical coordinate systems respectively.

1.2.2 Stress and Strain Caused by Thermal Loads

Besides the strain and stress caused by normal structural loading, e.g. applied forces or body forces, temperature difference induces thermal strain and stress in the heat treated component. The thermal strain is calculated as:

$$\varepsilon^{th} = \alpha (T - T_{ref}) \tag{1.5}$$

where α is the coefficient of thermal expansion and T_{ref} is the reference temperature at which thermal strain does not exist. If α is a function of temperature and T_{ref} is not set to be T_0 upon which the coefficient is based, an effective $\alpha(T)$ has to be computed as:^[69]

$$\alpha_{eff}(T) = \alpha(T) + \left(\frac{T_{ref} - T_0}{T - T_{ref}}\right) \left(\alpha(T) - \alpha(T_{ref})\right)$$
(1.6)

where $\alpha(T_{ref})$ is the average coefficient of thermal expansion based on T_0 , evaluated at T_{ref} .

The stress field is transient and it changes in magnitude with location during the process. If the stress magnitude exceeds the yield point, residual stress and distortion will remain in the component.

1.2.3 Influence of Phase Transformation on Thermal History

Phase transformation is the major characteristic associated with a quenching process. Quenching of a component may involve transformation of austenite to ferrite, carbide, pearlite, bainite or martensite, etc. The principle influence of phase transformations on the thermal analysis is the latent heat generated during the cooling of the component, represented by heat generation rate Q in Equations 1.1 and 1.2. The latent heat may disturb the temperature fields and show some abrupt changes in the thermal history of the component. Typically there are two kinds of transformation: diffusional and nondiffusional. As would be expected, the kinetics of the two types is very different. The diffusional transformations, such as austenite to ferrite, carbide, pearlite or even bainite, are shown by C-shape curves whereas two horizontal lines representing the starting and finishing of the transformation respectively display martensitic transformation, the diffusionless one. A large collection of transformation data of various steels such as TTT diagrams has been accumulated so far.^[70]

The model used widely for the isothermal diffusional phase transformation was proposed in a two-parameter equation, also known as Avrami equation^[43] which takes the form:

$$f_{i} = f_{i}^{\max} [1 - \exp(-b_{i} \cdot t^{n_{i}})]$$
(1.7)

where f_i is the volume fraction of a phase *i* at a time *t* and f_i^{\max} is the equilibrium volume fraction of the phase. The parameters b_i and n_i characterize the growth rate of the phase *i*. The growth rate depends on the temperature, materials, grain size and other factors. These parameters can be calculated from the TTT diagram.

It is important to be aware that the kinetics of these transformation reactions should be applied to a case of continuous cooling in the quenching process. Therefore the information provided by the isothermal transformation is of limited value when continuous cooling is considered. CCT diagrams are more appropriate, however, the availability of CCT diagrams is very limited, compared to the large number of TTT diagrams in contrast. Differentiation of the Avrami equation, however, allows the determination of the amount of transformation products over a small time interval, specifically,

$$\frac{df_i}{dt} = f_i^{\max} \cdot b_i \cdot n_i \cdot t^{n_i - 1} \cdot \exp(-b_i \cdot t^{n_i})$$
(1.8)

Phase transformation may not take place immediately. The corresponding delay is called incubation. The following summation represents the incubation time during the continuous phase transformation process. The transformation will start when the summation is equal to unity.

$$\sum_{i=1}^{n} \frac{\Delta t_i}{t_{i\tau}} = 1 \tag{1.9}$$

where Δt_i is the time span at the *i*th step, t_{iT} is the incubation time at the temperature that the component reaches at the *i*th time step, which can also be determined from TTT diagram.

The discretized calculation of latent heat of continuous cooling is described as follows:^[71,72]

Transformation fraction:

$$f_{n+1} = 1 - exp[-c(T) \cdot \theta^{n(T)}]$$
(1.10)

Fictitious time:

$$\theta = \Delta t + [ln(1 - f_n) / c(T)]^{1/n(T)}$$
(1.11)

Heat generation rate:

$$Q = \rho \cdot \Delta H \frac{f_{n+1} - f_n}{\Delta t}$$
(1.12)

where ΔH is the enthalpy change of the phase transformation.

Compared to the kinetics of diffusional transformation, modeling nondiffusional martensitic transformation is simple. The most popular model is the empirical relationship between the reduction in temperature below *Ms* and the amount of martensite present, proposed by Koistinen & Marburger:^[73]

$$f_m = f_m^{\max} [1 - e^{-\gamma (Ms - T)}]$$
(1.13)

where f_m is the volume fraction of martensite, f_m^{max} is the volume fraction of the material available for martensitic transformation, and γ is a constant, which equals to 0.011 in many steels.

1.2.4 Influence of Phase Transformation on Stress and Strain

A dramatic change of mechanical properties of the component after quenching is the fundamental target of commercial applications of the quenching process. The effects of microstructure changes on the mechanical properties of the component can be obtained via empirical studies. Principally different microstructures display different mechanical characteristics, such as strength, work hardening rate, etc.

Influence of phase transformation also involves removal of plastic damage accumulated in the parent phase during an earlier stage in the stress-generation process^[13]. For example, a martensitic transformation process produces an extremely high density of dislocations, as though it had been subjected to severe deformation. Therefore its forgoing plastic deformation may be minor in comparison, so that the previous small plastic deformation is eliminated by the subsequent significant plastic deformation.

Another factor influencing phase transformation modeling procedures is transformation plasticity. Two important phenomena associated with the phase transformation are:^[43]

- Volumetric change due to the difference in density between original and new phases. The strain generated by volumetric change is very similar to that of thermal stress in which no shear components will be generated.
- The presence of plastic deformation even when the stress level is well below the yield strength, which can be explained as a temporary loss of strength of the material undergoing phase transformation, local stress concentration, preferred orientation, etc.

This phenomenon has been known qualitatively for a relatively long time, although the attempts for its mathematical or physical models are quite recent. Several models have been presented, however, there are three most representative models which are described as follows:

Greenwood-Johnson Model and its Variations

Greenwood & Johnson^[43] proposed a model based on rigid-ideal plasticity, with the assumption that all the plastic flow occurred only in the weaker phases. Basically transformation plasticity was dependent on two components, one was linearly dependent upon the magnitude of the applied stress, while the other was dependent upon the orientation of the transformation front relative to the direction of the applied stress. Having studied the effects of these two components in a range of transformations, including the $\alpha \rightarrow \beta$ and $\beta \rightarrow \gamma$ in uranium and the $\gamma \rightarrow \alpha$ in iron, Greenwood and Johnson concluded that the second component was negligible, and presented the following expression based on the first component:

$$\varepsilon^{ip} = \frac{5\sigma}{6Y} \left(\frac{\Delta V}{V} \right) \tag{1.14}$$

where ΔV is the volume dilation (swelling), Y is the yield stress of the weaker phase and σ is the applied uniaxial stress.

Supporting evidence was found by Ankara & West^[43,74] in the $\gamma \rightarrow \alpha$ transformation in the nickel-chromium steels, at a stress of 1 MPa. A linear relationship between applied stress and the amount of transformation plasticity was found by Ankara *et al*^[43] in the $\gamma \rightarrow \alpha$ transformation in Fe-20%Ni steels, at stresses below 200 MPa. Other evidence of plastic flow proportional to applied stress was reported by de John & Rathenau^[43,75] in the study of transformation plasticity in iron and iron-0.2%C steels.

Different assumptions lead to variations of Greenwood & Johnson model. Such variations were reviewed by Abrassart,^[43] who introduced the following model:

$$\varepsilon^{*p} = \frac{3\sigma}{4Y} \frac{\Delta V}{V} \left(m - \frac{2}{3} m^{3/2} \right) \tag{1.15}$$

where *m* is the fraction of transformed structure, and when m = 1 the model becomes:

$$\varepsilon^{\,\wp} = \frac{1}{4} \frac{\sigma}{Y} \frac{\Delta V}{V} \tag{1.16}$$

More recently Desalos *et al*^[43] suggested a relationship in incremental form based on the experimental data obtained in a stress-dialatometer, and were specific to the alloy chemistry:

$$\frac{d\varepsilon_{ij}}{dt} = 3K(1-m)s_{ij}\frac{dy}{dt}$$
(1.17)

where s_{ij} is the deviatoric stress tensor and K is a constant.

Reduced Yield Stress Model

Basically the reduced yield stress model does not recognize the possibility of plastic flow at stresses below the yield point as a consequence of microscopic level local yielding. Consequently, it assumes that transformation plasticity is a result of the significant reduction of the yield stress during the progress of the phase transformation.^[43,76,77] Figure 1.4 shows schematically the reduced yield stress during the phase transformation. It can easily be understood from the viewpoint of mechanics, whereas its microscopic explanation of the phenomenon is based on the movement of atoms between new and original crystal lattice sites during the transformation. This model was the first to be used to simulate transformation plasticity associated with martensitic transformation.^[43,76,77] The major advantage of the model is that it is simple and easy to use, where only one type of plasticity is involved so that the classical theory of plasticity may be used directly to incorporate transformation plasticity.

On the other hand, the model experiences some major difficulties, since it does not examine the metallurgical and microstructural mechanisms associated with the transformation. Firstly, it suffers from insufficient and indirect experimental evidence, or in some cases it contradicts experimental data. Although only little evidence was found by Tamura^[78] and de Jong & Rathenau,^[75] evidence of reduced yield stress is hardly ever found. Other researches, such as Denis *et al*^[43,79,80] and Fletcher & Price^[81] found only a steady rise in yield stress with the formation of martensite. Secondly there are no direct data available to implement the model. Consequently, this model has lost popularity recently in favor of the Greenwood & Johnson model. However, it has been used occasionally in some studies due to its simplicity and ease of incorporation with classical thermal stress analysis.

Preferred Orientation Model

This model is based on Scheil's concept: when martensitic transformation occurs under stress, the product chooses an orientation minimizing the total energy. Magee^[43] proposed the following relationship as:

$$\overline{\varepsilon^{p^{r}}} = \frac{\int \left[\frac{1}{2}\gamma_{0}\sin 2\theta + \frac{1}{2}\varepsilon_{0}(1+\cos 2\theta)\right]d\theta}{\int_{\theta} f_{r}^{\sigma}(\theta)d\theta}$$
(1.18)

where the integral in the numerator is the deformation produced by the formation of a plate of martensite, and $f_t^{\sigma}(\theta)$ is the quantity of phase formed under stress for the orientation θ of the formed plate.

This model has hardly been used since various factors associated with it are very difficult to obtain. However, the model can explain transformation for materials that exhibits small $\Delta V/V$ and for which preferential orientations is evident, e.g. in a reversible transformation.

1.2.5 Influence of Stress and Strain on Phase Transformation

The major concern of such influence focuses on the effect of applied stress on the kinetics of martensitic transformation, essentially resulting in a variation of the martensite start temperature (Ms).^[80]

A quantitative criterion for the relationship between Ms and tensile, compressive or hydrostatic stresses has been given by Patel & Cohen,^[82] based on Scheil's concept:

$$\frac{dM_{s}}{d\sigma} = \frac{\frac{1}{2} [\gamma_{0} \sin 2\theta \pm \varepsilon_{0} (1 + \cos 2\theta)]}{\frac{d(\Delta G)}{dT}}$$
(1.19)

where γ_0 and $\varepsilon 0 ~(\cong \Delta V/V)$ are the shear strain and the normal component of the transformation strain respectively, θ the orientation between stress axis and the normal habit plane ($tan2\theta = \pm \gamma_0/\varepsilon_0$), ΔG the change in Gibbs free energy; the plus sign is for tension and the minus sign for compression.

The model described above shows typical effects of the stresses on the Ms temperature. The shear and normal component of the stress influence the Ms point differently. The shear and tensile normal stress always raises the Ms temperature while compressive normal stress and hydrostatic pressure lowers the Ms temperature resulting from the relative shear and dilation on the formation of martensite.

The Patel & Cohen^[82] model and its modifications are based on thermodynamics. They fail to account for all the observations in a specific steel and stress state, and very often need quantitative data regarding the way transformation occurs at a microscopic level. Thus their applications are very limited due to the complexity of the stress states developed during the transformation. Inoue^[83] has proposed another relationship between the Ms temperature, the mean stress σ and the second invariant of the stress tensor J_2 :

$$\Delta Ms = A\sigma_{mean} + B\sqrt{J_2} \tag{1.20}$$

where A and B are constants.

Denis *et al*^[43,84] have also proposed a similar relationship and obtained experimental evidence in a Ni-Cr-Mo steel.^[43,80]

In addition to the effect on the Ms temperature, the stress state also influences the progress of the austenite decomposition during the transformation. The effect of tensile stress on the relationship between temperature and quantity of the martensite product has been studied by Denis *et al*^[43,84], with a high Ms temperature associated with an enhanced amount of transformation product at any lower temperature down to the martensitic transformation finish temperature (M_f).

1.3 Numerical Approaches

Finding an appropriate way of implementing the model and achieving meaningful results is another major task of modeling analysts. Figure 1.5 shows schematically a typical modeling procedure. As discussed earlier, quenching models tend to be fairly complex, due to the complicated nature of the process. Thus closed-form solution of the model is very difficult or even impossible to achieve in most cases. Consequently, in the absence of solution techniques other than closed-form, models have to be very simple, in some cases, to the extent that they may have little or no value.

Numerical analysis and computer simulation has become a promising and powerful candidate for attempting realistic models, which may involve various forms of nonlinearity, complex geometry and loads. Although it yields approximate solutions instead of exact ones, the numerical approach may produce fairly accurate results provided appropriate procedures are carried out. Three commonly used analysis methods namely finite difference method (FDM), finite element method (FEM) and boundary element method (BEM), are discussed as follows:^[65,85-87]

Finite Difference Method (FDM) is based on directly discretizing the governing equation, using Taylor series, or directly establishing discrete finite difference equations through energy conservation. This method is fairly simple, straightforward and easy to understand and implement. The FDM gives a "pointwise" approximation to the governing equations, which discritizes the domain into a finite difference grid with nodes at intersections of the grid. Finite difference equations need to be established for every node, both inside and on the boundaries of domain. A set of finite difference equations must be solved simultaneously to get the solution of interest at the nodes. The results obtained from the FDM are "discrete" indeed, i.e. the solution in the domain other than the nodes are still unknown, which must be interpolated from the nodal values by an appropriate order polynomial function. One obvious disadvantage of the FDM is that it is clumsy in handling complex geometric domains, since most finite difference grids are rectangular in nature. However, more robust schemes have been developed to enable the FDM to deal with irregular shapes, for example, the algorithm used by a CFD code application Flow3D. The FDM is well-established in thermal analysis and fluid dynamics.

Finite Element Method (FEM) is a more capable numerical analysis technique for obtaining approximate solution to a wide variety of engineering problems. Unlike the FDM, which seeks the solution region as an array of grid points, the FEM seeks the solution region as built up of many small, interconnected sub-regions or elements. It gives a "piecewise" approximation to the governing equations. The basic premise of the FEM is that the solution region can be analytically modeled or approximated by replacing it with an assemblage of discrete elements. It has great flexibility for handling complex shapes, since the element size, element shape and the way of element assemblage can be selected in a flexible manner. Figure 1.6 shows the different approaches of discretizing the domain between the FDM and the FEM. Obviously, the FEM demonstrates a better approximation to the boundary shape, however, this figure is not intended to suggest that the FEM are decidedly better than the FDM in all models. The performance of the FEM in a particular problem will depend on the definition of the model, the quality of the finite element mesh, the element properties, e.g. the shape function, etc. Another important feature of the FEM is its ability to formulate a solution for individual elements before assembling them together to present the entire problem. This means a complex problem reduces to that of considering a series of greatly simplified problems.

There are basically four different ways to obtain element properties: namely the direct approach, the variational approach, the weighted residuals approach and the energy balance approach. The details of those approaches are covered in most finite element text books^[65,85].

Boundary Element Method (BEM) also known as boundary integral method, is another fairly popular numerical tool. In some applications, only the values on the boundary are of interest, while interior results are not required. For example, one might have a problem in which a potential is given on the boundary and the desired information is the gradient of the potential on the boundary. Boundary element method can be derived by the use of Green's formula for Laplace's equations. The BEM discretizes the boundary into elements and solves for values on the boundary. The method has the reputation of high accuracy. In addition, the BEM uses a lower dimension computational domain with regard to the problem domain, since the boundary of a three dimensional domain is a surface (2-D) and a two dimension domain is a curve (1-D). Therefore, the meshing can be much finer with a given computational capacity. Although discretization of the interior domain may be necessary for the non-homogeneous governing equations, e.g. involving body loads, etc., the interior can be fairly coarse without significant influence on the accuracy. Actually, the result of the BEM is not limited on the boundary only. The interior values can be derived after the values on the boundary are obtained.

1.4 Foreword, Scope and Outline of the Dissertation

Process modeling of steel quenching is a challenging discipline with enormous economic benefits. It has gained increasing attention from the heat treating society. Modeling of quenching involves many aspects of engineering disciplines including materials science, heat transfer, structural analysis, and cross coupling between various aspects. Various models and theories related to quenching practice have been established in the past several decades. However, difficulties of process modeling of quenching still exist which stem from the complexity of the problem being studied, uncertainty and incompleteness of the theoretical understandings of the phenomena. These are mostly caused by phase transformations associated with the quenching process. Limited or lack of availability of the data is another source of the difficulty. Heat transfer coefficients and materials data especially temperature dependent thermodynamic and mechanical data are difficult to obtain. Complicated geometry and limitation of modeling tools add another degree of difficulty to the problem. Evidently, systematic and efficient strategies are necessary to coordinate modeling practice in order to increase the degree of data sharing, modeling efficiency, and collaboration among various modeling research parties.

Work presented in this dissertation focuses on the important issues of process modeling including analyzing the effects of critical modeling parameters such as
obtaining reliable heat transfer coefficients, developing representative modeling procedures for thermal history, residual stress and distortion for practical quenching problems. Tools for advancing the state of knowledge in process modeling such as database construction and application tools are proposed and initiated. The work is intended to address the issues of quenching modeling both in depth and breadth. The procedure of "weak coupling" between thermal, mechanical and phase transformation has been discussed and used. Figure 1.7 illustrates the coupling effects and Figure 1.8 explains the details of coupling. Commercial finite element analysis codes ANSYS and SYSWELD were the main modeling tools used in this thesis work. Special utility tools are developed to address specific needs of the research. The rest of the dissertation is organized as follows:

Chapter 2 addresses the important modeling issues including challenges of modeling practice, remarks on current practices and proposed strategies to advance the state of knowledge. Major advantages of modeling and computer simulation are pointed out including numerical experiments and the concept of a virtual laboratory. Quantitative analysis has been performed on different modeling approaches for thermal analysis of problems with constant moving sources. The importance and the impact of the modeling strategy are addressed in terms of accuracy and cost, specifically CPU time and data storage requirements.

Chapter 3 focuses on the validation of measuring techniques of heat transfer coefficients using quenching probes. Heat transfer coefficient is one of the critical modeling parameters. It is highly nonlinear in nature and very difficult to obtain in practice. Quenching probe is the standardized methodology for studying the heat transfer characteristics between quenchants and the quenched components. The lumped capacitance model is one of the approaches to derive heat transfer coefficients from a quenching probe test. In chapter 3 a numerical experimental procedure to validate the applicability of the lumped capacitance model is proposed. Limitations of the model are pointed out and discussed, from which an improved model is presented. The improved model is then used to study some practical quenching probe test data.

Chapter 4 discusses the limitation of modeling capabilities of the quenching process in current commercial codes. Generic code customization is proposed to extend the functionality of existing tools. A template for incorporating metallurgical phase transformation was developed for the ANSYS code with the aid of the "ANSYS Parametric Design Language" (APDL). Issues regarding commercial code, code customization and in-house code are also addressed.

Chapter 5 focuses on the study of a practical quenching problem. A modeling procedure is established which covers thermal history, phase transformation products, residual stress and distortion associated with the quenching process. Qualitative discussions with respect to the cycle parameters and as-quenched properties to be expected are given.

Chapter 6 discusses the role of the computer in the process modeling of quenching practice. The significance of the computer other than being a finite element analysis tool is addressed. Two modeling applications for modeling prototyping and modeling utility are presented in this chapter. More importantly, the role of databases in modeling practice is emphasized. Both the relational database and object-oriented database are proposed to facilitate the modeling practice.

Chapter 7 concludes the work and highlights the achievements and significance of this dissertation and pertinent future research work is suggested.



Figure 1.1 Cooling curve and the corresponding cooling rate curve. Oil quenching of the ISO quenching probe (oil temperature: 40°C).



Figure 1.2 A schematic demonstration of the interactions among the temperature field, mechanical response, transformation behavior and microstructural development.



Figure 1.3 Schematic of heat transfer mechanisms involved in a quenching process.



Figure 1.4 Schematic of reduced stress model, which assumes transformation plasticity is the result of reduced yield stress during transformation.



Figure 1.5 Schematic of modeling procedure.



(b) Finite Element Method (FEM)

Figure 1.6 Domain discretization using finite difference method (FDM) and finite element method (FEM).



- 1: Influence of temperature on stress and strain
- 2: Influence of temperature on phase transformation
- 3: Influence of transformation on temperature filed
- 4: Influence of phase transformation on stress and strain

Figure 1.7 Weakly coupled approach used in this study.



Figure 1.8 Details of the weakly coupled approach.

CHAPTER 2

CHALLENGES OF QUENCHING MODELING AND STRATEGIES

Quenching remains a mysterious subject in the field of heat treatment. The problem is so complex that it deserves intensive study in both theoretical and applied perspectives. The difficulties stem from various aspects including the cycle itself, heat transfer, thermal mechanical response, phase transformation associated with the process, chemistry of quenchant, quenching equipment, the component heat treated, and experimental verification method. A comprehensive prediction methodology and control is still far out of reach, though significant progress has been made in theoretical studies, experimentation, as well as modeling and simulation of quenching processes. In particular, the focus of major research initiatives in heat treatment remain as follows:

- Heat transfer between quenchant and component.
- Thermal history, residual stress and distortion of the quenched component.
- Coupling of phase transformation in both thermal and thermal mechanical response.
- Reliable data of physical and mechanical properties.
- Modeling complex geometry of the component.
- Systematic and efficient modeling strategy.
- Materials selections.
- Heat treating cycle optimization.

2.1 Theory and Model Incompleteness and Model Limitation

The first step in process modeling procedure is to map a practical process into the modeling domain. Establishing metallurgical and mathematical models that describe the behavior of the process does this mapping. For example, isothermal transformation diagrams model the phase transformation progresses that quenched parts may experience from the metallurgical viewpoint, and corresponding models such as Avrami equation may be used to translates the metallurgical model into a mathematical model so that this transformation phenomenon can be studied quantitatively. The mapping requires sufficient knowledge of the practical process, however, many quenching aspects are too complicated to be mastered. For instance, the interaction between phase transformation and thermal mechanical response, i.e. influence of phase transformation on residual stresses and vice versa, is still far from being understood. Consequently, a lot assumptions and simplifications have to be adopted. Although assumptions and simplifications are part of modeling strategy, they can lead to a poor model or even an invalid model if they are used beyond reason. Due to the complexity of the quenching process to be modeled, a model may have to start with inherent deficiencies. The incompleteness of the theory and the model of a quenching process primarily stems from the phase transformation, namely the mechanism of the phase transformation and its influences to other modeling aspects, such as thermal, structural analysis and vice versa. Modeling latent heat and transformation plasticity, for instance, are still ongoing research areas that involve deep understanding of metallurgy, heat transfer and mechanics. All these point to the inherent deficiencies in current models, which will have to be improved with the aid of experiments.

Modeling is powerful, however, it is neither omnipotent nor all applicable. A model, even after verification, still has its limitations and its applicable domain must be examined before its use. For example, a model created for a quenching process cannot be applied directly to a heating process without adequate and appropriate modification.

Even one oil-quenching model may differ from another oil-quenching model depending on its equipment, quenchant, heat treated component, and so on.

2.2 Reliable Data

The complexity of a real heat treating process demands a nonlinear model. Reliable material properties and boundary conditions are critical and are always quite difficult to obtain. Examples include thermal conductivity, coefficients of thermal expansion, temperature dependent stress strain data of the materials and heat exchange coefficients. The data are extremely difficult to obtain at elevated temperatures. Without a reliable data set, the model cannot be correctly established and accurate results would be impossible to achieve.

As an example, the heat transfer coefficient, the critical boundary condition parameter, is very difficult to obtain due to the complexity of the heat transfer involved in a practical heat treating process. As discussed earlier, for example, a liquid quenching process may involve three stages, vapor blanket, nucleate boiling and liquid cooling^[2]. Not only is it difficult to obtain by theoretical analysis of the heat transfer mechanism, but also it is hard to establish by experiment. Moreover the heat transfer coefficient differs at various surface locations, for example, the value at a free top surface may differ dramatically from that at a inner hole's surface. In most cases an average heat transfer coefficient value over the whole surface of the part has to be used.

2.3 Difficulties related to Experimental Measurement and Validation

Modeling could not be considered complete without verification. Virtually modeling can do anything and produce desired results. A model must be verified before it can be used with confidence when applying it to an unknown case even under similar conditions. A model may go wrong at any stage of the procedure. For example, a model might be ill-defined or incorrectly established at the very beginning. It may do not reflect the nature of the problem being studied. A wrong numerical procedure might be adopted that does not faithfully reflect the original model intent. It is also likely that one might use a poorly implemented or even "buggy" in-house or commercial code. It is more common that the accuracy of the modeling results are jeopardized by inappropriate meshing quality, coarse time step, or even the limitation of the computational resources. It is worth to point out that although modeling and computer simulation is considered to be inexpensive compared to a practical experiment, it is not free at all. A model or modeling procedure should be considered advanced and sophisticated by the efficiency and accuracy not the size of the model. The cost of a modeling practice may easily become forbidding and even unacceptable without a careful examination of the requirement. An experienced modeling analyst may consider twice before extending his/her model.

There is no cure-for-all validation procedure in existence because of the complex nature of the problem being studied. Experiments are the most commonly accepted method although other ways of verification exist. Measurements taken and monitored in a typical modeling procedure could be the thermal history (time-temperature profiles), the fraction of materials transformed and the residual stress and final distortion.

In addition to the validation, experiments may have to be used as well to obtain the critical inputs of the model that are not available from other sources. It is common to carry out experiments to obtain, typically, the boundary heat transfer coefficients, mechanical and physical properties of the materials such as yield strength, work hardening characteristics, thermal conductivity, etc.

Validating a thermal model is somewhat easier than that of a residual stress. The typical method of measuring thermal response involves embedding the thermocouples in various locations of the component to be heat treated. A complete thermal history that the component has experienced can be obtained in a fairly straightforward manner, though the procedure may involve many measuring techniques to ensure the reliable and accurate results, such as reliable thermocouple contact and high data sampling frequency. On the other hand, validation of the whole model, especially measuring stress and strain during the process as well as proper representation of transformation plasticity, is rather

difficult. For example, it is very hard, or even impossible to trace the stress and strain history of the component during the whole process. In most practical applications only the residual stress and distortion are measured at the end of the quenching process^[88]. Only the final results of the process are available, without any information about what happens during the process, specifically how the stress and coupling effects behave in real time, etc. This makes the error backtracking extremely difficult since the model may go wrong at various points: thermal analysis, thermal stress analysis, phase transformation, method of coupling, material properties, boundary conditions, numerical treatment, meshing quality, or even the mathematical foundation of the model or theory.

2.4 Thermal-only vs. Thermal-stress Modeling Approach

Prediction of residual stress and final distortion is one of the ultimate goals of modeling work, which is driven by the forgoing thermal history. In spite of it attractiveness, the results of thermal stress and final distortion are much more costly and difficult to obtain as discussed above. It requires extra details of structural analysis and may involve incorporating additional theoretical or modeling uncertainties such as transformation plasticity. In addition, its experimental verification becomes much more challenging. In many cases, a careful thermal analysis has the potential of yielding enough information that serves as guidance and insight for heat treating practice. For example, acceptable practice in improving quenching quality is by minimizing temperature difference within the component, which can be achieved by thermal analysis including monitoring carefully the effects of cycle parameters and loading configuration. Depending upon the requirement and definition of the problem, a thermal-only approach could be a more reliable, efficient and cost-effective modeling approach.

However thermal-only analysis could not yield sufficient information. For instance if a quenched component is mechanically constrained during the quenching process, very limited information regarding residual stress and distortion can be obtained. In such case only a complete thermal stress and residual stress model is desired. As a

result a modeling analyst should select the efficient modeling procedure based on the problem to be studied.

2.5 Difficulties of Incorporating Phase Transformation in Existing Analysis Tools

Phase transformation is the most complicated phenomenon associated with quenching. As it was indicated in earlier sections, the model of interaction between phase transformation, thermal history and the mechanical behavior are not well understood and established, especially the phenomenon of transformation plasticity. Moreover most of numerical analysis tools, including ANSYS, are designed for the general use. Although their capabilities in the common analyses, e.g. thermal, structural, or even coupled thermal-stress analysis, are quite functional, special procedures have to be used to account for the phase transformations of the quenching process. However the potential of incorporating new features or functions is largely constrained by the interfaces provided by the existing FEA codes like ANSYS. It is also constrained by the complexity of the functions being added. Incorporating new functions into an existing code is type of nontrivial code customization. The task requires both computer programming and domain specific skills. For instance to add phase transformation functions into ANSYS code one need to have advanced programming skills in FORTRAN, understand the high performance algorithms for numerical calculations, be proficient in the ANSYS's existing functions and data structures. Finally one also need to understand the details of the phase transformation model to be implemented. Consequently if a desired new function involves significant amount of analysis, design and coding, code customization will be clumsy and may significantly degrade the performance of the original code. Alternatives have to been sought such as self-developed in-house code or another existing code.

2.6 Numerical Experiments

Experimental validation has become an well-accepted procedure, however, it is worthy to point out that it should not be regarded as the only procedure nor always correct. Due to the difficulties of setting up experiments and system error, a validation may yield erroneous results. In addition experimental validation may not be efficient or even not applicable in some cases such as evaluating the effects of mesh quality.

2.6.1 What is and Why Numerical Experiment

Numerical experimentation is one of alternative procedures that uses numerical procedures to validate some unknown aspects of the primary model of interest. There are several reasons for adopting numerical experiments as listed below:

- Comparatively low cost
- Comparing several alternative modeling procedures/approaches
- Analyzing the impacts of critical parameters
- Validating the model when traditional experiments may not help
- Isolating factors of particular interest from others. e.g. experimental system errors

Numerical experiment is purely a numerical analysis, which involve no or very little practical experiment. Therefore it is comparatively cheaper than a conventional experiment and it is easier to configure, more versatile and flexible. A typical example of numerical experiment is choosing appropriate meshing strategy in finite element analysis procedure. It is well known that mesh quality is a vital factor in finite element analysis. In general the denser the mesh the better the result. However increasing the mesh density will significantly increase the size of the model and thus may tremendously increase the CPU time and storage requirement. Therefore it is desirable to figure out a compromise mesh density which will yield good result without excessive overhead. In such a case, a numerical procedure is proposed to test the impact of the mesh density so as to find an optimum state. In reality more modeling strategies or approaches can be tested using numerical experiment. For instance, it is very easy to propose a numerical procedure to test the influence of critical boundary conditions, e.g. heat transfer coefficient, on the result of temperature simulation. One can simulate the temperature field with one heat transfer coefficient value, and then introduce some deviation, for example 10% of the original heat transfer value and do the simulation again. By comparing the result one can have better insight and a good understanding of the impact of heat transfer coefficient on the model. Obviously such kind of sensitive analysis is very difficult in a practical experiment, in which heat transfer coefficient is difficult to manipulate.

Another advantage of numerical experiment is that it can isolate critical factors from other complexities. In the example present above, we actually perform an ideal experiment in which only the deviation of the heat transfer is considered. A more detailed discussion will be presented in a later section of the thesis, in which a numerical experimental procedure is carried out to test the validity of the lumped capacitance model used for deriving heat transfer coefficient using quenching probe.

Numerical experiments help modeling analysts to determine the modeling strategy, not only in the modeling details like the critical parameters and mesh quality as mentioned above, but also in the higher level decisions such as domain selection, dimensionality of the model, i.e. one-, two- or three-dimensional model, and even the type of model to be used. The following example demonstrates the use of numerical experiment to compare the cost and applicability between two types of models, namely Eulerian (moving coordinate frames) and Lagrangian (fixed coordinate frames) approaches, for the thermal analysis of heat conduction in response to uniformly moving heat sources, as encountered in welding and other applications.^[89]

2.6.2 Determining Modeling Strategy by Numerical Experiment - A Case Study

Many welding applications involving computational modeling of welding thermal cycles using finite element analysis is usually performed as a transient problem with the heat source moved incrementally to correspond to the motion of the welding arc. Considerable spatial detail is required to represent a moving source about which there are

strong gradients. Problems are very time consuming, even on advanced modern computers, and make heavy demands on data storage. An alternative approach uses moving coordinate frames to correspond to the motion of the moving arc. Significant saving in both CPU time and storage would be expected since moving coordinate frames transfers the time-dependent problem into a static problem through mathematical treatment. The equivalence of the two models can be described as follows.

One dimensional time-dependent heat conduction problem is described by the following equation:^[89]

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot k \nabla T + Q \qquad (2.1)$$

In a coordinate system moving with speed v in the positive x direction, the time derivative is replaced by a spatial derivative

$$\rho c \, \frac{\partial T}{\partial t} = -\rho c \, v \, \frac{\partial T}{\partial x} \tag{2.2}$$

This leads to an equivalent static problem

$$\nabla \cdot k \nabla T + \rho c v \frac{\partial T}{\partial x} + Q = 0$$
(2.3)

In this moving coordinate frame, values of the x-coordinate correspond to time. Positive values of x correspond to the heating portion of the problem, i.e. to times before the center of the moving source reaches a particular location. Negative values of x correspond to the cooling portion of the problem.

A numerical experimental procedure was proposed. ANSYS, a commercial finite element code was used to carry out the numerical experiment. A set of two- and threedimensional test cases were performed with both fixed and moving coordinates. The parameters characterizing these cases are summarized in Table 2.1. Running times and data storage requirements for these cases are shown in Table 2.2. In these problems, a region in which the temperature is set equal to the melting temperature of steel represented the heat source.

Representative temperature distributions are shown in Figure 2.1 for the moving line source in two dimensions. They are displayed as functions of position relative to the source in the moving Eulerian coordinate frame. The Lagrangian coordinate results also are plotted

in this manner. Recall that there is correspondence between time and distance traveled. These distributions have certain general characteristics.

It also may be observed that the moving Eulerian coordinate system is more accurate than the fixed Lagrangian coordinate system for the same mesh detail. This has been found consistently to be the case for all levels of mesh refinement. Figure 2.2 shows that comparable results are obtained for 50-interval Eulerian and 80-interval Lagrangian calculations.

The higher accuracy of the Eulerian frame reflects the need to make an additional approximation in Lagrangian coordinates. The continuous motion of the heat source is represented by step-wise movement to fit the finite space and time intervals. The source will be at one location for a time step, then jump to the next location, where it will remain over the next time step. In other words, the Lagrangian formulation makes an approximation (not made in the Eulerian formulation) to the problem itself in addition to approximations made to the derivatives of temperature to solve the problem.

Figure 2.3 presents runtimes for two dimensional line source problems. Central processing unit (CPU) times for Eulerian problems are shorter than those for Lagrangian frames by one to two orders of magnitude, *i.e.* factors of 10 to 100, closer to 100. The factor of 100 applies to the comparable accuracy 50-division Eulerian and 80-division Lagrangian problems. Roughly speaking, time consumption of two-dimensional Eulerian problems in seconds corresponds to Lagrangian problems time consumption in minutes, and time consumption of three-dimensional Eulerian problems in minutes correspond to Lagrangian problems in hours.

Data storage requirement gains in solution files are comparable to CPU time gains. In Lagrangian problems, about ninety per cent of data storage is associated with the solution file, which dominates memory requirements. In Eulerian coordinates, the solution file is about half of the total storage requirement, with the data base file typically being the largest single file. These results are illustrated in Figures 2.4. The large storage requirements for Lagrangian problems have frequently led to inability to run cases.

Time consumption increases more rapidly with mesh detail in Lagrangian coordinates than in Eulerian coordinates, as may be seen from Figures 2.3 and 2.5.

Doubling the number of intervals for the Eulerian case led to less than doubling of running time, while doubling intervals in the Lagrangian case led to almost quadrupling running time. The normalized presentation of Figure 2.5 shows this clearly. These results may be understood in terms of the relative amounts of data in solution and data base files. In Lagrangian coordinates, most of the data, and most of the effort is associated with the solution file. CPU time tends to increase more rapidly than the number of elements, reflecting the nature of the solution processes used. In Eulerian coordinates, comparable data are associated with data base and solution files, and a significant portion of computational effort is in setup time.

Storage requirements also increase faster for Lagrangian problems, as can be observed from Figure 2.6. It therefore can be seen that there are higher prices to be paid, both in running time and in storage requirement, for refining mesh to increase accuracy in Lagrangian relative to Eulerian coordinates.

Similar results have been obtained in the other cases. Orders of magnitude gains have been achieved in both running time and data storage requirements relative to commonly used fixed coordinate modeling. The Eulerian formulation is found to be more accurate than the corresponding Lagrangian problem for the same spatial mesh detail. In addition, the Eulerian formulation is found to be amenable to accuracy improvement at no cost through non-uniform sizes of spatial divisions. The Lagrangian option, however, must include detail sufficient to represent temperature distributions as the source moves. Finally, the cost of increasing mesh detail is observed to be lower in the Eulerian formulation than in the Lagrangian.

2.7 Some Considerations for Choosing Modeling Domains

In practical quench process very complicated heat transfer occurs between the component, the quenchant and other surroundings. Since the interest of the thermal analysis mostly remains in the temperature response and history within the component during the quenching process, it is reasonable to choose the component as the modeling

domain and integrate the effects of surroundings into boundary conditions for the analysis. The advantages of this treatment are obvious: only heat conduction needs to been taken care resulting in a simple modeling procedure, and the domain is more efficient and thus reduces the computation significantly. This could be important since a finer meshing scheme can be carried out under the constraint of the capacity of the software and hardware. However, boundary heat transfer is usually very hard to characterize and it is a nonlinear term in most cases. Heat transfer coefficient strongly depends on the chemistry, thermodynamic properties of the quenchant, temperature of quenchant, surface temperature of the heat treated component, geometry of the component, loading configuration, agitation of the quenchant, design of quenching equipment, etc. Consequently it is extremely difficult to capture all of the details by using comprehensive coefficients, obtained either by experiments or from existing databases. A tactical approach extends the domain to include quenchants in the model, as shown schematically in Figure 2.7. For example, when modeling the thermal response of the component in a gas quenching process, the quenching chamber, together with the component, will be used as the simulation domain. The major advantage of this approach is that we move the boundaries away from the component to the wall of the quenching The original boundaries between the component and quenchant will be chamber. solid/fluid interfaces, which are automatically analyzed as a convective heat transfer process involving fluid dynamics. The new boundary conditions of the domain, namely wall of the chamber, are much easier to specify. In addition, the domain boundaries are usually far enough away from the component so that the errors associated with it may have less influence on the accuracy of the temperature within the component. The extended analysis also yields bonus information on the quenchant flow pattern which potentially aids to improve the quenching practice include finding equipment design hot spots and optimum load configuration. The extended analysis also make possible for establishing a heat transfer coefficient database with regard to different quenching configuration for later use.

Recently, considerable literature has reported on activity of research regarding the convective heat transfer involving fluid dynamics.^[90-94] However, extending modeling domains has several major limitations, as discussed below:

- It makes the analysis more complicated. Analysis of convective heat transfer is usually more difficult that of heat conduction. More unknown variables have to be solved and more sophisticated theoretical and numerical approaches have to be used.
- 2. Uncertainties and assumptions in the convective heat transfer are introduced into the model. Convective heat transfer, especially its fluid dynamics component, has to use some empirical models or assumptions to handle the uncertainties in its theory, such as turbulence characteristics of the fluids. One model may be best applied to only certain applications, i.e. one particular model may work fairly well in one application, whereas it may yields erroneous results in others. Thereby the accuracy of the quenching model may largely depend on the skills and experience of the modeling analyst to make appropriate decisions.
- 3. In some difficult applications, other heat transfer mechanism, such as radiation has to be incorporated in the convective heat transfer model. The typical application is a gas quenching process. Although conductive and convective heat transfer between the component and the surroundings has been integrated in the model, radiation has to be added to the model, since it represents a significant portion of the total heat transfer when surface temperature of the component is high. Other typical difficult problems are the vapor blanket forming in the early stage of the liquid quenching and the nucleate boiling stage thereafter. Coupling these complex mechanisms is clearly nontrivial, which makes the modeling quite difficult.
- 4. Modeling of convective heat transfer is extremely computational intensive. Due to the large simulation domain and fine meshes needed for a successful simulation, the cost of modeling increases dramatically. A very well

configured computer platform and sophisticated analysis codes would be a minimum requirement of carrying out this kind of analysis.

2.8 Database for Process Modeling of Quenching

Process modeling has become increasingly popular lately. Modeling practice has concentrated largely on model creation, procedure preparing and model implementation. Tremendous work has been done and vast amounts of results have been accumulated. On the other hand there has been little effort made regarding the organizing and sharing the existing information.

Databases and database technology forms a major branch of computer industry that has grown very fast in recent history.^[95-98] Database plays a critical role in most computer applications. Bibliographical databases, e.g. METADEX, are one of the major database applications in materials science in these days. A database system is a computerized record-keeping system, which provides the user a given facility for a variety of operations including adding new data, retrieving data and updating data or deleting data. However its applications are still very limited in process modeling practice. Significant advantages of the database applications in process modeling can be listed as follows:

• Systematic data organization: As we know fairly rich information has been stored in a quenching modeling practice, including the modeling results such as thermal history, phase products, residual stress and distortion of the component. Information on modeling procedure may also need to be added into modeling repository. Typical information includes type of the model, geometry, finite element mesh, solution strategy, and analysis tool and computer platform. Related data including heat transfer coefficient and its source are the part of modeling procedure that needs to be traceable. More importantly the definition and the specification of the problem including component is

the important information need to be stored. Database thus is able to organize and store the information and retain the traceability among the various data groups.

- More modeling analysis: Using database in process modeling encourages the pre- and post- analysis of the model. Before starting a modeling process, one needs to carefully study the problem and modeling procedure. Critical model parameters need to be identified and may be queried against database. Necessary data, guidelines or suggestions can be obtained from the past modeling practice. After completing the modeling, analyses are required to identify the useful information that will be added into the database. Therefore the model will be treated as the part of the modeling repository for later use instead of only for one specific problem.
- *Efficiency*: Database helps modeling practice with valuable suggestions from the previous results as well as the critical data. Therefore by incorporating the database one may avoid redundant work or establish a more sophisticated and efficient modeling procedure. The modeling practice therefore may eliminate the ad hoc state to a systematic approach.
- Concurrency: Database provides accurate and up-to-date to the information on demand at anytime.

Other benefits of the database are also applied including consistency, redundancy reduction, data sharing, common standards, security, integrity and requirements balancing. The benefits discussed above are more significant when database is applied into a multi-user group or even collaboration among various modeling parties.

2.9 Modeling and Simulation - A Virtual Laboratory

Mathematical modeling and computer simulation has become increasingly popular nowadays. It has shown great potential in various applications, such as structural analysis, heat transfer, fluid mechanics and many other fields of science and engineering. The general approach in computer simulation is to analyze directly the governing equations that drive the processes. In cases where direct analysis is too complicated and perhaps impossible, application of numerical methods that seek solutions to governing equations in an approximation approach. Such methods have evolved and developed significantly over the past two decays.

Modeling and simulation forms a virtual experimental platform or a virtual laboratory, which is so versatile that many unknown parameters such as the quenching process can be predicted and tested in advance of final part production. The benefits are directly implicit in production quality and costs. With modeling treatment, a real world quenching problem is mapped onto a mini world - a model, which can be solved with the assistance of mathematics, numerical methods and computer simulation. As a result, sophisticated modeling and simulation could turn to be a powerful virtual laboratory, where real world problems can be studied. Examples include conducting important experiments such as cycle prediction, optimization and validation can be carried out. Valuable information and suggestions could be drawn from the simulations with the goal of producing components with little or no post production distortion

Figure 2.8 illustrates an analogy between a virtual experiment and a traditional experiment. For successful modeling practice one should have the expertise in the application domain, e.g. quenching as well as possesses strong modeling skills. That person needs to understand the practical problem and find a way to map the problem from real world (practical application domain) into mini-world (modeling domain). The mapping must be legitimate and efficient. That means the mapping should capture the nature of the problem, for example several aspects including metallurgical behavior, heat transfer, mechanical response and coupling effects much be handled in the mapping procedure in a heat treating problem. The mapping is normally done by establishing mathematical representation, for instance partial differential equations, boundary condition, and initial condition. Mapping forms the foundation of the virtual laboratory. It is not wise and not possible to include all details of the problem into the model. Therefore a modeling analyst needs to decide what needs to be included, what need to be

simplified and what needs to be ignored. The knowledge and expertise of the modeling analyst as well as the problem drive such decisions at hand. One may not gain much from an over-detailed model except a significant overhead on modeling cost. On the other hand modeling results might not be representative of the problem that is being studied if a model is too rough or not properly established.

After mapping the problem into the modeling domain, an appropriate methodology must be chosen to retrieve most effective results. This procedure is similar to the design of an feasible experimental procedure, for example the decision on what kind of laboratory facility need to be used, the detail procedure of the experiment, and what kind of result is expected. In the virtual laboratory, a modeling analyst needs to decide the solution strategy, typically a closed-form or numerical approach. In general, numerical approach has to be used due to the model complexity. Closed-form approach is limited in very simple models, such as one-dimensional on those involving constant properties and simple boundary and initial conditions. More decision-making procedure could be necessary in order to refine the experimental procedure. For example, one needs to decide what kind of numerical procedure is to be used, finite element method (FEM), finite difference method (FDM), or boundary element method (BEM). One may also need to decide whether he/she would like to use an in-house code or find a good commercial code. Another important decision one may face is the mesh density and mesh quality that must be used in the discretization procedure of numerical analysis. Mesh quality is a critical factor that may directly influence the accuracy of the simulation result.

The computer code for numerical analysis and computer platform is a counterpart of experiment facility in a traditional experiment. An important practice in the virtual laboratory is the validation procedure. This procedure is required for establishing a new model for a new application. After getting the result, one need to analysis and validate the result, typically by comparison with the result of a reliable practical experimental test. After validation, the model is ready to be used in future practice.

2.10 Concluding Remarks

Modeling and simulation forms a virtual laboratory platform, in which practical quenching problems can be analyzed, predicted and optimized. However such modeling practice is challenging. Difficulties includes incompleteness and limitation of current theories and models, especially those intertwined with phase transformations. Limited availability of the reliable data and insufficient functionality of the existing modeling tools add an additional layer of difficulty. Due to the complexity of the problem being studied model validation procedures are not easy either.

Process modeling of quenching demands advanced skills and knowledge in modeling procedure, numerical analysis, as well as quenching practice. Efficient modeling procedure could be achieved through careful analysis of the modeling requirements and the nature of the problem. Decisions need to be made with respect to the size of the domain, type of the model, scope of the analysis and details of the model. Numerical experiment could be used as an auxiliary tool for the decision making and validation.

Problem Type	Geometry and FEM Mesh			
2D Line Source	 H=0.05 m (5 div.) Note: 1. Uniform mesh along both length L and height H 2. The inverse triangle represents the location of the heat source in all cases studied 3. Natural convection on both top and bottom surfaces 			
2D Point Source	W/2=0.15 m (5 div.) L=1 m (60/80 div.) Note: 1. Only half the plate is employed 2. Non-uniform mesh along the width W			
	 3. Uniform/Non-uniform mesh along length L in the different cases and a denser mesh near the source region when non-uniform meshing along L 4. Natural convection on the longitudinal edge L 			
3D Problem	H=0.05 m (5 div.) L=0.15 (40 div.) Note: 1. Only half the block is employed 2. Non-uniform mesh along width W and height H 3. Uniform mesh along length L 4. Natural convection boundary conditions at top, bottom, front and rear			
Other paramete	surfaces			
Thermal co	ponductivity: $k = 16.3 W/m \cdot K$ Density: $\rho = 8030 kg/m^3$			
Specific he	tat: $c = 502 J/kg \cdot K$ Moving velocity: $v = 2.5 \times 10^{-4} m/s$			
Initial temperature: $T_0 = 30 ^{\circ}\text{C}$ Bulk Temperature: $T_{\infty} = 30 ^{\circ}\text{C}$				
Heat transfer coefficient $n = 10 \text{ m/m} \cdot \Lambda$				
Adiabatic d	contention on the surfaces where it is not specified			

Table 2.1Parameters of different problem types.

Table 2.2 Runtime and storage requirements for the different cases studied.

2D Line Source									
,	Eulerian			Lagrangian					
	50 div.	100 div.	200 div.	50 div.	80 div.	100 div.			
CPU time (sec.)	15.4	27.4	49.4	547.8	1,476.6	2,164			
Database file (byte)	573,440	983,040	1,769,472	589,824	835,584	999,424			
Result file (byte)	196,608	360,448	688,128	7,061,504	17,760,256	27,574,272			
Total storage (byte)	770,048	1,343,488	2,457,600	7,651,328	18,595,840	28,573,696			

(The divisions listed in the table are all along the length L)

2D Point Source								
	Euler	ian	Lagrangian					
	60 div. Non-uniform	60 div. uniform	60 div. uniform	80 div. uniform				
CPU time (sec.)	29.8	30.6	1,507.3	2,689.7				
Database file (byte)	1,097,728	1,097,728	1,114,112	1,425,408				
Result file (byte)	393,216	393,216	17,727,488	31,260,672				
Total critical storage (byte)	1,490,944	1,490,944	18,841,600	32,686,080				

3D Problem					
	Eulerian	Lagrangian			
	40 div.	40 div.			
CPU time (sec.)	89	3,707			
Database file (byte)	2,293,760	2,359,296			
Result file (byte)	1,032,192	34,308,096			
Total critical storage (byte)	3,325,952	36,667,392			



Figure 2.1 Temperature distributions for 2D line source problems, path plot along the top surface.



Figure 2.2 Temperature distributions for 2D line source problems, path plot along the top surface.



Figure 2.3 Comparison of runtime for 2D line source problems.



Figure 2.4 Comparison of storage requirement for 2D line source problems.



Figure 2.5 Normalized runtime vs. problem size for 2D line source. (Normalized runtime = Runtime CPU sec. (problem size) / Runtime CPU sec. (50 divisions)).



Figure 2.6 Normalized storage requirement vs. problem size for 2D line source. (Normalized storage requirement = Storage in byte(problem size) / Storage in byte (50 divisions)).



Figure 2.7 Extended modeling domain including both solid (component) and fluid (quenchant).



Figure 2.8 Analog of a virtual laboratory to a conventional one.

CHAPTER 3

NUMERICAL VALIDATION OF HEAT TRANSFER COEFFICIENT DERIVATION BY LUMPED CAPACITANCE MODEL USING QUENCHING PROBE

Heat transfer coefficient is a critical boundary condition required for carrying out thermal analysis. Quenching into vaporizable liquids such as mineral oil, water and aqueous solutions involves at least four cooling mechanisms, shock film boiling, full film boiling, nucleate boiling, and convective (and some conductive) cooling. Therefore modeling of quenching heat transfer processes is much complicated. Heat transfer between quenchant and heat treated components is further complicated by the often complex shape of the part such as a gear or fastener.^[19,42,99-101] Due to the inherent complexity of the problem, it is often difficult to adequately model subtle and transient quenching phenomena. Cooling curve analysis is a widely used experimental procedure to study the heat transfer behavior during a quenching process.

Cooling curve analysis using an instrumented probe is a widely used method to characterize quenchants with respect to cooling temperature or cooling rate behavior, heat transfer coefficients and other quenching parameters in quenching practice.^[36,99,102-106] In general, the probe may be constructed from a high thermal conductivity material such as silver to achieve maximum sensitivity. Alternatively, probes may be constructed from stainless steel or Inconel600 for cooling temperature-time data that is more representative

of actual steel quenching as desired. Typically, a probe is constructed from bar or plate material of infinite shape. (Infinite shape is approximated by a length at least 4 times the diameter or the length and width of a plate being at least 4 times the thickness.) The thermocouple is inserted into a hole drilled precisely into the desired location for instance the geometric center of the material. The thermocouple may be held in position by soldering, such as silver solder, press fitting or with the use of a spring loaded thermocouple. Procedures are necessary to assure that the thermocouple maintains contact with the probe materials during the expansion that inevitably occurs upon heating.

To conduct the cooling curve analysis, the probe is heated to the desired austenization temperature, often 840°C for Inconel600 or stainless steel and then quickly immersed into the quenchant. The instrumented probe is attached to a computerized data acquisition system that accurately records the temperature-time profile (cooling curve) during the quenching process. A range of useful information can be derived from this test, including cooling rate, quenching severity, heat transfer coefficient, etc.

3.1 Methodology

Cooling curve analysis procedures have been standardized with regard to probe configuration and material in many countries, including Japan, France, China and the USA.^[99,102,103] Two representative configurations are the ISO 9950 (International Organization for Standardization) and JIS 2242 (Japanese Industry Standard). Figures 3.1(a) and (b) are the schematics of ISO and JIS probe configurations respectively.

A quenching probe is designed to be sensitive to heat transfer occurring on the probe surface. Cooling curve analysis probes should be free from phase transformation within the working temperature range so that the probe can be reused many times and also to eliminate the complexity of metallurgical transformations in the data analysis. Some standards, including the JIS, use silver for the probe material because of its high thermal conductivity. To further enhance sensitivity, the thermocouple is located at the surface of the JIS probe.

The probe used for the ISO 9950 standard was designed to better model steel quenching performance. Heat transfer that occurs on the surface of the probe is not only the function of surface temperature, but also many other factors, such as material, surface roughness, surface oxidation, etc. A part made of silver may perform quite differently from a steel probe even though it starts from the same austenization temperature and immersed into the same quenching tank. The ISO probe is made from Inconel 600 that more closely models the thermal conductivity of steel than silver does, and it is oxidation resistant. This probe contains a single Type K thermocouple inserted to the geometric center of the 12.5mm diameter, 60 mm long cylindrical bar.

Past experience has shown that highly sensitive probe configuration, for example a JIS silver probe, will respond to fast cooling processes, such as shock film boiling, and reveal some details of the quenching process that are not readily observable with the ISO 9950 Inconel probe. It is not necessary that the probe always be constructed in a cylindrical bar shape. A thin plate may also be used. The thermocouple can be located either at the center, near the surface, or at the surface.

In addition to above two standards, there are some other standard procedures used in various quenching analyses. For example, Liscic ^[36] proposed a thermal gradient testing bases on the measurement of temperature gradient at the surface region. This method uses a $\phi 50 \times 200$ mm stainless steel probe in which temperatures are sampled at the surface, 1.5mm below the surface and the center of the probe. Thus temperature gradient on the surface can be obtained by directly differentiating the data (e.g. $\frac{T_i - T_j}{\Delta_u}$) or though

certain mathematical treatment (e.g. quadratic fitting of temperature points and then obtain the thermal gradient at the surface). Heat flux or heat transfer coefficient may then be computed as:

$$q = -k \frac{\partial T_{surf}}{\partial r}$$
(3.1)

$$h = \frac{k \frac{\partial T_{surf}}{\partial r}}{T_{\infty} - T_{surf}}$$
(3.2)
The advantage of the thermal gradient method is that instead of temperature it provides temperature gradient at the surface, and thus simple and direct mathematical treatment (Eq.3.1 & 3.2) can be applied. It may not pose strict geometric and thermal conductivity constraints on the probe configuration, for instance, small dimension and high conductivity required by lumped capacitance model as discussed in section 3.2. In addition, thermal gradient method could be applied to not only laboratory quenching tests but also workshop practice. However the applicability of thermal gradient method is limited by the complexity of the probe configuration, extremely sensitivity to the accuracy of thermocouples and thermocouple embedding, and excessive disturbance of the temperature field because more thermocouples have to be embedded in the probe, compared to other standards.

This part of the thesis focuses on the methodology of deriving heat transfer coefficients from cooling curve temperature-time data. Although only ISO 9950 Inconel 600 type probes were used, the probe specifications for this study were extended to permit the simulation of the cooling behavior of a JIS silver probe with a surface thermocouple.

3.2 Lumped Capacitance Model

Heat transfer coefficient is a critical parameter for both quenching practice and computer simulation of quenching processes. It may be used as a quantitative criterion for the comparison between quenchants and it is a necessary boundary condition for modeling and simulating the quenching process. As discussed above, the overall quenching heat transfer mechanism is complicated. For example, oil quenching, exhibits at least three cooling phases: full-film boiling, nucleate boiling and convective cooling. Consequently it is difficult to directly model heat transfer between the quenchant and the part being quenched. Typically, heat transfer coefficients that are reported are not associated with a specific cooling process and they are derived from experimental temperature-time data. Lumped heat transfer analysis is a simple inverse heat conduction model used to derive heat transfer coefficients from temperature-time data obtained from the cooling curve data associated with a particular probe. The model is an example of an inverse heat conduction problem. The model is based on one-dimensional heat conduction and is illustrated as follows.

One dimensional heat conduction model:

Partial differential equation:

$$\frac{\partial}{r\partial r}(kr\frac{\partial T}{\partial r}) + Q = \rho C \frac{\partial T}{\partial t}$$
(3.3)

Boundary condition:

$$-\left.k\frac{\partial T}{\partial r}\right|_{r=R} = h(T_{r=R} - T_{\infty})$$
(3.4)

Initial condition:

$$T(r, 0) = f(r)$$
 (3.5)

Lumped capacitance analysis assumes that the temperature variations inside the bar are very small and thus considered being uniform. *i.e.* T(r, t) = T(t). If constant thermodynamic properties and zero heat generation rate Q are assumed, *i.e.* no phase transformation, the following lumped thermal equation can be applied:

$$\rho C V \frac{\partial T}{\partial t} = h A (T_{\infty} - T)$$
(3.6)

where V is the volume of the probe, A is the surface of the probe, C is the specific heat, and ρ is the density.

For this model to be successful, the bar dimension must be sufficiently small and thermal conductivity of the probe must be sufficiently high. A range of Biot number (Bi), a dimensionless parameter can be used to determine the validity of lumped capacitance approach.

$$Bi = \frac{hL}{k} < 0.1 \tag{3.7}$$

where L is the characteristic dimension that could represent the radius of the cylindrical bar or the half thickness of the thin plate. Biot number is a quantitative criterion for comparing the thermal resistance between the surface and interior domain. Figure 3.2 schematically illustrates the effects of Biot number on the temperature profiles. An efficient way of study the effects of thermal conductivity k, heat transfer coefficient h and dimension L is to use a thermal circuit, an analogy to an electric circuit. Biot number can be reformatted as:

$$Bi = \frac{\frac{L}{kA}}{\frac{1}{hA}}$$
(3.8)

where the numerator represents thermal resistance due to conduction while the denominator represents thermal resistance due to convection, as shown in the lower part of Figure 3.8. High Biot number means that the thermal resistance for conduction is significant and implies a significant temperature difference within the conduction domain. Low Biot number suggests that thermal resistance mainly come from convection on the surface and therefore the temperature within the conduction domain is small. In order to study the heat transfer coefficient, it is required that the convective thermal resistance composes a major part of the total thermal resistance. As a result one may study the heat transfer coefficient using temperature at the center of the probe (T_c) and the quenchant temperature (T_{∞}) by ignoring the contribution of conductive thermal resistance.

Based on the assumption of low Biot number, the lumped capacitance approach is used to derive the heat transfer coefficient from the cooling curve analysis temperaturetime data. Since the temperature at either the center or near the surface is recorded during the test, the heat transfer coefficient may be derived from Equation 3.6:

$$h = \frac{\rho C R \frac{\partial T}{\partial t}}{2(T_{\infty} - T)}$$
(3.9)

3.3 Numerical Experimental Procedure for Testing the Validity of Lumped Capacitance Model

Although any of those aspects of the quenching probe test is a non-trivial subproblem and still deserves further investigation, this section focuses on addressing the applicability of the lumped capacitance model to derive the heat transfer coefficient from a numerical modeling perspective. To simplify the problem, it has been assumed that there is no error in temperature measurement. This simplification is performed to isolate the lumped capacitance model from the other complexities of the test. Instead of experiments involving in-situ testing, it is proposed that numerical experiment such as the one described here be used. This procedure is schematically illustrated in Figure 3.3.

Basically there are three steps in the numerical experiment:

- Assume a heat transfer coefficient and perform a typical one-dimensional heat transfer analysis, either using a closed-form or numerical approach. This is the simulation of the real quenching probe test. Constant material properties are assumed. Temperature profile either at the center or near the surface, according to different test probes, can be obtained from the simulation. As discussed above this is the implementation of an assumed ideal test.
- 2. Calculate the heat transfer coefficient using equation 3.9. This calculation corresponds to post-processing of the result of a practical test, in which one uses measured temperature profile(s) to derive the heat transfer coefficient.
- 3. Compare the heat transfer coefficients between the one assumed in step 1 and the one calculated in step 2. This validation step represents the advantage of a numerical experiment over a real test. In practical applications it is impossible to validate the data we obtained since we do not know what the true heat transfer coefficients would be.

The numerical experiment is mostly dependent on the accuracy of step 1, *i.e.* the simulation will correctly reflect the thermal response during the test. Actually the simulation in the first step is simplified by assuming a one-dimensional heat flow and constant material properties. Several articles in the literature on computer simulations have shown that the simulation in step 1 is reliable enough to be the basis of numerical experiments. ^[28,32,65,67,86,105,107-111]

The ISO 9950 Inconel600 probe configuration was used for this part of study. Lumped capacitance analysis was performed using the temperature-time data of the center of the probe, simulating the reading of the thermocouple at the center of the Inconel600 probe. Data that would be expected from the JIS silver probe is simulated from ISO probe configuration by replacing the Inconel600 material properties with those of silver, and using surface temperature in the lumped capacitance model. The simulations were carried out by using ANSYS, a commercial finite element analysis code, running on a HP9000 workstation. Table 3.1 lists the material properties of the probes that were used and Table 3.2 summarizes the test cases analyzed.

3.4 **Results and Discussions**

The numerical tests were divided into two categories: linear and nonlinear. In linear analysis, constant heat transfer coefficients were assumed. Nonlinear analyses utilized heat transfer coefficients close to those found in quenching oils used in the workshop. It is this temperature dependence that accounts for a typical three-stage heat transfer in oil quenching process as shown in Figure 3.3.

Figure 3.5 illustrates the results of linear analyses. Constant heat transfer coefficients $500 \text{ W/m}^2\text{K}$ and $2000 \text{ W/m}^2\text{K}$ are used respectively. The results indicate that the heat transfer coefficients calculated by lumped capacitance model are in good agreement with the assumed values. However latencies in the initial stage of probe response were observed in all test cases.

The lumped model gives results of acceptable accuracy even when Biot number is as high as 0.74 (Inconel600 probe, $h = 2000 \text{ W/m}^2\text{K}$). This is much higher than the acceptable range for conducting a lumped capacitance analysis (Biot < 0.1). Simulations have shown that temperature difference is negligible for a silver probe (Biot << 1), however, the temperature difference between surface and center is not negligible for the Inconel600 probe as shown in Figure 3.6. It is interesting to find that the predictions are still acceptable after the Inconel600 probe passes the latencies. The reason is that the lumped capacitance model is more sensitive to the temperature rate ($\partial T/\partial t$) than the temperature itself. Because the assumed heat transfer coefficient applied at the probe surface is constant, the probe is able to overcome the latency and thus respond to the surface heat transfer condition to a certain extent. Nevertheless the basic rule still holds here, namely the lower the Biot number the better the prediction, not only in the overall accuracy, but also in the fast response and negligible latency.

The nonlinear tests used an assumed, more practical heat transfer coefficient, one close to a typical oil quenching, as shown in Figure 3.4. The assumed heat transfer coefficient reflects the highly nonlinear boundary conditions that a quenched component may experience in practice. The nonlinear boundary conditions make the simulation in step 1 of numerical experiment nonlinear.

Figure 3.7 shows that the silver probe responds to the surface heat transfer very quickly and therefore the lumped analysis reproduces the heat transfer coefficients very well. On the other hand the Inconel600 probe suffers significant dumping in the peak region due to a high Biot number value, as shown in Figure 3.8. Unlike the tests for constant heat transfer coefficient, a low Biot number becomes extremely important in highly nonlinear tests since there will be no time for a low sensitivity probe to catch up with the fast changing heat transfer at the probe surface.

ISO Inconel 600 probes have been widely used in quenching practice and their tests have been designated more representative of actual steel quenching. As shown in the numerical experiment, however, they exhibit significant dumping (the predicted value is lower than the assumed heat transfer coefficient) and thereby are unable to capture the details of the heat transfer occurring at the surface of the probe. This significantly jeopardizes the applicability of the probe. Although other alternatives are applicable, the procedure proposed by this study modified the lumped capacitance model with a modification factor as a function of Biot number:

$$h_{new} = \frac{\rho C R \frac{\partial T}{\partial t}}{2(T_{\infty} - T)} \cdot f(Bi) = \frac{\rho C R \frac{\partial T}{\partial t}}{2(T_{\infty} - T)} \cdot f(\frac{hL}{k})$$
(3.10)

The choice of modification as a function of Biot number is legitimate since it has been shown that the dumping is less significant in low Biot number tests (e.g. silver probe) and dramatic in high Biot number test (Inconel 600 probe). However this approach poses another numerical difficulty in the model, namely nonlinearity. Since Biot number is a function of heat transfer, the model described by Equation 3.10 becomes nonlinear. To simplify the procedure, the following two-run approach is proposed:

- 1. Calculate the *h* using Equation 3.9 in the first run.
- 2. Calculate h again using equation 3.10 in the second run, in which the Biot number in function f(Bi) uses the heat transfer coefficient calculated in the first run.

The modification function used in this study is exponential and is shown in Equation 3.11:

$$h_{new} = h \cdot f(Bi) = h \cdot f(\frac{hL}{k}) = h \cdot 1.5^{\frac{hL}{k}}$$
(3.11)

The number 1.5 is not arbitrary. It was determined by careful observation of the results. By applying this approach, the predicted computational results showed significant improvement as shown in Figure 3.8. This treatment is not limited to Inconel 600 probes undergoing nonlinear quenching processes, improvements were also found when it was applied to linear cases and silver probes.

One may also find that besides dumping, there is also a shift of peak value, e.g. the peak value of the predicted heat transfer coefficient (at 400°C) is different from that of the assumed (at 350°C). A further modification can be adopted to handle this shift. In this study, a modification based on quadratic function of Biot number was used to shift the temperature in the h-T curve:

$$T' = T - 60 \times Biot^2 = T - 60 \times \left(\frac{hL}{k}\right)^2$$
(3.12)

Figure 3.9 shows the predicted heat transfer coefficient value after modifications proposed in both Equations 3.11 and 3.12. Significant improvement was found.

Another important fact that has been realized from the experiment is that the location of thermocouple in the probe is not critical when Biot number is low, for example in a silver probe. As shown in Figure 3.7, predictions for center and surface nodes are both very good. Embedding a thermocouple at the probe center would be easier and more reliable than locating it at the probe surface. Therefore locating thermocouple in the center of the silver probe is recommended based on work from this study. On the

other hand, the location of the thermocouple causes significant difference for the Inconel600 probe since the temperature is not uniform within the probe. Figure 3.10 shows the predicted heat transfer using temperature profiles at center and surface nodes respectively. The results illustrate the large differences between these two approaches, in which heat transfer coefficient is over predicted by using temperature profile of surface node. As a result, in highly nonlinear situations like a practical quenching process, the results will be sensitive to the location of the thermocouple.

3.5 Concluding Remarks from Heat Transfer Coefficients Studies Using the Improved Lumped Capacitance Model

Several conclusions can be drawn from the numerical experiment:

- 1. The lumped capacitance model works very well with high sensitivity probes such as silver probes in all cases, linear and nonlinear.
- 2. The lumped heat capacity model is capable of producing good results when the probe undergoes a constant heat transfer coefficient process, even though for the low sensitivity ISO Inconel600 probe.
- 3. Significant dumping effects can be found in an ISO Inconel600 probe undergoing a highly nonlinear process, for example a practical liquid quenching process. The lumped heat capacity model, however, could still be applicable if reasonable modifications can be adopted, as demonstrated in this study.
- 4. The location of the thermocouple is not significant for a probe with low Biot number, for example a silver probe. Locating the thermocouple in the midsection of the probe is recommended.

Figures 3.11-3.13 show some examples of practical use of measuring heat transfer coefficient using ISO quenching probe with the modified lumped capacitance model, namely Equations 3.11-3.12. As a standard methodology important aspects of heat

transfer coefficient can be studied by quenching probe tests. In practice there are two important factors, namely the effects of quenchant temperature and quenchant agitation. In many modeling procedures, heat transfer coefficients are nonlinear. A common type of heat transfer coefficient is in the format of h = h(T). For example, heat transfer coefficient is treated as a function of surface temperature. However, at least study has shown that significant differences could be expected due to the quenchant temperature as well.^[2] Sometimes the heat transfer coefficient is treated as a function of both probe surface temperature and quenchant temperature, for example an averaging temperature. However this improvement is generally not good enough either. Figure 3.12 shows a case study for the effect of quenchant temperature using an ISO quenching probe. A set of results were obtained in a water solution with the same agitation but different temperature ranging from 40°C-90°C. The result shows that when water temperature goes up the temperature corresponding the peak value shifts towards lower temperature and duration of vapor blanket stage increases significantly. Although water temperature does not change peak values significantly the shift and longer duration of vapor blanket stage implies a much slower quenching process.

3.6 Difficulty with Quenching Probe Test and Future Work

The difficulties associated with the quenching probe test have been widely documented, including test methodology, probe configuration, sensitivity, and stability.^[102,103,112] Use of quenching probes is intended to acquire information on the quenching process which is assumed similar to what happens in a workshop practice. Although the procedure involved in a quenching probe test may be simple, there are many aspects that significantly affect the accuracy and the applicability of the test result.

First of all one must realize that the data obtained from a quenching probe test may not reflect the workshop quenching of a practical part even though the part is quenched in the same quenching tank as the quenching probe. Quenching probe test can be used as a standard methodology for comparing various quenching configurations, for instance quenchants, quenching tank designs, agitation etc. Quenching of a practical part, however, may differ significantly from quenching of a probe, because of the geometry, materials, agitation, quenchant temperature, etc. For example, one may use a JIS probe to obtain the temperature dependent heat transfer coefficient. Unfortunately the data may not represent exactly the heat transfer coefficient of a practical quenching of a steel part. Several factors contribute to the discrepancy:

- The heat transfer behavior on a steel surface is different that of a silver surface
- The local heat transfer coefficients may differ significantly with regard to the location of the surface. For example heat transfer in a hole is much different from that of a free surface.
- The quenchant temperature when quenching a big part may be raised higher than that of a quenching probe.
- The flow pattern of the quenching tank when practically loaded may significantly differ from that of quenching probe test.

Using the quenching probe test to obtain heat flux or heat transfer coefficient is a inverse heat conduction problem (IHCP). The problems of the nonlinear tests are actually inherited from the nonlinear inverse conduction. Inverse conduction is known to be an ill-posed problem and known to be much more difficult than a well-posed heat conduction problem. Detail investigations on inverse heat conduction can be found in references^[113,114]. The difficulties of the inverse heat conduction analysis, for example the lumped approach discussed in this paper, stems from two major aspects: dumping and extremely sensitive to measurement errors. In general it is not surprising to get a noisy temperature profile from a data acquisition system. Smoothing out the noise can introduce significant error to the time differential of temperature $\partial T / \partial t$, which is a crucial experimental input in deriving heat transfer coefficient in the model. Other important aspects one needs to be aware of is that a quenching probe test may differ according to probe geometry, probe material, surface condition, quenchant type, quenchant temperature, quenchant agitation, and so on.

In this section, the problem was addressed from a pure modeling perspective. In practical applications, many issues arise from both the algorithm and system configurations such as the accuracy of thermocouple, data sampling, and so on. The system error is critical to both actual tests and numerical experiments since lumped analysis is extremely sensitive to errors.^[113] One may argue that the simulation in step 1 may introduce errors that lead to inaccurate prediction. It is true that there is no perfect validation methodology, especially for nonlinear problems such as oil quenching. In an actual test system, errors could be more significant and lead to erroneous results. Given the flexibility and advantages of numerical experiments, another numerical experimental procedure is desired to study the influence of system error on the derivation of heat transfer coefficient via lumped analysis. For example by introducing noise artificially, the impact of data smoothing can then be investigated. More desirably, a numerical procedure may need to be examined and the impact of the heat transfer coefficient on the result of simulation results, thermal history or even residual stress state. This can give a quantitative understanding of the importance of quenching probe test.

Other future work may study the effects of nonlinear material properties, including temperature dependent thermal conductivity and heat capacity, the sensitivity. It is also interesting to compare the results between different modeling approaches, including lumped capacitance model, temperature gradient method and other inverse heat conduction procedures.^[115] Future efforts could also be made to study the effects of other experimental details, such as thermocouple sensitivity and disturbance of the temperature filed within the probe due to the thermocouple(s) embedded.

Material types	Thermal conductivity	Specific Heat	Density
	(W/mK)	(J/kgK)	(kg/m^3)
Inconel600	17	460	8000
Silver	400	230	10500

Table 3.1Probe Material Properties.

Table 3.2	Test	Config	urations.
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Test case	Material types	Probe diameter (m)×10 ⁻³	Heat transfer coefficients* (W/m ² K)	Biot number $\frac{hR}{k}$
#1	Inconel600	12.5	500	0.18
#2	Inconel600	12.5	2000	0.74
#3	Silver	12.5	2000	0.031 ***
#4	Inconel600	12.5	oil**	0.92 ***
#5	Silver	12.5	oil**	0.039 ***

* These are the assumed heat transfer coefficients used in the first step of numerical experiment.

** The heat transfer coefficient for "oil quenching" is shown in Figure 3.4.

*** The maximum Biot number corresponds to the peak value of heat transfer coefficient.



Figure 3.1 Schematics of probe geometry.



Figure 3.2 Effect of Biot number on temperature profile. Static heat conduction with constant temperature on the left wall and convection on right wall.



Figure 3.3. Comparison between an actual test and the numerical experiment procedure.



Figure 3.4 Assumed heat transfer coefficient in numerical experiment step 1.



Figure 3.5 Predictions of constant heat transfer coefficients. The reference heat transfer coefficients are indicated in the parentheses.



Figure 3.6 Temperature profiles of surface and center node of Inconel600 probe.



Figure 3.7 Predicted heat transfer coefficients by silver probe. Predictions use both center (ISO suggested) and surface nodes (JIS suggested).



Figure 3.8 Predicted heat transfer coefficients by Inconel 600 probe. Lumped model uses temperature at center of the probe.



Figure 3.9 Predicted heat transfer coefficient after adopting improvements suggested in this study. Inconel 600 probe using center node, nonlinear test.



Figure 3.10 Predicted heat transfer coefficients using surface and center nodes respectively (Inconel 600 probe).



Figure 3.11 Heat transfer coefficient of quenchant A. Data using both pure lumped capacitance model and modified model are plotted.



Figure 3.12 Heat transfer coefficient of quenchant B. Data using both pure lumped capacitance model and modified model are plotted.



Figure 3.13 Heat transfer coefficients of quenchant C with different levels of addictive. Calculated by modified lumped capacitance model and curves represent 5%, 10% and 15% addictive respectively.



Figure 3.14 Effect of water temperature on the heat transfer coefficient. Calculated by modified lumped capacitance model and water temperature ranges from 40°C-90°C.

CHAPTER 4

INCORPORATING PHASE TRANSFORMATION IN THE ANSYS PROGRAM

The core of heat treatment processes is the control of temperature. Heat transfer is therefore always one of the most important topics in heat treatment. The complexity as well as the fundamentals of heat treatment is based on the phase transformations associated with the heat treated component during a heat treating cycle. A typical heat treatment cycle, e.g. hardening, involves heating up to an austenite temperature followed by cooling down to the room temperature. During the heating stage, the component undergoes phase transformation from the phase(s) at room temperature, e.g. pearlite for eutectic steel, to austenite. After a holding period at austenite temperature the component is then cooled down at a specific rate, according to the desired end microstructure, to room temperature. In hardening, as mentioned before, fast cooling process, such as oil quenching or even water quenching is used to obtain martensite, a high hardness state of the material. The phase transformation process in heat treatment is so complicated that it may involve incubation, continuous transformation over a temperature range and more than one kind of phase transformation. Isothermal transformation (IT) or timetemperature-transformation (TTT) diagrams and continuous-cooling-transformation (CCT) diagrams are two major metallurgical tools used for studying phase transformation and cycle design in heat treatment. Figure 4.1 shows a schematic of a typical heat treating cycle involving both heating and cooling periods.

4.1 In-house Code vs. Commercial Code

Many modeling procedures use computer programs to solve the mathematical equations that describe the problem being studied. Solutions are usually not easy to obtain due to the complexity of the problem. Occasionally a close-form solution can be achieved, however, in most cases numerical procedures have to be adopted and then implemented into a computer code. There are two main choices of a computer program, namely developing an in-house code or purchasing commercial codes. In-house coding requires that code developers have sophisticated computer skills as well as deep understanding in problem specifications, numerical procedure and efficient algorithms. In addition vast amount of man-hours are necessary for problem analysis, code design, implementation, debugging and maintenance. Therefore it is not a general approach for large-scale models. However, an in-house code is generally more problem-oriented. It can accommodate the specific requirements of the problem, such as transformation plasticity in the residual stress analysis of a quenching process. It also gives the flexibility of implementing user-developed or customized models or algorithms. On the other hand, commercial code is a multi-purpose tool that one can purchase from a store or vendor. Thanks to the fast development of digital computer and software engineering there are many scientific calculation programs available, ranging from finite element analysis to solution post-processing. For instance the ANSYS program is a finite element analysis code for general research purposes, including heat transfer, structural, magnetic and coupled analyses. A commercial code is normally developed to be as general as possible in order to accommodate as many types of application as possible. It is developed under the joint efforts of software engineers and the domain experts with expertise in specific applications, for example numerical analysis, heat transfer, structural mechanics, fluid mechanics, etc. The code is normally well developed and sophisticated from the perspective of software engineering. It is user-friendly, robust and efficient in most cases. It saves tremendous amount of efforts for the end users, however, it may not meet all requirements of solving a specific problem. In certain cases a user needs to customize the code to incorporate specific functions into the existing code. Quenching,

for example, requires incorporation of phase transformation with thermal and thermal stress analysis. The ANSYS program, although quite a versatile code already, can only accommodate simple transformation phenomena and can not handle a metallurgical transformation process at the current release. An ANSYS user thereby will have to find ways of code customization, for example either ANSYS Parametric Design Language (APDL) or user developed routine. Many advanced commercial codes recognize the potential needs of extension and thus provide code customization capability often in a variety of methods.

There is still a debate on whether a serious modeling researcher should use an inhouse code verse a commercial one. Some people argue that one should have full control over the modeling procedure. In that case only in-house coding becomes a viable option. By in-house coding one can understand the algorithms that are used, the model implementation, efficiency of the numerical procedure, the details of the actual behavior of the program, the sources of the error and the limitation of the code. The commercial codes often give limited information about these critical issues. Therefore a modeling procedure may easily go wrong due to undocumented misleading functions or unknown bugs in the software. On the other hand, many people tend to use commercial codes, which provide user-friendly interface and versatile functionality. Some in the debate point out that it was not the responsibility of an application domain user to do programming, but only know how to use the code as a tool for solving the model. Also they argue that in-house code is not an efficient way of doing modeling practice. Inhouse code has other limitations such as less portability, difficult to use and buggy. In many cases in-house code can only handle simple models such as 1-D or 2-D problems

Knowledge and experience with in-house code development become very valuable in efforts of customizing general-purpose codes. For successful customization of the ANSYS program the author relied on the prior knowledge of in-house code development for application in cycle design and optimization in heating and gas carburizing processes. The reward for the laboring programming task is the full control over the functionality and algorithms. Although it is not a trivial task, incorporating metallurgical functions like phase transformation is made possible and can be embedded

into the code smoothly. In the current research commercial codes were the main tools used to carry out thermal history analyses, CFD computations and residual stress analysis in quenching process. It is the author's experience and recommendation that one should take advantage of commercial codes as much as possible. As a result of multidisciplinary efforts, commercial codes are generally well designed and implemented. It is user-friendly, well tested, robust, and portable. If some aspects of a specific problem were not supported, one would be better of customizing commercial codes than developing in-house capabilities. An advanced commercial code will provide ways of user customization, in which new functionality can be added to certain extend, such as the user programming feature of ANSYS. In-house code is probably the last choice if no appropriate user customization is provided by the commercial code, or when the problem to be studied is very simple, such as one-dimensional analysis or simple data processing. In contrast to the need to spend a majority effort in programming and debugging in-house coding, one may spend valuable research time in problem analysis and modeling troubleshooting. For example, the author spent more than half of the effort required to complete an MS thesis developing an in-house three dimensional heat conduction code. On the other hand, customizing a commercial code only took 10% of the effort thus freeing up as much as 90 percent of research time to study the problems and build correct models in commercial codes like ANSYS or SYSWELD.

From software development point of view software engineering is extremely complex. No matter how well a piece of software is developed, it is very difficult to eliminate all errors or bugs. One important thing that a user needs to be aware of is that whatever functions that a commercial code may provide one needs to understand the theory, numerical procedure and the nature of the problem just like doing a in-house programming. This is very important for the efficient and appropriate use of the commercial codes. Commercial codes are usually robust and always seem to be able to yield "impressive" results. However without sufficient knowledge, it is impossible for a user to know the limitation of the code, correct use of the program parameters defining the problem, let alone the model troubleshooting and data interpretation. It is the author's opinion that the boundary between in-house and commercial code is not that important. When the size of an in-house code is big and the functions are many, the code is close to a commercial one since the details of the code would be hard to understand and controlled by one end user. Therefore it is not a problem of in-house or commercial code but how to use the code efficiently and correctly.

4.2 Incorporating Latent Heat of Phase Transformation into ANSYS

Simulations in this part of study were carried out using ANSYS, a commercial FEA code. ANSYS is a finite element analysis code for general purpose. It implements generic modeling requirements including heat transfer, structural analysis, fluid dynamics, magnetic field, electric field as well as coupled phenomena such as coupling between thermal and stress, thermal and fluid flow, electric and magnetic analysis. In general ANSYS is a quite versatile tool for solving modeling problems. Unfortunately ANSYS is not strong enough to handle the metallurgical phase transformation of a quenching process, even though it provides phase transformation functionality.

Using the phase transformation function in ANSYS requires knowing of transformation temperature range and transformation progress with respect to temperature before hand. For instance, if the specific heat temperature curve is known, the area below the spike, the transformation region, represents latent heat (Figure 4.2). The ANSYS program used this approach in its early version. After revision 5.0, phase transformation is specified in terms of enthalpy instead of specific heat (Figure 4.3). This new approach is recommended because the enthalpy-temperature curve is smooth and thus can be treated more efficiently. Unfortunately phase transformation in quenching processes involves a continuous transformation over a large temperature region. It may involve several kinds of transformation, for instance, austenite to ferrite, austenite to pearlite, austenite to bainite and austenite to martensite. Moreover it is not necessary that the transformations in heat treating depend on the entire thermal process. According to different cooling histories, a quenched part may experience quite different phase

transformations and results in different transformation products. Therefore modeling phase transformation requires a dynamic procedure which strongly couples it with the calculation of the thermal history. Due to the limitation of ANSYS the coupling between phase transformation and thermal history has to be incorporated by code customization.

There are two ways of customizing code to incorporating metallurgical nature phase transformation into the standard ANSYS, namely ANSYS Parametric Design Language (APDL) or user routine. The idea behind the incorporating phase transformation is that during every time step, latent heat is calculated according to the previous history and metallurgical transformation information like TTT or CCT, and then is applied in to model as heat generation rate term. Recall the heat conduction model in Chapter one:

$$\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + Q = \rho C p \frac{\partial T}{\partial t}$$
(4.1)

The main task is the calculation of heat generation rate Q base on metallurgical and thermal history. Calculating latent heat for martensitic transformation is straightforward using Koistinen & Marburger^[73] model, which is temperature dependent only. The volume fraction of martensite at temperature T is calculated by:

$$f_n = f_n^{\max} [1 - e^{-\gamma (Ms - T)}]$$
(4.2)

where f_n is the volume fraction of martensite transformed, f_n^{max} is the volume fraction of the material available for martensitic transformation, and γ is a constant, which equals to 0.011 in many steels. The heat generation rate due to latent heat is calculated according to the volume of martensite transformed during a time step:

$$Q = \Delta H_{\gamma \to a} \frac{f_{n+1} - f_n}{\Delta t}$$
(4.3)

where $\Delta H_{\gamma \to \alpha}$ is the enthalpy change of the phase transformation.

Calculating the latent heat for diffusional phase transformations is more complicated. The transformation behavior depends on not only the temperature itself, but the entire thermal history. The model needs CCT or TTT diagrams to calculate the incubation and volume fraction transformed. The transformation must overcome the incubation period before start. The incubation finishes if the following criterion is met:

$$\sum_{i=1}^{n} \frac{\Delta t_i}{t_{iT}} = 1$$
(4.4)

where Δt_i is the time span at *i* th step, t_{iT} is the incubation time at temperature that the component reaches at *i*th time step. This can also be determined from TTT diagram.

The calculation of latent heat of continuous cooling is described as follows:

Transformation fraction:

$$f_{n+1} = 1 - exp[-c(T) \cdot \theta^{n(T)}]$$
(4.5)

Fictitious time:

$$\theta = \Delta t + \left[\frac{\ln(1-f_n)}{c(T)}\right]^{\frac{1}{n(T)}}$$
(4.6)

Heat generation rate:

$$Q = \Delta H \frac{f_{n+1} - f_n}{\Delta t}$$
(4.7)

where ΔH is the enthalpy change of the phase transformation, C(T) and n(T) are material properties that can be determined from the TTT curve. The details of the procedure are discussed in detail elsewhere^[71].

The latent heat is finally incorporated into ANSYS as heat generation rate via command "BF" or "BFE^{"[69]}. Latent heat is calculated using "backward" scheme, i.e. the latent heat at t+1 is calculated from the information at time t. Therefore it is highly recommended that very fine time step is used when transformation starts. Alternatively an iterative algorithm, though not implemented in this study, can be developed without much difficulties. Figure 4.4 shows the flowchart of a generic procedure to incorporate phase transformation in this manner.

4.3 Simulation of the Latent Heat in Austenitic and Martensitic Transformation

Two case studies are presented in this section to demonstrate the procedure for customizing the ANSYS code to incorporate latent heat of phase transformation. Figure 4.5 shows an axisymmetric model of the component used in one of the studies. The

material is M2 tool steel. A typical hardening treatment was studied, which involves austenization followed by oil quenching. The heating up was done in a salt-bath with bath temperature at 1200°C. The austenite transformation starts at 730°C. The transformation calculation used a step-wise approach such as the one shown in Figure 4.6. The quenching was done in mineral oil. The Ms point is 350°C and the oil temperature is 80°C. The cooling involved a highly nonlinear heat transfer mechanism as discussed in earlier sections. Figure 4.7 shows the thermodynamic properties and heat transfer coefficient used in this simulation.

Calculation of latent heat for the heating up process used the method discussed in the earlier section, namely Equations 4.4-4.7. The implementation uses ANSYS Parametric Design Language (APDL). Figure 4.8 is the APDL code for incorporating latent heat of austenization transformation. The generic template pattern has been marked on the code segment. Although the details might be different, the procedure is proposed as a generic method for phase transformations. The content of each section may need to be changed when the template is used for other specific phase transformations.

M2 steel is of high hardenability, which can be through hardened, in a wide cooling range. This characteristic is shown in its isothermal transformation (IT) diagram or temperature time transformation (TTT) diagram.^[70] Therefore only martensite transformation is of concern in the simulation. Incorporating martensitic transformation is easier since the martensite volume fraction in the model is only a function of temperature. Therefore the code can be much simpler in the section of transformation fraction calculation, as shown in Figure 4.9. In the simulation the martensitic transformation starting temperature is assumed to be 350°C. Figures 4.10-4.11 show the temperature profiles of the component at points A and B. Figure 4.10 shows the temperature profiles for salt-bath heating cycle while Figure 4.11 shows oil quenching. Compared with those temperature profiles without phase transformation, the effect of the phase transformation is significant. Some oscillation was encountered in the simulation. To minimize solution oscillation, finer time steps had to be used.

Another case study involved a design issue of heat treating cycle for a practical application. The heat treated component is a step roll used for rolling mill application.

Different hardness is desired on the surface of the body and necks of the step-roll, as

illustrated in Figure 4.12. High hardness is required on the surface however lower hardness is targeted for the necks to achieve certain level of toughness. In the original cycle, the component was heated and quenched as whole and local tempering was applied on both necks to reduce the hardness. Based on the knowledge of the influence of temperature on the metallurgical transformation and resultant hardness, a new cycle was proposed which used partial heating and quenching as illustrated in Figure 4.13. In the new cycle, the step-roll was partially immersed into the salt bath at 860°C for a period of time t_1 and then totally immersed into the oil for another period of time t_2 . This kept the upper neck at a lower temperature state. As a result the as-quenched hardness of the upper neck could be lower than the rest of the body. Quenched in a similar manner, the step-roll was turned up side down and the original lower neck stayed above the oil for a while to reduce the cooling rate of that neck so as to reduce its as-quenched hardness. After quenching both necks would have lower hardness than the surface. Local tempering is not necessary for the necks. In the new cycle however, the duration of partial heating and quenching is critical. The cycle parameters and feasibility must be simulated and tested before the actual implementation. The final proposed heating cycle involved a 900-second partial immersion followed by a 300-second whole immersion in the salt-bath. The quenching cycle used a 300-second partial quenching followed by additional a 2100-second whole quenching period. To simplify the simulation only martensite phase transformation is considered in the quenching stage. Figures 4.14-4.15 show the temperature profiles during the heating and quenching cycle. The simulation illustrates the significant effects of partial heating and quenching as well as the latent heat of phase transformations. The results show that the temperature of one neck was kept lower than the rest and that slower cooling of the other neck during the quenching cycle resulted from partial quenching. The body of the step-roll remained at the expected high austenization temperature and then was subject to a high cooing rate. Unfortunately the metallurgical consequences of the cycle can not be directly predicted from the thermal history of the component. One may notice that the difference between the austeniting temperature in the different locations of the component is in the range of 10-30°C.

Without the prediction of the phase products and the CCT associated with the new cycle, one is unable to conclude whether the temperature differences will result in difference at various surfaces of the component. A full coupling of phase transformation with thermal history is thus needed if a qualitative or quantitative analysis of the as-quenched properties is desired.

The simulation results show the importance of the phase transformation in the thermal analysis of the heat treatment. Modeling phase transformations in the case studies was relatively straightforward since only martensitic and austenitic transformations were studied. In the cases involving multiple transformations, for instance the as quenched products that have pearlite, bainite and martensite, the procedure would be much complicated.

4.4 Limitation of Code Customization

Code customization is not a trivial task in some cases. It not only depends on the programmable interfaces that a commercial code provides but also the complexity of the functionality that need to be added. Fully incorporation of the transformation latent heat and transformation plasticity is tedious and inefficient. In ANSYS, for example, one needs to use APDL or user routines predefined in the ANSYS code. In order to add the full capability of phase transformation module, tremendous lines of code would be needed. For example multiple types of phase transformations including austenite to ferrite and bainite would have to be considered and a flexible way of incorporating CCT or TTT diagrams would be necessary. Finally phase transformation plasticity would need to be integrated into the residual stress and distortion procedure. Consequently tedious programming and debugging would still be required resulting in tremendous modeling overhead. A more metallurgy specific code would thus be desirable.

There are a few metallurgy specific codes in the market place or that have been developed in-housely by some research teams. SYSTUS/SYSWELD+ is an example that has been developed by FRAMATOME, a French software company. SYSWELD is an

example of commercialized customization of an existing FEA code. SYSWELD is an additional metallurgical module that was built on the top of the SYSTUS, another commercial FEA code. It uses the existing utilities of pre-processor, solver and post-processor available in SYSTUS. For example, building a quenching model follows the same standard procedure of conventional FEA model as that in SYSTUS. However metallurgical information such as CCT or TTT diagram, thermodynamic and mechanical properties of individual phases are the additional information that are required by the SYSWELD module. Additional degrees of freedom such as volume fraction of phases will be obtained after solving the problem. Post-processor facilities in SYSTUS can be used to review the results. Simulation of a practical oil quenching application will be demonstrated in the next chapter. Phase transformations such as austenite to ferrite, austenite to bainite and austenite to martensite can be computed. Moreover the residual stress and distortion calculation incorporates transformation plasticity.





A - Austenite, P - Pearlite, F - Ferrite, Ms - start of Martensite transformation Ac₁ and Ac₃ - critical temperature associated with Fe-Fe₃C diagram.



Figure 4.2 Schematic of heat capacity approach.



Figure 4.3 Schematic of enthalpy change versus temperature where $H = \int \rho \cdot C dT$.



Figure 4.4 Procedure for incorporating phase transformation into ANSYS.



Figure 4.5 Geometry of the component used in the simulation showing the location of point A and B corresponding to the temperature profiles in Figures. 4.11 and 4.12.



Figure 4.6 Schematic of stepwise transformation calculation. Subdivision of heating profile superimposed on the TTT diagram.



(b) Thermal conductivity of M2 steel

Figure 4.7 Heat transfer coefficients and thermal conductivity used in simulation.



Figure 4.8 Sample APDL code for incorporating latent heat of austenization process with generic pattern marked on the code.





Figure 4.10 Temperature profiles of the heating cycle.


Figure 4.11 Temperature profiles of the quenching cycle.



Figure 4.12 Step-roll used in the simulation, different hardness is required on the different part of the roll.



Figure 4.13 Schematic illustration of new cycle using partial immersion or quenching. Total cycle time $t = t_1 + t_2$



Figure 4.14 Temperature profiles during the heating and quenching cycle, representing center and surface points of the upper and lower neck of the step-roll.



Figure 4.15 Surface temperature profiles of the different parts of the step-roll.

CHAPTER 5

THERMAL, RESIDUAL STRESS AND DISTORTION PREDICTION OF FASTENING RING

In civil engineering structures, such as bridge, highway and tunnel, many concrete constructions are reinforced with steel wires. One reinforcing method is proposed as follows:

The concrete is cast into the desired shape and steel rods are inserted into concrete structure by special equipment. The fastening rings are located at the both ends of the structure. The rod goes through from the side with larger hole to the opposite small hole. A certain amount of tension is applied on the steel rod. Both steel rod and fastening rings will be embedded in the concrete construction until it is fully solidified. The fastening rings serve as both supporting and fastening devices and they will experience large stress during the concrete construction process. In practice cracks have been found in the hole region of the ring. The original method used 40Cr steel oil quenched at 850°C. To reduce the material cost a new heat treating procedure has been proposed successfully in which the plain carbon steel 1045 is used instead of alloy steels. The heat treating involves pre-cooling in air from 850°C austenizing temperature to 830°C. The ring is then quenched in a water solution or a specific solution quenchant. The objective of the computer modeling and simulation is reported herein to qualitatively understand the thermal history distortion and residual stress associated with the quenching process so as to validate the feasibility of the new process.

This study demonstrates an integrated analysis approach to simulate and predict the results of a typical quenching process. The analysis involves obtaining heat transfer coefficient form quenching probe, thermal history analysis coupled with phase transformation, prediction of volumetric fractions of phase products, and thermal and residual stress analysis coupled with transformation plasticity.

5.1 Phase Transformation Model in SYSWELD

As discussed in Chapter 4, phase transformation plays a critical role in both thermal and thermal-stress analysis. The major aspects of phase transformation in the process modeling of heat treatment are latent heat, volumetric fraction of phase transformation products, and transformation plasticity.

There are several ways of dealing with the latent heat of phase transformation. Most heat transfer analysis codes incorporate temperature dependent heat capacity or enthalpy. For instance, to model a heat transfer process involving solid to liquid transformation like ice to water, one may simply specify a temperature dependent enthalpy curve with a steep change at the melting point region. This kind of analysis can easily be carried out in a commercial code like ANSYS. Another way of modeling latent heat can be by calculating the heat generation rate incrementally during the simulation process. This approach is more difficult but more powerful. It can be used to handle the latent heat of a continuous transformation process like that encountered in heat treatment. A good example of such an approach used to extend the capability of ANSYS program to handle latent heat of a heat treating process is covered in Chapter 4 of this thesis. The heat generation rate can be calculated based on the temperature field development and metallurgical input, for example time-temperature-transformation (TTT) information.

The code used in this part of study is SYSWELD, another commercial FEA code developed by a French company, FRAMASOFT. The main advantage of SYSWELD over ANSYS is that it has full capability of incorporating metallurgical behaviors into traditional finite element analysis procedure. SYSWELD's phase transformation models

are mainly based on Leblond's work.^[44-46,56,62,116-119] which will be discussed briefly as follows.

SYSWELD incorporates latent heat of phase transformation as follows:

$$H(T) = \int_{T_0}^{T} C dT + Q_L$$
 (5.1)

where Q_L is the latent heat of phase transformation. Thus the heat conduction equation becomes:

$$div[k \cdot grad(T)] = \rho \frac{dH}{dt} + Q$$
(5.2)

where k is the thermal conductivity, ρ the density, H the enthalpy and Q the volumetric heat source other than phase transformation.

The law of mixtures is used to calculate the equivalent material properties, for example:

$$H = \sum_{phase=1}^{n} p_i H_i, \quad k = \sum_{phase=1}^{n} p_i k_i \text{ or } \rho = \sum_{phase=1}^{n} p_i \rho_i$$
(5.3)

where p_i is the volumetric fraction of the individual phases, for instance, martensite, austenite, etc.

With above treatment, the heat conduction equation will be:

$$div[k \cdot grad(T)] = \left(\sum_{phase=1}^{n} p_{i}\rho_{i}\frac{\partial H_{i}}{\partial T}\right)\frac{\partial T}{\partial t} + \sum_{phase=1}^{n} \dot{p}_{i}\rho_{i}H_{i} + Q$$
(5.4)

In the above equation, \dot{p}_i represents the transformation rate of a specific phase

developed in the process and the term $\sum_{phase=1}^{n} \dot{p}_{i} \rho_{i} H_{i}$ accounts for the effect of phase transformation in the heat conduction. The transformation rate \dot{p} is a function of the heat treating cycle, metallurgical property of the material, thermal history etc. To summarize, one may express as following:

$$\frac{dp}{dt} = f(T, p) \tag{5.5}$$

Leblond Model^[116] is incorporated in SYSWELD^[120] as follow:

$$\frac{dp}{dt} = \frac{p_{eq}(T) - p}{\tau(T)} f(\dot{T})$$
(5.6)

where p_{eq} is the maximum volumetric fraction of the phase that can be obtained at equilibrium state, and $\tau(T)$ is the delay time. $f(\dot{T})$ is the modification function used for tuning the model.

SYSWELD provides a tool with graphical user interface (GUI) to correlate the parameters from an input continuous-cooling-transformation (CCT) curve. The method of incorporating phase transformation involves building a metallurgical data file with the parameters extracted from the CCT curve and then using the file later in the thermal calculations. The detail description of the correlation procedure can be found in SYSWELD user manual.^[120]

The important aspect of phase transformation in the thermal and residual stress analysis is the additional transformation strain contributed to the total strain and the possible dramatic changes in the material properties due to the new phase products. The total strain is described as following:

$$\varepsilon^{total} = \varepsilon^e + \varepsilon^p + \varepsilon^{th} + \varepsilon^{ph} \tag{5.7}$$

where ε^{e} and ε^{p} are the elastic and plastic strain respectively, ε^{th} is the thermal strain and ε^{ph} is the strain due to phase transformation. The transformation strain is composed of two parts; strain due to the volume changes between old and new phases, and the strain due to transformation plasticity. The transformation plasticity has been modeled as following:^[120]

$$\dot{\varepsilon}_{ij}^{ph} = -\frac{2}{3} \cdot \frac{2\Delta\varepsilon_{r\to a}^{ih}}{\sigma_{y}^{r}} \cdot \ln f_{r} \cdot S_{ij} \cdot h\left(\frac{\sigma_{eq}}{\sigma_{y}}\right) \cdot \dot{f}_{r}$$
(5.8)

where

 $\Delta \varepsilon_{r \rightarrow a}^{ih}$ is the thermal strain difference between austenite and martensite

 f_{γ} is the volume fraction of austenite

 σ_v is the yield strength of the bulk material

 σ_{v}^{γ} is the yield strength of austenite

 S_{ii} is the strain deviator

$$h\left(\frac{\sigma_{eq}}{\sigma_{y}}\right)$$
 is the nonlinear term used when the applied stress is more than half of σ_{y}

 σ_{eq} is the Von Miss equivalent stress

5.2 Facilities and Procedures

Figure 5.1 shows the machine drawing of the ring used in SYSWELD model analysis. The ring is cylindrical in shape with six tapered holes. Due to the symmetry of the geometry and cooling condition that the ring will experience, only $1/12^{\text{th}}$ of the ring needs to be used in the model for analysis. Benefit of reducing the modeling domain through symmetry has already been pointed out in an earlier section, that is, this presents a more efficient model which yields equivalent results with less computation time and storage requirement. Figure 5.2 shows the solid model of the domain to be studied. In the thermal analysis, convective heat transfer boundary conditions are specified on the surfaces of the ring, i.e. surfaces A-F. Symmetry boundary conditions are defined on the symmetry surfaces, i.e. surfaces G-I. Heat transfer coefficient and quenchant temperature are the two critical parameters that need to be specified in the convective heat transfer boundary condition.

The heat transfer coefficients were measured using a non-standard quenching probe. Instead of the standard thin cylinder, the probe was in the shape of a thin plate as shown in Figure 5.3. Three thermocouples were embedded in the plate as shown in the figure. The advantage of the plate probe over a cylinder plate is that it has a large surface and thereby will give a better averaging of the heat transfer between plate and quenchant. A high frequency data acquisition system (100 points per second) was used to record the thermocouple readings.

Quenching process using water solution was simulated. The starting ring temperature was assumed to be 830°C. The water bath temperature was 20°C. To study the effect of quenching cycle, another quenching process using polymer quenchant was also simulated. SYSWELD was used to carry out the simulations of thermal, phase transformation and thermal-stress of the component during quenching processes. The code ran on a HP 9000 platform running a UNIX operating system.

Figure 5.4 shows the CCT diagram obtained from the literature^[121] which is close to the steel studied. Some material properties are given in Figure 5.5 as well. The details of the model and all material properties can be found in the appendix to this chapter. A metallurgical file was created which contains the information necessary for incorporating phase transformation progress. The convective and symmetric boundary conditions are specified on the domain surfaces A-H as shown in Figure 5.2.

In addition to the quenching probe tests, the research partner of this study, namely Shanghai Jiao Tong University, Shanghai, China experimentally measured thermal response of the component.^[122] Two thermocouples were located inside of the component when it was water quenched. Figure 5.6 is the finite element mesh used in the simulation. In addition it also shows the way and the locations of the thermocouples being embedded into the component. The data measured at these two positions, namely location 1 and 2, were used to compare with the corresponding nodal temperature values of the thermal simulation. Location 3 and the plot path indicated in the figure will be used in the thermal-stress analysis.

5.3 **Results and Discussions**

5.3.1 Obtaining heat transfer coefficients

The heat transfer coefficient is one of the most difficult parameters that need to be defined in advance in the model. A discussion on the challenges of simulating real materials processes was covered in Chapter 3. Figure 5.7 shows the temperature profiles obtained from the thermocouples. Raw test data were found to be noisy due to the violent heat transfer that the probe had experienced as well as due to other errors such as thermocouple response or data acquisition equipment. This data could not be used directly for further processing. Large oscillation or significantly amplified noise was found if cooling rate was used directly from them. The temperature value used in the analysis was the average of values read from three thermocouples. Smoothing was applied to filter out the noise. Figure 5.8 shows the smoothed temperature profile of average temperature and its corresponding cooling rate.

One may notice that the Biot number of the probe is not small enough to satisfy the lumped capacitance analysis requirement. For instance the Biot number will be as high as 1.5 if heat transfer coefficient goes as high as 3000 W/m²°C. This large Biot number implies significant dumping and shift of the peak value. The modified lumped capacitance method proposed in Chapter 3 was therefore used, i.e. Equation 3.11-3.12. Heat transfer coefficients of both water solution and polymer solution were obtained as shown in Figure 5.9.

5.3.2 Thermal history and phase products of water quenching process

Figure 5.10 displays temperature profiles at locations 1 and 2 of the component as shown in Figure 5.6. The temperature profiles at the upper right window show the temperature responses during the first 30 seconds of the quenching process. The simulated results are in good agreement with the experimental test data. The isotherms at 30 seconds after quenching are shown in Figure 5.11. The temperature profiles indicate that the component experienced a fairly fast cooling process.

Figure 5.12 shows the volumetric fractions of martensite developed after water quenching process. The plot is in transparent mode representing the volumetric fractions at the Gaussian integration points. The values at Gaussian points are the initial solution set on which the nodal solutions are derived. The figure shows that considerably large amount of martensite was obtained. One design goals was to obtain sufficient hardness and strength in the hole region. Figure 5.13 shows the martensite distribution at the hole region. Due to the fast cooling of water quenching, reasonable amount of martensite was developed at this critical region, and consequently good strength and hardness could be expected.

The simulation results have shown that the major phase constituents are pearlite, bainite and martensite. Figure 5.14 shows the development of phase products at location 2 of the component, as shown in Figure 5.6. Figure 5.15 shows the development of martensite at locations 1 and 2 in Figure 5.6 and the center of the component. Very little ferrite and retained austenite were found. Figures 5.16-5.17 show the distributions of pearlite and bainite respectively. In comparison to the CCT diagram of the steel, one may

find that the simulated total amounts of bainite and pearlite were reasonable, however, it over-predicted the bainite and under-predicted the pearlite. The error is caused by the difficulty of accurately representing CCT diagram in the SYSWELD program. In SYSWELD, a CCT curve needs to be simplified and parameterized into a metallurgical file.^[120] Simplifying and parameterizing the CCT diagram shown in Figure 5.4 is nontrivial and thus errors are inevitable. To minimize the error, one may treat pearlite and bainite together rather than separately.

From a metallurgical point of view, the quenching cycle will yield the desired combination of microstructures which will provide required mechanical properties in service. This objective can be achieved from the thermal-only analysis as described in this section. More information may be obtained from the thermal analysis, for example the temperature gradients, a good indication of the thermal stress states that might be developed in the quenching process. In general, the greater the gradient the greater the expected residual stress. Actually thermal-only analysis is a good method to be used to spot high stress regions in a cost-effective way. A detailed discussion on this issue can be found in Chapter 2.

5.3.3 Thermal stress, residual stress and distortion of water quenching process

As discussed earlier in Chapter 2, simulating a structural response due to the thermal load, phase transformation and normal mechanical load or constraints during a quenching process is much more difficult and challenging than a thermal or metallurgical analysis. The ability to predict and control residual stress and distortion is one of the ultimate goals of heat treaters.

Structural response during a quenching process was simulated utilizing the mechanical simulation engine of SYSWELD FEA code. In the thermal structure model the load comprised of thermal load only with volumetric changes and transformation plasticity occurring during the phase transformation. No significant mechanical constraints were applied except at the symmetric surfaces. To prevent the component from rigid body movement, a full constraint, zero displacement in all x, y and z directions, was applied on the node at the origin of the coordinate system. Simulation

used temperature dependent yield stress and bi-kinematic strain hardening model. The yield strengths of the phases are temperature dependent as shown in Figure 5.5. Details of the model can be found in the appendix of this chapter.

Figures 5.18-5.21 show the results of residual stress states. Figure 5.22 illustrates final distortion of the component and Figure 5.23 displays the distortion in three different views. In most cases compressive stress is desired on the surface of the component in order to improve the fracture and fatigue properties. In a normal cooling process where no martensite transformation occurs, compressive stress state is expected on the surface region while tensile stress is expected in the core. The reason behind this phenomenon is that the outer region experiences contraction first. Tension is generated at the surface region and compression at the inner region. Yielding might occur at this stage due to high stress state and probably low material strength. Later in the cooling stage, the core experiences contraction and is restrained by the hard outer surface. This reverses the stress state and leads to tension in the core and compression at the surface. If martensitic transformation is involved during the cooling process a more complicated situation can be expected. This is because martensitic transformation will introduce volumetric expansion which is opposite to the contraction during cooling process. If expansion due to martensite transformation dominates, a reversed stress state can be observed in the as quenched component. This is more likely to happen in a through-thickness hardening process. The case encountered in this study is more complicated. Figure 5.24 show the residual stress states at hole region. In the current case study considerable amount of martensite was developed in the component. However both compressive and tensile stresses has been found in the hole region which implies a complicated residual stress situation. Pure compressive or tensile stress may not easily be obtained in the hole region due to the geometric complexity, thermal history and material properties.

Cracks are mostly likely to be initiated at the locations with the thinnest crosssection where high thermal or residual stress occurs. In the current study the hot spots were in the hole region. The path shown in Figure 5.6 indicates the location of interest in this study. Figure 5.25 shows the residual stress values along the path and Figure 5.26 shows the development of thermal-stresses during the quenching process at the hot spot as shown in Figure 5.6. In Figure 5.26 a change of stress states can be found. The change starts at 3rd second of the quenching process and ends at 6th second. Referring to the austenite decomposition curve, one may notice that this is also the period of transformation including martensite formation. Thus the change of stresses could be contributed by the phase transformations.

5.3.4 Study of the alternative quenching cycle using polymer quenchant

Thermal history, phase products and the subsequent thermal and residual stresses are highly dependent on the quenching cycle. One of the most important cycle parameters is the selection of the quenchant. The water quenchant used in the study is categorized as a type of fast quenching media. Other widely used quenchants include mineral oils, polymer solutions and gases. When designing the quenching cycle one of the candidate quenchants was a polymer solution which has a lower quenching power. Its heat transfer coefficient is shown in Figure 5.9(b). Another quenching cycle was proposed using this polymer quenchant with bath temperature at 50°C. The validity of the cycle was tested by another simulation procedure.

A similar simulation procedure was carried out for the proposed polymer quenching process. The difference between the two modeling procedures lies in the boundary conditions. In this case the heat transfer coefficient of the polymer quenchant was used and the bath temperature was 50°C instead of 20°C of the water quenchant.

Figure 5.27 shows the martensite distribution at the end of the polymer quenching process. It is very obvious that less martensite was developed due to the slower quenching. The martensite at the hole region (Figure 5.28) is found to be lower than that of water quenching too. Consequently polymer quenching may not be able to yield sufficient strength for the component in service. The water quenching thus yields suprior results of thermal-only analysis. On the other hand, quench cracking was another major concern in the cycle design. In general slower quenching will reduce the thermal and residual stresses, which is desirable in order to avoid quench cracking. Figures 5.29 and 5.30 shows the evidences of such expectation by comparison of Von Mises equivalent

stresses and final distortion respectively, between water and polymer quenching processes.

The simulations give a good demonstration of the importance of the cycle parameter, namely the quenchant. If quench cracking is a severe problem associated with the quenching process that needs to be controlled, one may need to solve this by reducing the cooling rate. One may try to find an appropriate quenchant that has an intermediate quenching power. Another approach could use timing quenching or interrupted quenching. One may use water quenching during the initial quenching process and then change to a salt bath at an elevated temperature, e.g. 300°C, at certain time. The duration of the water quenching could be studied by an appropriate modeling procedure. An example is the heat treating cycle for the step-roll as presented in Chapter 4. Other strategies are also possible, for instance using a water quenchant with higher temperature based on the fact that the higher the quenchant temperature the lower the quenching power.

5.4 Some Comments on Metallurgical Modeling

SYSWELD implements the metallurgical models related to the materials thermal treatment. Phase transformation, for example, is one of the major advantages over other general purpose FEA codes like ANSYS. Nevertheless, the power of SYSWELD's metallurgical modeling engine has been largely limited by the lack availability of material properties, especially those of specific phases. For instance a quenching model involving phase transformation may require data like enthalpy, thermal conductivity, yield strength, thermal expansion coefficient and other material properties of individual phases which may appear during the metallurgical development. To incorporate the metallurgical models accurately, these material properties are critical. As it has been indicated earlier in this dissertation, one of the biggest difficulties of quenching modeling is the very limited availability of material property data. This difficulty turns out to be much more severe when dealing with individual phases instead of bulk material. The simulations in

this part of study used some data of another steel on the assumption that those material properties do not vary significantly. For example the yield strengths of the phases are borrowed from the steel coming with SYSWELD tutorials. It is highly desirable that a comprehensive material database be available as a utility tool to modeling analysts. This task demands tremendous investments and data sharing among a variety of research parties.



Figure 5.1 Machine drawing of the fastening ring.



Figure 5.2 1/12th of the original geometry of fastening ring. Surfaces A-F are specified with convective heat transfer boundary conditions while surfaces G-I are symmetric surfaces.



Figure 5.3 Non-standard plate-type quenching probe. Three thermocouples are embedded.



Figure 5.4 CCT diagram of the steel used in the simulation



(b) Yield stress of five phases involved in simulation





Figure 5.6 Finite element mesh and locations of interest. ① and ② are the locations of the thermocouples being embedded. The arrows show the way of the holes being drilled. The indicated path and location ③ will be used in the discussions of thermal-stress analysis.



Figure 5.7 Temperature profiles obtained from a quenching probe test. Data sampling frequency is 100 points per second, and three curves represent the readings of three thermocouples.



Figure 5.8 Smoothed average temperature T mean and the corresponding cooling rate.



Figure 5.9 Heat transfer coefficients used in the simulations. Obtained from nonstandard quenching probe (plate probe) tests.



Figure 5.10 Temperature profiles at the locations 1 and 2, as shown in Figure 5.6. The upper right window shows the comparison between the experimental data and the calculated data in the first 30 seconds.



Figure 5.11 Isotherms at time = 30 seconds.



Figure 5.12 Volumetric fraction of martensite at the end of quenching process. The data are the values at Gaussian integration points and plotted in transparent mode



Figure 5.13 Martensite distribution in hole region.



Figure 5.14 Phase evolution at the location 2 of the component shown in Figure 5.6.



Figure 5.15 Development of martensite at location 1 & 2 (shown in Figure 5.6) and the center of the component.



Figure 5.16 Pearlite distribution (transparent mode). The data are the values at Gaussian integration points and plotted in transparent mode.



Figure 5.17 Bainite distribution (transparent mode). The data are the values at Gaussian integration points and plotted in transparent mode.



-

Figure 5.18 Residual tress state, σ_x .



Figure 5.19 Residual tress state, σ_y .



Figure 5.20 Residual tress state, σ_z .



Figure 5.21 Residual tress state, equivalent stress σ_{eqv} .



Figure 5.22 Final distortion of the component.



Figure 5.23 Final distortion displayed in three different views, XY, YZ, and XZ.



Figure 5.24 Residual stress states in hole region.



Figure 5.25 Residual stresses along the path shown in Figure 5.6.



Figure 5.26 Thermal-stresses developed during quenching process. Stress values are corresponding to point 3 in Figure 5.6 and dashed line represents the austenite.



Figure 5.27 Martensite distribution after polymer quenching.



Figure 5.28 Martensite distribution in hole region.



Figure 5.29 Comparison of Von Mises stress along the plot path between water and polymer quenching.



Figure 5.30 Comparison of final distortion along the plot path between water and polymer quenching.

Appendix

SYSWELD Input files:

NAME PAN

SEARCH DATA 2

DEFINITION

quenching- Thermal history

OPTION THERMAL METALLURGY SPATIAL

RESTART GEOMETRY

MATERIAL PROPERTIES

ELEMENTS GROUP \$BODY\$ / C= -101 KX=-100 KY=-100 KZ=-100 --

MATE=1 RHO= 7824

CONSTRAINTS

ELEMENTS GROUP \$hole\$ \$side\$ \$top\$ \$bottom\$ / KT= 1 VARI 400 LOADS

1 quenching/ ELEMENTS GROUP \$hole\$ \$side\$ \$top\$ \$bottom\$/ TT=20

TABLE

100/1 20 47.68 100 43.53 200 40.44 300 38.13 400 36.02 * 500 34.14 600 31.98 700 28.66 800 26.49 900 25.92 101/1 20 472 100 480 200 498 300 524 400 560 * 600 700 700 854 755 1064 800 806 900 637 400/1 0 3000 100 3500 200 4000 300 4250 400 5000 * 500 5100 600 4000 700 2250 800 1000 850 300 RETURN NAME PAN SAVE DATA 1000

```
NAME PAN
SEARCH DATA 1000
RENUMBER ITERATION 10
RETURN
TRANSIENT NON-LINEAR EXTRACT 0
BEHAVIOUR METALLURGY 5
ALGORITHM BFGS IMPLICIT 0.5 ITERATION 200
PRECISION ABSOLUTE NORM 0 FORCE 1*-8 DISPLACEMENT 1*-4
METHOD SYMMETRICAL TEST 1 DIRECT
INITIAL CONDITIONS
   NODES / TT 830
   ELEMENTS GROUP $body$ / P 0 0 0 0 1
TIME INITIAL 0
     50 STEP 1 / STORE 1
    200 STEP 10 / STORE 1
    500 STEP 100 / STORE 1
RETURN
NAME PAN
SAVE DATA TRAN 1001
MATERIAL 1 PHASE 5
REACTION
 5 1 cooling peg table 10 tau table 11 f table 12
 5 2 cooling peq table 20 tau table 21 f table 22
 5 3 cooling peq table 30 tau table 31 f table 32
 5 4 cooling ms 340 km 0.011
TABLE
 10/1 649 0 650 1 740 0
 11/1 650 150 780 150
 12/1 -80 1 -71.43 3 -26.67 5 -8.75 5.4 -2.31 2.5 -0.3126 1 -
0.00833 1
 20/1 599 0 600 1 650 0
 21/1 600 1 650 1
 22/1 -63.16 0.1 -14.83 0.2 -11.43 0.4 -10 1
 30/1 339 0 340 1 600 0
```
```
31/1 340 2 600 2
 32/1 -137.5 0.05 -50.0 0.2 -47.5 1 -32.86 0.4
END
NAME PAN
SEARCH DATA 1001
DEFINITION
extrusion die quenching
OPTION THREE-DIMENSIONAL THERMOELASTICITY SYMMETRY
RESTART GEOMETRY
MATERIAL PROPERTIES
ELEMENTS GROUP $body$ / E=-10001 YIELD=-10005 LX=-10002 LY=-
10002 --
LZ=-10002 MODEL=3 NU=0.3 SLOPE=-10010 PHAS=5 MARTENSITE=4
CONSTRAINTS
PLANE nodes 11 8 2595 / UY
PLANE nodes 11 8 2081 / SYMMETRY
NODES 11 / UX UY UZ
nodes 1to10 / UX UY
LOAD
1 quenching/ NOTHING
TABLE
 10001 / 1 80 200*9 900 120*9
 10002 / -10003 -10003 -10003 -10003 -10004
 10003 / 1 80 0 900 0.01
 10004 / 1 80 -0.01024 900 0.01
 10005 / -10006 -10006 -10007 -10008 -10009
 10006 / 1 20 320*6 100 310*6 200 290*6 300 280*6 400 260*6
         500 240*6 600 180*6 700 100*6 800 60*6
     *
 10007 / 1 20 460*6 100 450*6 200 420*6 300 400*6 400 350*6
     * 500 280*6 600 210*6 700 110*6 800 60*6
 10008 / 1 20 660*6 100 650*6 200 620*6 300 550*6 400 400*6
     * 500 350*6 600 250*6 700 125*6 800 60*6
 10009 / 1 20 220*6 200 200*6 300 180*6 400 150*6 500 120*6
     * 600 95*6 700 75*6 800 60*6 900 45*5
 10010 / -10011 -10012
```

METHOD SYMMETRICAL TEST 1 DIRECT TIME INITIAL 0 0 / STORE 1 RETURN

NAME

SAVE DATA TRAN 2001 ASSIGN 19 TRAN2001.TIT BINARY

```
TRANSIENT NON-LINEAR STATIC EXTRACT 0
BEHAVIOUR PLASTIC METALLURGY 5
ALGORITHM BFGS IMPLICIT 0.5 ITERATION 60
PRECISION ABSOLUTE NORM 0 FORCE 1 DISPLACEMENT 1*-6
STEP DTMINI 0.0025 EPSC 5000 EPSP 300 FACP 4 EXTRACT
METHOD SYMMETRICAL TEST 1 DIRECT
INITIAL CONDITION RESTART CARD 1
TIME INITIAL 0
50 STEP 1 / STORE 1
200 STEP 10 / STORE 1
500 STEP 100 / STORE 1
```

RETURN

SAVE DATA TRAN 3000

CHAPTER 6

THE ROLE OF COMPUTER IN PROCESS MODELING OF QUENCHING PROCESS

Computer technology has grown in leaps and bounds in recent history. Nowadays the computer has found it way in almost all parts of human life including manufacturing, education. banking, office automation, electronic communication and home entertainment. Computer technology has already been widely accepted and used as a powerful tool in many engineering disciplines such as aerospace, automobile, materials CAD/CAM/CAE has subsequently become a very active and civil engineering. subdivision of modern engineering. Although its application somewhat lags behind other computer intensive disciplines, computer acceptance and usage is constantly gaining in heat treating society. Process modeling, computer simulation, process control, electronic documentation, materials related database and information are the witnesses of this progress. Despite the exciting achievements, applications of computers in materials science and heat treating practice are still very limited. The quality and quantity of the software and databases are not satisfactory. With the rapid grown of Internet such as World Wide Web (WWW), electronic mail and file transfer protocols (FTP) facilities, more work need to be done in order for material scientists to fully take advantage of this fast growing significant technologies.

Unfortunately the use of computer technology in materials science is not an easy task at all. The reasons can be explained from several perspectives. First of all, materials science itself has many uncertainties that limit the application of the computer technology. Successful use of the computer is driven by the nature and the mechanism of the problem to be computerized. As an example the success of finite element analysis in mechanical engineering lies in the fact that mechanical engineering is a well-developed engineering discipline. The theories and mechanisms of structural behavior or heat transfer are well understood. With the solid understanding of theoretical foundations the computer becomes an accurate and efficient tool for mechanical engineers. Secondly, computer software engineering is an very complex discipline. Software engineering is a young discipline. It is dynamic and subject to change which makes software engineering differ from other engineering disciplines and extremely difficult to manage. Many software development fiasco are the witness of such difficulty. Thirdly, successful computer application in materials science requires interdisciplinary knowledge in both computer science and materials science. Isolated efforts can not guarantee efficient materials science specific software tools or services. A computer software engineer may not understand the complexity of the materials science and the requirements of materials scientists. For instance one may not understand the difficulties of modeling phase transformation during a metallurgical process and its related theory and limitations. On the other hand a materials scientist would not know clearly what a computer can do and what it cannot. Therefore it is no surprise to see that a materials engineer expects too much from a computer application. An efficient and good materials application thus can be developed only under smoothly integrated efforts from both disciplines. Finally the day that extensive application of computer technology in materials science may come if only the importance and the advantage of computers can be widely accepted by materials scientists. Generically speaking the training for materials scientists and engineers focuses on the theoretical learning, laboratory skills and problem solving skills. Less emphasis has been addressed in the advanced use of computer software and hardware. This stems from the nature of materials science and engineering, whose research largely based on

experimental tests and analyses. Experience constitutes majority of the source of success. People are easily overloaded by the tedious laboratory work and on-site practical practice and thus have less time to spend on computer, a "fancy" but forbidding toy. As mentioned above, however, successful use of the computer in materials science is an extremely difficult task that requires interdisciplinary efforts from both materials science and computer science. Moreover setting up a computer laboratory for process modeling is non-trivial in both financial and technical issues. Consequently, without the recognition of its importance and significant supports form materials community that day could remain a distance dream.

Thanks to the pioneering multidisciplinary work, computer applications in materials science and engineering is gradually becoming increasingly popular. Its power and potential and power is becoming more widely recognized. As an example, process modeling in heat treatment has gained worldwide attention and is showing even greater potential. Computer prediction, modeling and simulation has become a hot button issue lately. Two recent international conferences^[8,123] sponsored by the American Society of Materials (ASM International) highlighted recent advances of computer simulation of materials processes. Other pertinent references are also given in the literature review of this thesis.

Another interesting aspect of computer application comes with the rapid expansion of Internet. Internet and in particular the World Wide Web (WWW) is growing exponentially and is increasingly accessible to every people. Public databases, services and convenient communication media provided by the Internet have resulted in dramatic impact on the way of information sharing in research activities. One of the most successful examples is the bio-Web service, which provide broad and comprehensive research information and tools for researchers and scientists in the bioscience disciplinary. Taking advantage of the information highway provided by the Internet, most recent discovery, news and research tools can be freely accessed by numerous researchers and scientists. Although not as advanced as that of bioscience, the power of Internet and WWW has been recognized by increasingly more people in materials science and engineering. Many universities and organizations have hosted materials databases and resources that can be used by materials scientists for various purposes. For example METADEX, a major database of literature resource in materials science and engineering, can be accessible via the WWW. The database contains information dating back to 1966. The service becomes one of major information sources for material scientists. A special committee, ASM-HTS International On-line Process Modeling Committee, which dealt with the coordination of process modeling challenges based exclusively on the Internet communications was formed under the umbrella of the ASM International. The first chair of the committee is the supervising professor of this thesis and the Web master of the committee is the author of this thesis. The committee is still in its infancy, however, it provides useful tools and services to its fellow colleagues.

Typical roles of computer in the process modeling of quenching process can be summarized as following:

- Model Implementations
- Analytical solution: for small and simple problem
- Commercial analysis codes: for large modeling procedure
- Databases
- Materials property database
- Bibliographic database, e.g. METADEX
- Special designed database, e.g. for modeling results
- Utilities & tools
- Visualization, graphical user interface (GUI)
- Data post-processing
- Fast prototyping of the models
- Internet and WWW
- Information shearing
- Client-server applications and services
- Fast and high accessibility, 24 hours/day, 7 days/week

Process modeling depends heavily on computer. Modeling software like ANSYS or SYSWELD is the computer implementation of the model and it forms the backbone of

the modeling practice. It makes the quenching modeling routinely, especially the largescale modeling. The case study in Chapter 5 is an excellent example in which thermal history, phase transformation and residual stress of a practical quenching problem can be studied efficiently. This chapter will demonstrate the role of computer in other aspects of process modeling including special databases for process modeling of quenching process, modeling prototyping and utility tools.

6.1 Database for Process Modeling of Quenching Process

The quenching process is extremely complex. There are so many factors involved and intertwined which makes modeling process so challenging but interesting. As a matter of fact process modeling of steel quenching has become increasingly popular and attracts more and more analysts. Two recent international conferences on quenching and control of distortion^[8,123] are the testaments of such progress. Because of the challenge and complexity, following an efficient path becomes increasingly important for modeling analysts to maximize results with minimum practice. It is highly recommended that advanced methodologies and efficient strategies be used.

In this section a useful methodology, namely database, will be explored to fit into the category of process modeling practice. As a widely used and fast growing computer related technique, database has found applications in nearly all walks of human life where computers are used.^[95-98] In generic terms a database is basically a collection of data. More technically a database represents another mini-world that reflects some aspects of a real world. For instance an administrative database of an organization represents the employees' real world information such as names, addresses, phone numbers, office locations, etc. In addition a database is designed and established for specific purposes. Database is a logical coherent collection of data. A database management system (DBMS) like ORACLE, INFORMIX, DBASE, ACCESS or PARADOX provides its users with tools and programming power to create, maintain and query against the database. The intention of this part of discussion is neither to present an in-depth expose of database technique nor an introduction to database principles. One may reference to a good text book on these topics.^[96] The objective is to demonstrate and propose the database approach in quenching modeling practice.

6.1.1 Relational Database for Heat Transfer Coefficients

One very obvious use of a database is to build good and comprehensive material property repositories. As discussed earlier such kind of databases are in tremendous need. Most current material property databases store the data in constant value format and thus provide very limited nonlinear functionality. Moreover quenching modeling also demands process related data like heat transfer coefficients, in addition to the material related data such as thermal conductivity, heat capacity, Young's modulus and yield strength. Heat transfer coefficients, as discussed in Chapters 1 and 3, are critical to the quenching process. A large amount of heat transfer coefficient data has been accumulated from both experimental tests and practical quenching practice. However it is very difficult to correlate data from one test to another since heat transfer coefficients are functions of many factors including quenchant chemistry, quenchant temperature, quenchant flow characteristics, surface temperature of the component, surface condition of the component and loading configuration of the quenching tank. Correlating these effects requires extensive study in heat transfer, chemistry and quenching mechanism. Thus a database can be used in such as situation to coherently relate the various parts of concern and to provide a searchable interface to users.

A relational database was proposed for storing heat transfer coefficients. The design of the database requires careful analysis of the aspects related to the heat transfer coefficient. In the current proposal, heat transfer coefficient was considered to be a function of quenchant chemistry, quenchant temperature, and quenchant agitation. In addition, heat transfer coefficient was also considered to be dependent on the component material, its surface conditions and the loading conditions of the quenching process including loading quantity and loading type. Figure 6.1 presents the database in terms of entity relationship diagram (ERD). ERD^[96] describes the database in term of entities, relationships and attributes. Entities represent the "things" in the practical application.

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An entity could be an object in the application or a conceptual object. Each entity has specific properties that are called attributes. A more detailed explanation will be presented in the database design discussion as follows.

In the current proposal three entities are identified in the database, namely "Quenchant", "Component", and "Material". The "Quenchant" entity in the database is corresponding to the quenchant to be used in quenching practice, which is the critical aspect of the concerns for the heat transfer coefficient value. All quenchants to be stored in the database will have the properties of quenchant chemistry, temperature and agitation. They are the important parameters that need to be taken into consideration as well. The entities in the ERD will be implemented in the database as tables in most cases. Therefore a water quenchant, for instance, will be put into database as an entry of "Quenchant" table, and it will have fields such as composition, temperature and agitation condition. Another important entity in the database is the "Component". To determine the heat transfer coefficient, one may also need to know what type of component to be quenched in addition to what type of quenchant to be used. The reason to include the surface orientation and surface condition of the component lies in the fact that the heat transfer coefficient may differ significantly according to the surface orientation of the component or surface condition of the component. The "Material" entity is an extended function of the heat transfer coefficient database. To determine the heat transfer coefficient the material properties of the component are not critical, however it would be nice for the user to get most useful additional information of the component in the database. Identification numbers, namely QuenchantKey, ComponentKey and MaterialID respectively, are the keys of the tables. In database technology entity key is the identification attribute of the entity, and thus the key of the entry must be unique.

Entities represent the important data parties in the database. Relationships identify the relationships between the entities that maintain the traceable paths among the entities. The critical relationship of the database is the "Quenched_in" which represents the relationship between "Quenchant" and "Component. This relationship can be easily identified since a component needs to be quenched in certain type of quenchant. The critical property of the relationship is the heat transfer coefficient data, namely h_Data as

shown in the ERD. In the proposed database it was assumed that the heat transfer coefficient data were determinable if both quenchant and component were specified and the parameters of loading configuration of quenching process were given. Two important loading parameters, namely loading quantity and loading type, are thus the attributes of the "Quenched_in" relationship as well. The number pair labeled on both sides of the relation, namely "M" and "N" is the cardinality ratio^[96] which specifies the number of relationship instances that an entity can participate. The "M:N" ratio in this case means that multiple components can be quenched in several types of quenchant and vise versa. Relations can be implemented as table too. The key of the relationship "Quenched_in" in this case is the combination of the foreign keys borrowed from "Quenched_in" was implemented as a table. Similar technique can be applied to the "Material" entity and the "Made_of" relationship.

Figure 6.2 shows the tables to be used in the database. Database management systems will provide the user with built-in facilities for data storing, data updating and data accessing. To access data in the database, for example the heat transfer coefficient data with respect to quenchant and component to be quenched, queries can be issued against the database. For example, in order to obtain the heat transfer coefficient data of a quenching process with follow parameters: Steel: 1045, Surface Orientation: Vertical, Quenchant: UCON, Quenchant Temperature: 60 °C, Agitation: Medium and Loading Type: Solitary, following query can be issued using standard query language (SQL):^[96]

select	Quenched_in.h_Data
from	Quenchant, Component, Quenched_in, Made_of, Material
where	Quenchant.Chemistry = UCON AND
	Quenchant.Temperautre = 60 AND
	Quenchant.Agitation = Medium AND
	<pre>Quenchant.QuenchantKey = Quenched_in.QKey AND</pre>
	<pre>Quenched_in.LoadingType = Solitary AND</pre>
	Quenched_in.CKey = Component.ComponentKey AND
	Component.SurfaceOrientation = Vertical AND
	Component.CID = Made_of.CID AND
	Made_of.MID = Material.MID AND
	Material.Name = "1045"

The proposed database is quite straightforward and simple. The reason is that only most important factors have been considered. A database for the simulation results could be much more complicated because more factors including modeling parameters have to be incorporated. This demands more entities, relations and consequently more tables and attributes or properties. In the proposed database it was assumed that the heat transfer coefficient data h_Data would be in the format of heat transfer coefficient value versus surface temperature of the quenched component, i.e. h = f(T). The other factors such as surface condition, quenchant chemistry, quenchant temperature etc. are the attributes of the entities or relations in the database.

A database prototype was established using Microsoft Access. Figure 6.3 shows the tables created in Access. Figure 6.4-6.6 shows the query forms and results of retrieving heat transfer coefficients with various criteria. Figure 6.4 retrieves the heat transfer coefficients of UCON quenchant. Figure 6.5 is the result of heat transfer coefficients of quenching a 1045 steel component in 60°C UCON quenchant. Figure 6.6 is the result of the heat transfer coefficient of the vertical surface of a 1045 steel component quenched in 60°C UCON quenchant. One may notice that more specific heat transfer coefficient data will be retrieved when more detailed quenching configuration is specified.

6.1.2 Object-Oriented database for Quenching Modeling

From a database point of view designing a relational database needs to identify the entities, the relationships among the entities and the attributes. Sometime it may difficult to design a relational database when an application is more self-contained and less relational.

The information and the results of a quenching model are quite rich and complicated to manage. When sizable modeling data have been accumulated, finding an efficient way of data storing and data accessing becomes increasingly important. To facilitate the modeling practice and systematically manage the existing modeling results, building a specific database will be an efficient approach. Not only will the database provide the coherent storage and fast access to the valuable data generated by modeling practice, but also it keeps the traceability of the model information and encourages the detail analysis of the modeling procedures and results.

Building a relational database for quenching modeling data however, could be clumsy and difficult, since modeling results are self-contained and relationships among the different parts of the modeling data are complex and sometimes vague. An alternative to the relational database is the fast growing object-oriented database (OODB). OODB is found to be more competent for engineering applications, for instance computer-aided design (CAD) applications.^[97,98]

OODB stores the data as objects which are self-contained. An object in computer's object-oriented paradigm is a piece of encapsulated data presentation, which has both data members and methods. The data members are the information that an object obtains. For instance if one designs a QuenchingProbe object, the object will have the data members like probe name, probe type, probe geometry, etc. An object may store another object as its member as well. For example, instead of storing the material properties of the probe like thermal conductivity, heat capacity and density as the separate data items, the QuenchingProbe object can have a data member of the Material object, another type of object that groups up all material properties. This embedded object data member not only simplifies the data management but also keeps traceable links between QuencingProbe objects and Material objects.

In addition to the data members, objects know how to response to the requests from outside. A set of functions, called methods, are defined by the object. The methods can be either public or private. The private methods are the help functions used by the object itself. The public methods constitute the public interface of the object. A welldefined object is thus an analogy to a mini-computer. The object, if receiving requests, called messages, can change the state of the object or provide services to the requesters. For example if the QuenchingProbe object has the method to answer the type of the probe, then one can send the request to the objects if he/she wants to know the type of quenching probe, e.g. ISO or JIS type probe.

Object-oriented database technology is thus more capable of representing modeling results. Figure 6.7 shows the logical relationship among the objects used to

store the information of the modeling data. To build the database, one needs to define the types of the objects in term of classes. Classes can be thought of as factories that manufacture objects. The class defines the type of the object, data members and methods that an object will have. Objects are thus instantiated from the class with the same interface and the same data members but possibly different values. For example if two objects *UCON* and *Water* are both instantiated from class Quenchant, they both will have the same methods including public interface. In addition both of them will have data members like quenchant name, quenchant temperature and so on. However what distinguish these two objects are the values of the data members, i.e. "UCON" and "Water" for quenchant name respectively, 80°C and 30°C for quenchant temperature respectively, and so on.

To define an OODB for quenching modeling one needs to decide what to be stored and how the data will be arranged. Currently modeling data will be broken down into six categories: generic modeling description, finite element model, quenchant, material data, heat transfer coefficient, and the quenching probe used to obtain the heat transfer coefficient. Consequently six classes are defined. The class ModelingData contains the generic information necessary for modeling data, form which one may retrieve the results of a modeling practice, for example thermal history, phase products, and so on. Another advantage of OODB is that the results are able to be stored in variety formats, such as images, animation or audio presentations. From the ModelingData objects one can have a good understanding of what have been done so far. The ModelingData object have an embedded object called FEAModel, which describes the information of finite element model including geometry, mesh quality, and other model parameters. The FEAModel object gives the user the idea of the finite element modeling procedures used to get the modeling results stored in the ModelingData objects. Similarly the FEAModel objects maintain links to other types of objects, namely the HeatTransCoeff object and the Material object. To obtain the information on the heat transfer coefficient, one may follow the link to the corresponding HeatTransCoeff object. Moreover one is also able to get additional information of the quenchant and quenching probe test from which the heat transfer coefficient data were obtained, if he/she follows

the subsequent links in HeatTransCoeff object. As discussed earlier these links maintain the traceable paths among the objects and thus any information about the model can be retrieved by careful and efficient implementation of the access methods.

The major part of class definitions in term of C++ syntax was shown in the appendix of the chapter. The OODB approach makes a clear semantic representation of the quenching modeling database. Using object oriented database management system (OODBMS) like ObjectStore, GemStone or O2, one can store the modeling results persistently and systematically. Queries can be issued against the database using query language or programming language. User friendly graphical interfaces or utility tools may be developed in collaboration with the database.

6.2 Model Prototyping and Utility Tools

The role of computer is not confined to heavy computation only such as largescale finite element analyses. The computer can also be used in modeling practice for fast prototyping the models and developing utility tools. In certain cases one may need a good representation of the model which requires a less expensive implementation and user friendly interface. Prototyping does not mean causal modeling, but a light-weighted and efficient implementation of small or simple modeling requirements. Developing modeling related utility tools is another application area of the computer. With a large collection of prototyping and utility programs for various modeling purposes, modeling practice will be less expensive and more efficient and attract a larger audience and more participants.

WinJominy and WinProbe to be presented in the next sections are examples of modeling prototyping and utility tools. Both computer applications described here are neither as big as nor as versatile as commercial finite element codes. However they show other aspects of the role of computer role in facilitating the work in modeling practice.

6.2.1 WinJominy - A Windows based simulation program for Jominy test

Jominy test is a standard test procedure for studying the hardenability analysis of steels. However, the test yields very limited information about the thermal history, intermediate transformation and the correlation between the different aspects, such as steel chemistry, quenching parameters, etc. The objective of this program is to develop a simulation-based software which provides a "virtual Jominy test laboratory". It will allow users to study the thermal history of the Jominy test, effects of the material properties, quenching parameters and qualitatively predict the final phase products of a quenching test.

The current program is a prototype of the proposed project. The final objective of the project aims at quantitatively analyzing and visualizing the test process with the aid of computer simulation. The thermal history analysis used a one-dimensional model. This is based on the fact of that the heat will be removed mainly from the end of the Jominy test bar and the heat exchange from the other surfaces of the bar is negligible. Consequently it is reasonable to assume that the heat flow is thereby parallel along the Jominy test bar. To ease the analysis it is also assumed the constant material properties and boundary conditions such as thermal conductivity, heat capacity, density and heat transfer coefficient. Analytical solution was used to calculate the heat conduction in the Jominy test bar. The following equations were used to solve the transient temperature field:

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha} \frac{\partial T}{\partial t}$$
(6.1)

$$T(x,0) = T_{init} \tag{6.2}$$

$$\frac{\partial T}{\partial x}\Big|_{x=0} = 0 \tag{6.3}$$

$$-\frac{\partial T}{\partial x}\Big|_{x=L} = h[T(L,t) - T_{\infty}]$$
(6.4)

The analytical solution can be expressed as

$$T(x,t) = T_{\infty} + (T_{init} - T_{\infty}) \sum_{n=1}^{\infty} C_n \exp(-\xi_n^2 F_0) \cos(\xi_n^2 \frac{x}{L})$$
(6.5)

where Fo is Fourier number (= $\alpha t/L^2$) and the coefficient C_n is

$$C_n = \frac{4\sin\xi_n}{2\xi_n + \sin(2\xi_n)} \tag{6.6}$$

The discrete values (eigenvalues) of ξ_n are positive roots of the transcendental equation

$$\xi_n \tan \xi_n = \frac{hL}{k} \tag{6.7}$$

The analytical solution used first hundred terms. Although this kind of analytical heat conduction simulation is simple, important information can be derived from it, such as cooling curve and possible phase transformation products if the CCT or TTT curve can be superimposed onto the cooling profiles. The advantage of this kind of analytical simulation is the low computational overhead and thus ease of implementation and user-friendly graphical user interface (GUI). The program provides:

- 1. A visualized simulation environment for the virtual Jominy test.
- 2. Cooling profiles corresponding to different locations from the quenching end.
- 3. Superimposed TTT/CCT curve onto the cooling profiles, so that a qualitative analysis of phase transformation is made possible.
- 4. A way to study the effects of material and quenching parameters.
- 5. An expandable steel library.

The program is design to be user-friendly. Figure 6.8 is the data input window in which one may specify the material properties and quenching parameters. The user is allowed to import the data, including material properties necessary for heat conduction simulation, i.e. thermal conductivity, heat capacity and density.

The steel library is a collection of separate files with the file extension prp (i.e. *.prp). The files are in ASCII format so that they can easily be created and modified by users. The format of the files is shown in Figure 6.9. Basically there are three segments in the file: material properties, TTT/CCT and other related information. Detail information of the contents and the format of the steel library entry will be defined in the appendix of this chapter.

Figure 6.10 shows the main window of the program. Cooling profiles can be plotted in the drawing area. User has the visualized control over the profiles to be plotted corresponding to the locations on Jominy bar by dragging the slide bar. TTT/CCT curve can be drawn in the drawing area too, if the data has been already loaded from the steel library. Thus qualitative analysis of the phase products as a function of the distance from the quenching end can be made.

Figure 6.11 is the window showing additional information of the steel that corresponds to the last section of the steel property file (Figure 6.9). Information such as steel chemistry, austenization temperature, grain size, etc. are recommended to be provided in this window.

The program is currently prototype in nature. There is a lot of future work that need to be done as listed bellow:

- Software improvement
 - More functionalities
 - More robustness
- Large and comprehensive steels database
- Nonlinear capabilities
 - Temperature-dependent material properties
 - Nonlinear boundary condition, for example h = f(T)
- Coupling between thermal and phase transformation
- Quantitative phase transformation analysis
- Quantitative hardness prediction
- Visualized continuous transformation

Software improvement

In the later revisions of this product, more functionalities need to be added, such as cooling rate information and controllable plotting. The software needs to be more robust and easy to use. A print function may be necessary in order to record the results of the virtual tests. Probably a fully functional database needs to be considered and into the program. This may become critical after a big number of steel data have been accumulated. A visualized or animated transformation is also desirable. It will be quite desirable if we can make the program as a distributed application. In such a case, a server may be built with extensive resources, e.g. a comprehensive steel library, while many users could access to the server and perform their tests via the Internet.

Modeling work

It is necessary to point out that the backbone of this project is the modeling component, not the fancy GUI of the software. Currently the project only incorporates a closed-form heat conduction model. However it is far away from the practical requirements from a heat treatment standpoint. Even for heat transfer analysis itself, one may need to consider the material and boundary non-linearity, such as temperature dependent thermal conductivity and complex heat transfer between specimen and quenchant. As a result, the closed-form approach is no longer capable of solving the problem, and we have to use a numerical approach, e.g. finite difference or finite element method. This change will in turn influence the software design and implementation in various aspects. However much more difficulties will be expected from the metallurgical part indeed. Coupling between thermal history and phase transformation is a non-trivial task, let alone the problem's heavy dependency on the understanding of the transformation mechanism and reliable data that is normally hard to obtained. Knowing that many empirical models, for example those typically encountered in a phase transformation class, have many obvious limitations, the author suggests Avrami equation based numerical model. The approach is a stepwise isothermal incremental method that is based on existing TTT/CCT diagrams.^[71] The advantage of this approach is that a continuous record of transformation can be obtained during the simulation. As a result the transformation fractions can be used not only to predict the hardness profile of the specimen, but also as the inputs for visualized progress of the transformation. Although the above approach is still a difficult task, it is envisioned that this will be a legitimate and efficient implementation in the final analysis.

6.2.2 WinProbe - A Windows based program for post-processing quenching probe test data

As discussed in Chapter 3, quenching probe test is a standardized measuring method for studying the heat transfer behavior during the quenching process. The raw data are generally the temperature-time profile(s) of the thermocouple(s) that are embedded inside a quenching probe. Significant data post processing work is needed to visualize the data, derive the new information such as cooling rate, quenching severity, heat flux or heat transfer coefficient.

The motivation behind this project is to create an integral software environment for post-processing the data obtained from typical quenching probes including ISO and JIS probe. Typical calculations such as cooling rate, heat flux and heat transfer coefficient should be carried out in the software with a user-friend graphical user interface. It is also designed to carry out virtual quenching probe test via simulating the probe's thermal response during the test. This feature provides the capability of numerical experimental analysis of quenching probe test.

The WinProbe program is designed for practical used and therefore the understanding of the practical requirements is extremely important. Valuable suggestions and information have been collected from many people who have special expertise in quenching probe test. Some suggested functionalities have already been implemented and some will be incorporated into WinProbe later in the development process. Winprobe is a multi-document interface application. User may open multiple test data and work simultaneously. However due to the integrity concern of the test data, processing is confined in the same test only and no cross boundary processing is allowed. For instance one can not copy a piece of data fraction from one test and then paste it into another test.

WinProbe accepts ASCII format data files. The format of the file is shown as following.

```
# of rows, # of columns
description 1, description 2, ..., description n
data00, data01, ..., data0n
data10, data11, ..., data1n
.....
```

It is based on the general format of the data obtained from an acquisition system of quenching probe test. The details of the data format can be found in the appendix of this chapter.

The test data are generally noisy, especially when data are sampled at high frequency. Figure 6.12 for example shows a portion of data obtained from a practice quenching probe test at a data sampling frequency of 100 points per second. It is obvious that the raw data can not be used directly. Data smoothing must be done before further processing.

Data smoothing is the first step of data processing. The quality of data smoothing is extremely important because it is not the temperature but the cooling rate $\left(\frac{\partial T}{\partial t}\right)$ that will be a crucial parameter for the calculation of heat flux and heat transfer coefficient. Data smoothing changes the original data values explicitly in order to reduce the noise and produce smooth curves. It is very obvious that data smoothing can alter the cooling rates slightly or significantly depending on the quality of the raw data and the smoothing algorithm. It is hoped that data smoothing only filters and smoothes out the erroneous data points and keeps the good ones. Unfortunately it is not an easy task for noisy data. Data smoothing itself becomes a nontrivial task of experimental methodology. Professor Reti and his research group^[124] made some valuable analysis and study on the effects of data smoothing algorithms. Currently two smoothing algorithms have been incorporated in the program, namely 5-point cubic smoothing algorithms including those studied by Reti will be implemented in the later release. The current program implements three most useful data processing functions, namely calculation of cooling rate, heat flux and heat transfer coefficient. Figure 6.13 shows the main window. The test data are placed in a spreadsheet and data processing is "column-driven", i.e. user needs to select a specific column of data before performing calculations such as cooling rate. The first column must be time and many other calculations will depend on the correctness of the time information. In addition to basic file operations like opening or saving data, some simple data edit functions are also implemented.

The program's main functions include following options:

• *Cooling rate*: calculate the cooling rate by central different scheme. The finite difference scheme is described as following:

$$\frac{\partial T}{\partial t} = \frac{T_{i+1} - T_{i-1}}{t_{i+1} - t_{i-1}} + O(\Delta t^2)$$
(6.8)

Heat flux: calculation of the heat flux is by lumped capacitance model as described in Chapter 3. When invoked, this function will bring up an input window in which the user is asked to input information necessary for the calculation. Figure 6.14 is the screen shot of the input window. In the window the user needs to specify the material properties such as thermal conductivity, heat capacity and density. Other data, for instance probe characteristic dimension and quenchant temperature, are also required. The program can process the data obtained from standard testing probes like ISO and JIS probe. Meanwhile it can process data from nonstandard probe for example plate shape probe. This information is also demanded for calculating heat transfer coefficient. Therefore this window will pop up when heat transfer coefficient is to be calculated. The calculation uses following equation:

$$HF = \frac{\rho CL}{2} \frac{\frac{\partial T}{\partial l}}{2} \tag{6.9}$$

where L is the characteristic dimension which is plate thickness for plate and radium for cylinder.

• *Heat transfer coefficient*: Heat transfer coefficient is calculated by lumped capacitance model as described in Chapter 3.

Data visualization is made possible in a plot window as shown in Figure 6.15. A few sophisticated plot functions have been implemented, including axis control, data item selection and graph enhancement. Details of the functionality of the program can be found in the chapter appendix.

Future work needs to be done to improve both software and data processing functionality. It is desirable to implement more robust and efficient smoothing algorithms. Inverse heat conduction algorithms need to be added into the program to improve the calculation of heat flux and heat transfer coefficient. To turn the program into a virtual laboratory it is also recommended to implement a set of simulation tools in the program so as to carry out the numerical experiment as described in Chapter 3.

6.3 Concluding Remarks

In summary process modeling needs the computer and there are still many modeling aspects needed to be explored with the aid of the computer. Developing computer tools for modeling practice demands efforts from both materials science and computer science. Computer methodologies such as database and application tools will facilitate process modeling practice and become increasingly important in the future.

The databases proposed here form a key blueprints of future work. Building a database is a very difficult task and mainly depends on the quality and quantity of the data accumulated. The task also requires careful design of testing and modeling procedure so that information can be derived efficiently from the results obtained. When too many factors are intertwined, orthogonal design technique or reasonable modification and justifications may need to separate and isolate the effects. It is the author's opinion that developing various purposes databases for process modeling in material science and engineering will be an important and imperative task in the near future.



Figure 6.1 Entity relational diagram for heat transfer coefficient database.

Quenchant	QuenchantKey	Chemistry	Temperature	Agitation
	1	UCON	70	Medium
	2	UCON	30	Medium
	3	Water-1	30	High
	4	Polymer-A	40	Medium
		•••		•••

Component	ComponentKey	SurfaceOrientation	SurfaceCondition
	1	Bottom	Smooth
	2	Vertical	Smooth
	3	Тор	Rough
			• • •

Quenched in	QuenchingKey	QKey	CKey	Quantity	LoadingType	h_Data
	1	1	1	1	Solitary	hf_1.dat
	2	1	2	1	Solitary	hf_10.dat
	3	2	2	1	Solitary	hf_5.dat
	4	1	2	4	Stacked	hf_8.dat

Material	MaterialID	MaterialName	ThermalCond	HeatCapacity	YieldStress	
	1	1045	k1045.dat	C1045.dat	1045.ys1	
	2	1050	k1050.dat	C1050.dat	1050.ys2	
	3	1080	k1080.dat	C1080.dat	1080.ys	

Made_of	MID	CID
	1	1
Γ	1	2
F	2	3

Figure 6.2 Tables of proposed heat transfer coefficient database.

The data of some fields are store in file format. For example the h_Data field of the Quenched_in table is of type of ASCII file, which stores the data in the format of temperature and heat transfer coefficient pairs, i.e. h=h(T).

(in	hf : Database		_ [Materia	Teb	le						_	
E	To D a B Fd		nd 🛷 Mi		Materia		ateria	INa Th	erm	alCor	HeatCar	dat	YieldStress	Y(A
Γ	Component		Open			2 10	050	k '	1040	dat	C 1050	dat \	Ys 1050 dat	E-
	Made_of		Jasian			3 10	080	k '	1080	dat	C 1080.	dat Y	Ys 1080.dat	E
	Material		Zeongii			4 H	13	k_ł	H13.	dat	C_H13.d	lat \	Ys_H13.dat	E1
	Quenched_in		New	R	ecord: 14			1 🕨	H	▶ * 0	if 4	4		• 1
	Quenched_jn Tat	ule.						_ 0	×	III M	lade_of : Tal	ble		
	QuenchingKey	QKey	CKey	Quantit	ty Load	lingTy	h_	Data			MID		CID	
	1	1	1		1 Solita	iry	hf_1	.dat		•		1		1
•	2	1	2		1 Solita	iry	hf_1	0.dat				1		2
	3	2	2		1 Solita	iry	hf_5	.dat				2		2
	4	1	3		4 Stack	ked	hf_8	.dat	1	Bec			1	*I of
	5	3	3		1 Solita	iry	hf_2	0.dat		[1000000000		
*		0		1	0						omponent	Table	-	
Re		2	PI P *	015						(Compone S	urfac	eOr Surfac	eCor-
	Quenchant Table	a survey and							×	•	1 B	ottom	Smooth	
	QuenchantKey	Chemi	stry	Tempe	rature	As	jitatio	n			2 V	ertica	al Smooth	
•	11	JCON			60	Mediu	Jm				3 T	ор	Rough	
	21	JCON			30	Mediu	um			*	0	·		×
	3 V	Vater-1			30	High				Hec		1		
	4 F	olymer			40	Mediu	Jm		-					
Red	cord: 14 4	1 🕨	>1> *	of 4										

Figure 6.3 Prototype of proposed heat transfer coefficient database.

all af-UCON	l : Select Qu	ery	_ 🗆 🗙		
Quenchant * QuenchantK Chemistry Temperatur	iey	Ouenched_in * OuenchingKey OKey CKey	1		
Agitation		Quantity LoadingType h_Data		hf-UCON : Selec	t Query 🗾 🗖 🗙
Field: Table:	h_Data Quenched_in	Chemistry Quenchant		h_Data	
Show: Criteria: or:		"UCON"		hf_10.dat hf_5.dat hf_8.dat	
			F		1 ▶ ▶ ▶ ★ of 4

Figure 6.4 Retrieving heat transfer coefficients of UCON quenchant.

	ey P Su antity adingType Data		MaterialNa ThermalCo HeatCapa YieldStres: YoungMoo PoisionRa	Ime Inductivity city s Julus tio
Field: h_Data Table: Quenched_in	Chemistry Quenchant	MaterialName Material	Temperature Quenchant	<u>A</u>
Sort Show: V Criteria: or:	"UCON"	"1045"	60	
			WithoutOrientation	n : Se 🗕 🚺
			h_Data	

1 _ 1

1 . 1

£

Figure 6.5 Retrieving heat transfer coefficients of 1045 steel component quenched in a 60 °C UCON quenchant.







Figure 6.7 Object representation of the database for quenching modeling. Only data members of the objects are illustrated. The links in the diagram point to the data member of another object.

material Properties	-	Continuo
I hermal conductivity	50	Continue
Density	7900	Reset
Heat capacity	500	Steel Libra
Quenching Parame	ters	
Initial Temperature	850	
Ouchant Temperature	80	Cancel
Heat transfer coeff	2000	-

Figure 6.8 Data input dialog.

* High Strength Steels: USS Strux * Conductivity, 40 Density, 8001 Heat Capacity, 501 ---- TTT data ----* A -> F/C * - start set -, 17 temp, 468,496,504,523,532,546,568,573,590, 607,627,656,690,718,735,746,763 time, 1.9,2.0,2.1,2.4,2.8,3.5,4.5,4.7,4.83, 4.6,4.0,3.4,3.3,3.4,3.6,4,5 - end set -, 0 temp time * A -> P * - start set -, 7 temp, 600,621,648, 676, 704,721,725 time, 4.9,4.6,4.45,4.41,4.5,4.7,4.8 - end set -, 0 temp time * Bainite Transformation * - start set -, 9 temp, 302, 351,427, 454, 474,482,504,517,521 time, 2.13,2, 1.87,1.85,1.9,2, 3, 4, 5 - end set -, 5 temp, 260, 316, 343, 371, 407 time, 4.15, 3.95, 3.9, 4.1, 5 * Martensite Start * 302 ---- Other Information----C - 0.39, Mn - 0.89, Si - 0.48 Ni - 0.68, Cr - 0.95, Mo - 0.50 V - 0.03, B - 0.002 Austenitized at 1550 F Grain size: 7.5

Figure 6.9 Sample steel data file for WinJominy.



Figure 6.10 The main plot window.



Figure 6.11 Additional steel information.



Figure 6.12 Quenching test data at the data sampled at 100 points/sec.



Figure 6.13 Major graphical user interfaces of WinProbe program.

There all a services (cons	lany	ОК
I nermal conductivity k	17	
Density p	8000	Cancel
Heat capacity C	460	- Prohe Type
		ISO probe
Probe Geometry		C JIS probe
Diameter D	0.0125	C Custom
Quenchant Temperature		Plate
Bulk temperature Tb	80	

Figure 6.14 Specification window for calculating heat flux and heat transfer coefficient.



Figure 6.15 Winprobe's Plot window.

	Transfer and the second by the second s	UN
time	Click on the color	Cancel
	box below to	
HF2	preferred color	

Figure 6.16 X-Y plot data selection window.

X-Y Customi	ration		OK
$\min X$ value	0	X main ticks 10	
maxXvalue	50	X minor ticks 2	Cance
min Y value	0	Y main ticks 10	
max Y value	500	Y minor ticks 2	
Captions			
X axis label	time		
Y axis label	dT/dt and h		
Figure Title	Probe test data		

Figure 6.17 Plot window's axis control.
Appendix

. . .

```
Class Definitions of Objects in C++ Syntax
class Quenchant
{
     // class representing quenchant
   private:
     // data members for quenchant
     String qName;
                         // quenchant name
     String chemistry; // quenchant chemistry
     String manufacturer;
     String description;
     int Agitation;
     float Temperature;
     . . .
   public:
     // public interface for query, set and maintain data
     string getChemistry(); // get quenchant chemistry
     int getTemerature(); // get quenchant temp.
     . . .
}
class MAT
     // class representing material properties
{
 private:
     String mName; // material name, e.g. "H13"
                         // thermal conductivity
     MPData k;
     MPData C;
                         // heat capacity
     MPData H;
                         // enthalpy
                         // Young's modulus
     MPData E;
                         // yield strength;
     MPData Y;
     String composition; // Steel composition
```

// more data

```
public:
     // public interface for accessing, setting
     // and modifying data
     . . .
}
class QuenchingProbe
{
     // class representing quenching probe
  private:
     // data members for quenching probe
     String pName; // probe name
     String pType; // probe type, e.g. "ISO", "JIS",etc.
     MAT material; // link to Material object
     GEOM geometry; // probe geometry
     String description;
                    // more data
     . . .
  public:
     // public interface for query, set and maintain data
     . . .
}
class HeatTransferCoeff
     // class representing heat transfer coefficient
{
  private:
     // data members for heat transfer coefficient
                               // designated name
     String hName;
     Quenchant quenchant; // link to Quenchant
     QuenchingProbe component; // link to quenching probe
                              // h value h = f(T)
     HeatTransferData hData;
                                // more data
     . . .
  public:
     // public interface for query, set and maintain data
     . . .
}
```

```
class FEAModel
{
     // class representing finite element model
  private:
     // data members for FEA model
     String fName;
                    // FEA model name
     GEOM geometry;
                         // model geometry
     MESH mesh;
                         // FEA mesh
     HeatTransCoff h; // link to heat transfer coeff.
                     // link to material library
     MAT matProp;
     float ausTemp;
                         // austenization temp.
     String description;
                         // more data
     . . .
  public:
     // public interface for query, set and maintain data
     . . .
}
class ModelingData
{
     // class representing generic modeling data
  private:
                        // model name
     String modelName;
                        // link to FEA model
     FEAModel model;
     MODELRESULT result; // modeling result
     String description; // additional info on the model
                          // more information
     . . .
  public:
     // public interfac for accessing and displaying,
     // modeling results
```

```
}
```

User's Manual for WinJominy

The program developed with this study provides:

- 1. A visualized simulation environment for the virtual Jominy test.
- 2. Cooling profiles corresponding to different locations from the quenching end.
- 3. Superimposed TTT/CCT curve onto the cooling profiles, so that a qualitative analysis of phase transformation is made possible.
- 4. A way to study the effects of material and quenching parameters.
- 5. An expandable steel library.

The program is design to be user-friendly. Figure 6.8 is the data input window in which one may specify the material properties and quenching parameters. The user may allowed to import the data, including material properties necessary for heat conduction simulation, i.e. thermal conductivity, heat capacity and density. TTT/CCT data of steels can be input from the steel library by clicking the button "Steel Library". The steel library as discussed in the next includes both thermodynamic and metallurgical data. User will be prompted by a standard file dialog in which an input file can be selected.

The steel library is a collection of separate files with the file extension prp (i.e. *.prp). The files are in ASCII format so that they can easily be created and modified by users. The format of the files is shown in Figure 6.9. Basically there are three segments in the file: material properties, TTT/CCT and other related information. Due to the current design limitation, user has to strictly follow the template. User should only replace or fill in the fields as highlighted in the example.

The first line specifies the name of the steel, and the next three lines specify the thermal conductivity, density and heat capacity respectively. These data are critical to thermal analysis. In practical use these data need to be found according to the steel and the cycle being studied.

The second section describes the transformation curves. It covers ferrite, carbide, pearlite, bainite and martensite transformations. Except for the martensitic

transformation, which is represented by martensite start point (Ms), transformations are represented by start and end curves. We use a set of data pairs (temperature-time) to describe a curve. It is required to determine the exact number of data points to be used before inputting the data, for example "17" in the 7th line of Figure 6.9. Please note that the temperature must be in ascendant order and no identical values are allowed. The program will interpolate the data to form a smooth curve. The time is specified in logarithm scale. The origin is at 0.1 second. Therefore one should use 5 for a real time 104 (*i.e.* t' = log(t) +1). The comma "," in the file is the field divider. Consequently, for example, if there is no data for ferrite end curve, its corresponding field for describing the data pairs needs to be 0. In addition the subsequent temperature and time fields need to be empty (no commas after the keywords temperature and time). Ferrite transformation and carbide precipitation curves are in the same slot, because it is not possible to have both curves appearing in the diagram simultaneously.

The last section of the input file is for additional steel information such as steel chemistry, austenization temperature, grain size, and other useful information. Only this section is free from the restrictions. User can put as much information as he/she wants without worrying too much about the format. Whatever is typed here will appear in the information window, as described later.

Figure 6.10 shows the main window of the program. By clicking the "TTT/CCT" button in the program main window the TTT/CCT curve will be drawn in the drawing area, if the curve has been already loaded from the steel library. User can click "Plot" button to draw the cooling profile corresponding to the specific location.

User has the visualized control over the profiles to be plotted corresponding to the location on Jominy bar by dragging the slide bar. The small window below "Plot" will tell the distance from the quenching end. The text window below "Help" button gives the locations of all the cooling profiles you have plotted.

To distinguish the multiple cooling curves user can click button "Pen's color" to define the color of cooling profile plotted. This control is also valid for TTT/CCT curves, such as Ferrite/Carbide, Pearlite, Bainite, and Martensite transformation. By default the program will avoid redundant calculation. If the profile of a location has already been

plotted, it will not be plotted again when that location is chosen again. However if the "Multiple plots" option is checked, this redundant checking will be bypassed. Therefore if a user wants to have multiple sets of profiles simultaneously, for example in order to study the effects of material properties and quenching parameter, he/she may plot the first set as usual. Then the user can click the "Modify" button to bring up the data input window. At this stage the user can directly change the data in the input fields or load another steel data file from the library. The user can click the "Continue" button to let the change take effect or, on the other hand, click the "Cancel" button to discard the modification. The "Reset" button will bring back the program's default values. It is important to notice that whenever a set of steel properties is loaded from the library, the TTT/CCT data cannot be canceled. It means that if clicking the "Cancel" or "Reset" button after loading the steel properties from the library, only material properties and quenching parameters can be undone, while the TTT/CCT data will be retained. Assuming a user does want to see the difference caused by modification, he/she may superimpose the new plots onto the previous drawing. In order to let this happens, he/she must check the "Multiple plots" and probably needs to change the drawing color as well so as to see the visual difference.

Figure 6.11 is the window showing additional information of the steel, which corresponds to the last section of the steel property file (Figure 6.9). Information such as steel chemistry, austenization temperature, grain size, etc. is recommended to be provided in this window.

User's Manual of WinProbe

WinProbe accepts ASCII format data files. The format of the file is shown as following.

```
# of rows, # of columns
description 1, description 2, ..., description n
data00, data01, ..., data0n
data10, data11, ..., data1n
.....
```

It is based on the general format of the data format obtained from an acquisition system of quenching probe test. For example, typical input data could be as following:

137,3
time,T_surf,T_cen
0.1,833.086,849.999
0.2,824.97,849.984
0.3,818.691,849.914
0.4,813.316,849.72
0.5,808.502,849.326
0.6,804.077,848.679
0.7,799.941,847.756
0.8,796.029,846.557
0.9,792.296,845.096
1,788.708,843.399
40.1,220.311,233.527
41.1,214.643,227.325
42.1,209.204,221.374
43.1,203.984,215.663
44.1,198.976,210.183
45.1,194.17,204.924
46.1,189.558,199.877

The above sample test data has total 137 rows and 3 columns. The first column of the data must be time. It will be used in the calculations including cooling rate, heat flux and heat transfer coefficient. The descriptions of the data columns are time, T_surf, and T_cen respectively. T_surf and T_cen are temperature profiles corresponding to the nodes of surface and center of the probe. The amount of data that can be read into the program is limited by the memory size of the computer. A large data file, for example 9000 rows, may not be able to be read into the program in a computer with 16 MB RAM. This limitation could be improved in the later release. The data items are separated by "," instead of space. If one's original data is separated by spaces, he/she may use other utility to convert the format. Due to the limitation of current implementation the data format has to be followed strictly.

The current program implements three most useful data processing functions, namely calculation of cooling rate, heat flux and heat transfer coefficient. Figure 6.13 shows the main window. The test data are placed in a spreadsheet and data processing is "column-driven", i.e. user needs to select a specific column of data before performing calculations such as cooling rate. The first column must be time and many other calculation will depends on the correctness of the time information. In addition to basic file operations like opening or saving data, some simple data edit functions are also implemented such as following:

- Cut Delete a data column
- Copy Copy a data column
- Paste Paste data into the first available free column, i.e. append

The data processing function includes following options:

- Cooling rate: calculate the cooling rate by central different scheme.
- *Heat flux*: calculation of the heat flux is by lumped capacitance model. When invoked, this function will bring up an input window in which the user is asked to input information necessary for the calculation. Figure 6.14 is the screen shot of the input window. In the window the user needs to specify the material properties such as thermal conductivity, heat capacity and density.

Other data, for instance probe characteristic dimension and quenchant temperature, are also required. The program can process the data obtained from standard testing probes like ISO and JIS probe. Meanwhile it can process data from nonstandard probe for example plate shape probe. This information is also demanded for calculating heat transfer coefficient. Therefore this window will pop up when heat transfer coefficient is to be calculated.

• *Heat transfer coefficient*: Heat transfer coefficient is calculated by lumped capacitance model as described in Chapter 3.

Other auxiliary data processing utilities are available:

- *Invert the value*: change the sign of the data, i.e. negative to positive and vise versa. This may be useful to change the value of cooling rate or heat flux from negative to positive for a better plotting image.
- *Smoothing*: two data smoothing choices are available: 5-point cubic spline and least square smoothing. The least square method is not recommended in most cases. More sophisticated smoothing algorithms will be implemented in the later versions.

Data visualization is made possible in a plot window as shown in Figure 6.15. The plot is in X-Y format. User can select the X-Y axes from the available data columns (Figure 6.16). Multiple data columns can be selected by holding Ctrl and mouse pointer. Double clicking a data item or clicking the color box can control the curve color. To achieve better plot result user can control the range of the X-axis and Y-axis, labels, ticks, etc. as shown in Figure 6.17. X or Y axis captions and graph title can be redefined here or by double clicking the labels in the plot window. User also has control over the grids. The graph legend can be turned on or off and can be dragged over the window. The legend uses the descriptions in the data spreadsheet and consequently modifying legend have to be done in the spreadsheet by double clicking on the descriptions.

CHAPTER 7

SUMMARY AND FUTURE WORK

Modeling and simulation forms a virtual laboratory platform, in which practical quenching problems can be analyzed, predicted and optimized. However modeling quenching processes is challenging. Difficulties include incompleteness and limitation of current theories and models, especially those intertwined with phase transformations. Limited availability of reliable data and insufficient functionality of the existing modeling tools add an additional degree of difficulty. Due to the complexity of the problem being studied model validation procedures are not easy either.

Some important issues of process modeling of quenching processes have been tackled, including obtaining heat transfer coefficients by quenching probes, incorporating phase transformation by code customization, modeling of the practical quenching problem, and establishing special databases for process modeling of quenching processes.

The heat transfer coefficient is the critical boundary condition needed by heat conduction. The work presented in this dissertation validated and improved the widely used lumped capacitance model. The numerical experiment procedure presented in the dissertation could be used to study many aspects of modeling practice, including the validity of the model and sensitivity analyses of the model parameters such as the mesh quality, boundary conditions and even the modeling procedures.

Code customization is one of the advanced modeling skills necessary for the modeling analysis to extend the functionality of the existing modeling analysis tools. A weakly coupled modeling procedure was used to aid the design of a practical quenching problem. The power of the virtual laboratory was demonstrated in this practical modeling problem. Useful information on thermal history, phase transformation products, thermal and residual stresses were obtained and consequently valuable design suggestions could be made.

Databases for process modeling of quenching processes were proposed as a systematic and efficient methodology to avoid ad hoc modeling practice. The significance of the modeling specific databases is providing modeling practice with the systematic data organization, traceable links among various modeling parts as well as the efficient and concurrent repository for modeling data. Although modeling specific databases are still in infancy, they will turn to be an important component of the modeling practice in the near future.

7.1 Modified Lumped Capacitance Model for Deriving Heat Transfer Coefficients using Quenching Probes

An efficient numerical experiment procedure was proposed to validate a widely used model, namely lumped capacitance analysis approach, for deriving heat transfer coefficients in quenching probe tests. The limitation of the lumped capacitance model was discussed, especially when it was used for low sensitivity probes, for example the ISO quenching probe. A modified lumped capacitance model described by Equation 3.11 and 3.12 was presented based on the careful analysis of the numerical experiment results. The new model tackled both dumping and peak shift problems of the original lumped capacitance model. The new model, which required very limited work added into the original model, adopted a two-run improvement procedure. The new model was deemed to be feasible and efficient in the study of practical data of quenching probe tests. Several conclusions can be drawn from the numerical experiment: 1. The lumped capacitance model works very well with high sensitivity probes such as silver probes in all cases, linear and nonlinear.

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- 2. The lumped heat capacity model is capable of producing good results when the probe undergoes a constant heat transfer coefficient process, even though for the low sensitivity ISO Inconel600 probe.
- 3. Significant dumping effects can be found in an ISO Inconel600 probe undergoing a highly nonlinear process, for example a practical liquid quenching process. The lumped heat capacity model, however, could still be applicable if reasonable modifications can be adopted.
- 4. The location of the thermocouple is not significant for a probe with low Biot number, for example a silver probe. Locating the thermocouple in the midsection of the probe is recommended.

In the thesis the quenching probe problem was addressed from a pure modeling perspective. In practical applications, many issues arise from both the algorithm and system configurations such as the accuracy of thermocouple, data sampling, and so on. The system error is critical to both actual test and numerical experiment since lumped analysis is extremely sensitive to errors.^[113] Given the flexibility and advantages of numerical experiments, another numerical experimental procedure may be demanded to study the influence of system error on the derivation of heat transfer coefficient via lumped analysis. For example by introducing noise artificially, the impact of data smoothing can then be investigated. More desirably, a numerical procedure may need to be examined and the impact of the heat transfer coefficient on the result of simulation results, thermal history or even residual stress state. This can give a quantitative understanding of the importance of quenching probe test.

Other future work may study the effects of nonlinear material properties, including temperature dependent thermal conductivity and heat capacity, the sensitivity. It is also interesting to compare the results between different modeling approaches, including lumped capacitance model, temperature gradient method and other inverse heat conduction procedures.^[115] Future efforts could also be made to study the effects of other

experimental details, such as thermocouple sensitivity and disturbance of the temperature field within the probe due to the embedded thermocouple(s).

7.2 Incorporating Phase Transformation in the ANSYS code

A feasible procedure to incorporate latent heat of continuous phase transformation during the quenching processes was presented. A generic template for ANSYS program was generated. The customized codes were used to incorporate the latent heat of austenitic transformation and martensitic transformation. The customization was proved to be feasible and efficient.

Code customization is a desirable advanced skill for modeling practice. Nevertheless code customization is not a trivial task in some cases. It not only depends on the programmable interfaces that a commercial code provides but also the complexity of the functionality that need to be added. Full incorporation of the transformation latent heat and transformation plasticity is tedious and inefficient. In order to add the full capability of phase transformation module, numerous lines of code would be needed.

The template of code customization presented in the dissertation is for the latent heat of the phase transformation. To generalize the template, it is desirable to extend the template to accommodate the multiple phase transformations, including austenite to ferrite or carbide, austenite to pearlite, austenite to bainite and austenite to martensite. In addition the procedure for incorporating phase transformation plasticity need to be developed so that the phase transformation phenomena can be fully incorporated into the existing generic modeling analysis tools.

7.3 Modeling in Practical Quenching Design

A practical modeling procedure was presented to aid the quenching cycle design for a practical application, namely a kind of fastening ring used in civil engineering applications. A proposed new water quenching cycle was validated using a weakly coupled modeling procedure. The thermal history and thermal-stress were simulated by incorporating with the phase transformations. The simulated thermal results were in good agreement with the experimental test data. The simulation showed that reasonable amount of martensite was developed at the desired region. Complex residual stress states were found in the component after the quenching process. The simulation proved the validity of the water quenching cycle based on the as quenched phase products and consequently expected mechanical properties. In addition to the water quenching, a candidate polymer quenching process was also studied. The simulation showed that only limited amount of martensite was developed due to the slower quenching process. However lower thermal stresses were developed compared to those of water quenching, which was another major design issue. Some suggestions to the new cycle design were made based on the simulation results. This modeling practice demonstrated the power and the versatility of the virtual laboratory.

Future work can be focused on the extension of the current modeling to study other possible cycles, including different quenchants and interrupted or timing quenching processes. Experimental validations are demanded, for example the quantitative microscopy to validate the prediction of phase transformation, and the experimental measurements to validate the residual stress and distortion predictions.

7.4 Specific Databases for Modeling Practice

Process modeling needs the computer and there are still many modeling aspects needed to be explored with the aid of the computer. Developing computer tools for modeling practice demands efforts from both materials science and computer science. Computer methodologies such as databases and application tools will facilitate process modeling practice and may become increasingly important in the future.

Databases for heat transfer coefficients and modeling data were proposed in the dissertation. The objectives of developing modeling databases are for the systematic and

efficient modeling practice. Relational and object-oriented databases are two major database techniques so far, however, object databases are more capable of managing modeling data.

The databases proposed in the dissertation form the blueprints of future work. Building a database is a very difficult task and mainly depends on the quality and quantity of the data accumulated. The task also requires careful design of testing and modeling procedure so that information can be derived efficiently from the results obtained. The author envisions that developing multi-purpose databases for process modeling in material science and engineering will be an important and imperative task in the near future.

REFERENCES

- Ericsson, T., "Principles of Heat Treating of Steels", <u>Metals Handbook</u>, 10th ed.,
 Vol. 4, ASM International, Materials Park, Ohio, 1991, pp. 3-32.
- [2] Bates, C.E., Totten, G.E., and Brennan, R.L., "Quenching of Steel", <u>Metals</u> <u>Handbook</u>, 10th ed., Vol. 4, ASM International, Materials Park, Ohio, 1991, pp. 67-120.
- [3] Persampieri, D., Roman, A.S., and Hilton, P.D., "Process Modeling for Improved Heat Treating", <u>Advanced Materials & Processes</u>, Vol.139, No.3, 1991, pp. 19-23.
- [4] Gergely, M., Somogyi, S., Reti, T., and Konkoly, T., "Computerized Properties Prediction and Technology Planning in Heat Treatment of Steels", <u>Metals</u> <u>Handbook</u>, 10th ed., Vol. 4, ASM International, 1991, pp. 639-766.
- [5] Reti, T., Felde, I., Horvath, L., Kohlheb, R., and Bell, T., "Quenchant Performance Analysis Using Computer Simulation", <u>Heat Treatment of Metals</u>, Vol.23, No.1, 1996, pp. 11-14.
- [6] Reti, T., Gergely, M., and Szilvassy, C.C., "Property Prediction of Quenched and Case Hardened Steels Using a PC", <u>Conf. Proc. Quenching and Carburising</u>, <u>Melbourne</u>, <u>Australia</u>, 1991, The Institute of Materials, London, UK, 1993, pp. 267-280.
- [7] Doyama, M., "Computer Applications to Materials Science and Engineering", <u>Mater. Trans.</u> Vol.32, No.2, 1991, pp. 105-113.
- [8] <u>Quenching and Distortion</u>, Ed. Totten, G.E., ASM International, Materials Park, Ohio, 1992.
- [9] Hu, M., Chen, X., and Pan, J., "Computer Simulation of Finite Length Cylindrical Parts during Heating Process and Reasonable Utilization of Energy", <u>Conf. Proc.</u> <u>Environmental and Energy Efficient Heat Treatment Technologies, Beijing,</u>

China, 15-17 Sept. 1993, International Academic Publishers, Beijing, China, 1993, pp. 40-45.

- [10] Inoue, T., and Uehara, T., "The Japanese Sword: Computer Simulation of Quenching Process", <u>Conf. Proc. Phase Transformations During the</u> <u>Thermal/Mechanical Processing of Steel, Vancouver, British Columbia, Canada,</u> <u>20-24 Aug. 1995</u>, Canadian Institute of Mining, Montreal, Canada, 1995, pp. 373-385.
- [11] Palafox, M.G., and Colas, R., "Computer Modeling as A Predictive Tool for Heat Treating", <u>Conf. Proc. Second International Conference on Quenching and the</u> <u>Control of Distortion, Cleveland, Ohio, USA, 4-7 Nov. 1996</u>, Eds. Totten, G.E., Howes, M.A.H., Sjostrom, S., and Funatani, K., ASM International, Materials Park, Ohio, 1996, pp. 315-320.
- [12] Baker, A.J., Manhardt, P.D., and Orzechowski, J.A., "On a FEM Platform for Simulation of Quenching/Heat Treating Operations", <u>Conf. Proc. Second</u> <u>International Conference on Quenching and the Control of Distortion, Cleveland,</u> <u>Ohio, USA, 4-7 Nov. 1996</u>, Eds. Totten, G.E., Howes, M.A.H., Sjostrom, S., and Funatani, K., ASM International, Materials Park, Ohio, USA, 1996, pp. 283-290.
- [13] Pan, J., Hu, M., She, X., and Ruan, D., "Development of Gas Carburizing CAD Software", <u>Heat Treatment of Metals (China)</u>, Vol.7, 1997, pp. 6-8.
- [14] Dymova, L.G., Sevastyanov, P.V., and Timoshpol'skii, V.I., "Comparative Analysis of Mathematical Models for Thermal Stress and Deformation Generation in a Solidifying Ingot", <u>J. Eng. Phys. (USSR)</u>, Vol.60, No.1, 1991, pp. 99-103.
- [15] Liscic, B., and Filetin, T., "Computer-Aided Determination of the Process Parameters for Hardening and Tempering Structural Steels", <u>Heat Treat. Met.</u> Vol.14, No.3, 1987, pp. 62-66.
- [16] Tanigawa, Y., and Komatsubara, Y., "Thermal Stress Analysis of a Rectangular Plate and its Thermal Stress Intensity Factor for Compressive Stress Field", Journal of Thermal Stresses, Vol.20, No.5, 1997, pp. 517-542.

- [17] Petrus, G.J., Krauss, T.M., and Ferguson, B.L., "Distortion Prediction Using the Finite Element Method", <u>Quenching and Distortion Control</u>, Ed: Totten, G.E., ASM International, Materials Park, Ohio, USA, 1992, pp. 283-286.
- [18] Wallis, R.A., Garwood, D.R., and Ward, J., "The Use of Modeling Techniques to Improve the Quenching of Components", <u>Conf. Proc. Heat Treating: Equipment</u> and Processes, Schaumburg, Illinois, USA, 18-20 Apr. 1994, ASM International, Materials Park, Ohio, USA, 1994, pp. 105-116.
- [19] Ramakrishnan, R.I., "Quench Analysis of Aerospace Components Using FEM" in <u>Quenching and Distortion Control</u>, Ed: Totten, G.E. ASM International, Materials Park, Ohio, USA, 1992, pp. 235-242.
- [20] Tian, H., and Stefanescu, D.M., "Experimental Evaluation of Some Solidification Kinetics-Related Material Parameters Required in Modeling of Solidification of Fe--C--Si Alloys", <u>Conf. Proc. Modeling of Casting, Welding and Advanced Solidification Processes. VI, Palm Coast, Florida, USA, 21-26 Mar. 1993</u>, The Minerals, Metals & Materials Society, Warrendale, Pennsylvania, USA, 1993, pp. 639-646.
- [21] Tszeng, T.C., Wu, W.T., and Semiatin, L., "A sensitivity study of the process model for predicting the distortion during heat treating", <u>Conf. Proc. Second</u> <u>International Conference on Quenching and the Control of Distortion, Cleveland,</u> <u>Ohio, USA, 4-7 Nov. 1996</u>, Eds. Totten, G.E., Howes, M.A.H., Sjostrom, S., and Funatani, K., ASM International, Materials Park, Ohio, USA, 1996, pp. 321-327.
- [22] Denis, S., and Simon, A., "Modeling of Heat Treatment of Steels: from Concepts to Process Simulation", <u>Conf. Proc. Second International Conference on</u> <u>Quenching and the Control of Distortion, Cleveland, Ohio, USA, 4-7 Nov. 1996</u>, Eds. Totten, G.E., Howes, M.A.H., Sjostrom, S., and Funatani, K., ASM International, Materials Park, Ohio, USA, 1996, pp. 239-240.
- [23] Krauss, G., "State-of-the-Art Developments in the Heat Treatment of Ferrous Alloys", <u>Mater. Sci. Forum</u>, Vol.163-165, 1994, pp. 15-35.

- [24] Yao, S.C., and Ericsson, T., "Computer Simulation for Quenching Process", <u>Heat</u> <u>Treat. Met. (China)</u>, No.8, 1987, pp. 25-32.
- [25] Seabrook, J.B., Brunot, A.W., Toney, S., and Melilli, A.S., "Prediction of Large Component Response to Heat Treatment by a Simulation Technique", <u>Computer</u> <u>Simulation for Materials Applications, Nuclear Metallurgy</u>, Vol.20, No.2, 1976, pp. 1051-1061.
- [26] Spalding, D.B., and Afgan, N.H., <u>Heat and Mass Transfer in Metallurgical</u> <u>Systems</u>, Hemisphere Publishing Corp. Washington, D.C. 1981.
- [27] Fukuda, S., Yoshihara, N., Ohkubo, Y., Fukuoka, Y., and Takushima, S., "Heat Transfer Analysis of Roller Quench System in Continuous Annealing Line", <u>Trans. Iron Steel Inst. Jpn.</u>, Vol.24, No.9, 1984, pp. 734-741.
- [28] Arola, R., Martikainen, H., and Virta, J., "Computer Aided Simulation of the Temperature and the Distortion of Components During Heating Up in Heat Treatment Furnaces", <u>Materials Science Forum (Switzerland)</u>, Vol.102-104, No.2, 1992, pp. 783-790.
- [29] Liscic, B., "State of the Art of Computer Simulation in Quenching", <u>Conf. Proc.</u> <u>Heat & Surface '92, Kyoto, Japan, 17-20 Nov. 1992</u>, Japan Technical Information Service, Tokyo, Japan, 1992, pp. 551-556.
- [30] Hasson, J., "Quenchants: Yesterday, Today, and Tomorrow", <u>Quenching and</u> <u>Control of Distortion</u>, Ed. Totten, G.E., ASM International, Chicago, Illinois, 1992, pp. 22-25.
- [31] Kovalenko, G.V., and Kobasko, N.I., "Modeling of the Unsteady-state Boiling Process in Water Quenching of Metals", <u>Heat Transfer Sov. Res.</u>, Vol.20, No.1, 1988, pp. 69-78.
- [32] Reti, T., Felde, I., Horvath, L., Kohlheb, R., and Bell, T., "Quenchant Performance Analysis Using Computer Simulation", <u>Heat Treatment of Metals</u>, Vol.23, No.1, 1996, pp. 11-14.
- [33] Fletcher, A.J., and Griffiths, W.D., "Heat Transfer during Vapor Blanket Stage of Quench", <u>Materials Science and Technology</u>, Vol.9, November 1993, pp. 958-965

- [34] Majorek, A., Muller, H., Macherauch, E., and Scholtes, B., "Influence of Heat Transfer on the Development of Residual Stresses in Quenched Steel Cylinders", <u>Steel Res.</u>, Vol.65, No.4, 1994, pp. 146-151.
- [35] Segerberg, S., and Bodin, J., "Investigation of Quenching Conditions and Heat Transfer in the Laboratory and in Industry", <u>Conf. Proc. Quenching and</u> <u>Carburising, Melbourne, Australia, 1991</u>, The Institute of Materials, London, UK, 1993, pp. 177-188.
- [36] Liscic, B., Svaic, S., and Filetin, T., "Workshop Designed System for Quenching Intensity Evaluation and Calculation of Heat Transfer Data", <u>Quenching and</u> <u>Distortion Control</u>, Ed. Totten, G.E. ASM International, Materials Park, Ohio, USA, 1992, pp. 17-26.
- [37] Reti, T., Horvath, L., Sutto, A., and Felde, I., "Comparative Analysis of Quenching Performance of Quenchants using Computer Simulation", <u>Conf. Proc.</u> <u>Euromat 94. Vol. IV, Balatonszeplak, Hungary, 30 May-1 June 1994</u>, Hungarian Mining and Metallurgical Society (OMBKE), Budapest, Hungary, 1994, pp. 1315-1319.
- [38] Reti, T., Czinege, I., Reger, M., and Takacs, J., "An Indirect Method for Quantitative Characterization of the Quenching Power of Quenching Media", <u>Quenching and Distortion Control</u>, ASM International, Materials Park, Ohio, USA, 1992, pp. 301-309.
- [39] Hernandez-Morales, B., Brimacombe, J.K., and Hawbolt, E.B., "Application of Inverse Techniques to Determine Heat Transfer Coefficients in Heat Treating Operations", <u>Journal of Materials Engineering and Performance</u>, Vol.1, No.6, 1992, pp. 763-771.
- [40] Fletcher, A.J., and Griffiths, W.D., "Model of Heat Transfer during Quenching in Sodium Polyacrylate Solutions", <u>Materials Science and Technology</u>, Vol.11, March 1995.
- [41] Tajima, M., Maki, T., and Katayama, K., "Study of Heat Transfer Phenomena in Quenching of Steel (An Analysis of Cooling Curves Accompanied with Phase

Transformation)", <u>JSME International Journal, Series II</u>, Vol. 31, February 1988, pp. 98-104.

- [42] Lally, K.S., Kearny, M.W., and Totten, G.E., "Quench Tank Agitation", <u>Quenching and Control of Distortion</u>, Ed. Totten, G.E. ASM International, Materials Park, Ohio, 1992, pp. 95-105.
- [43] Fletcher, A.J., <u>Thermal Stress and Strain Generation in Heat Treatment</u>, Elsevier Applied Science, London and New York, 1989.
- [44] Leblond, J.B., and Devaux, J., "Interactions Between Transformation Plasticity and Strain Hardening Phenomena in Steels", <u>Conf. Proc. International Conference</u> <u>on Residual Stress. ICRS 2, Nancy, France, 23-25 Nov. 1988</u>, Elsevier Applied Science, Barking, Essex, UK, 1989, pp. 410-415.
- [45] Leblond, J.B., "Mathematical Modelling of Transformation Plasticity in Steels. II. Coupling With Strain Hardening Phenomena", <u>Int. J. Plast.</u> Vol.5, No.6, 1989, pp. 573-591.
- [46] Leblond, J.B., Devaux J, and Devaux JC, "Mathematical Modelling of Transformation Plasticity in Steels. I. Case of Ideal--Plastic Phases", <u>Int. J. Plast.</u> Vol.5, No.6, 1989, pp. 551-572.
- [47] Inoue, T., Ju, D., and Arimoto, K., "Metallo-Thermo-Mechanical Simulation of Quenching Process--Theory and Implementation of Computer Code "Hearts"", <u>Quenching and Distortion Control</u>, Ed. Totten, G.E. ASM International, Materials Park, Ohio, USA, 1992, pp. 205-212.
- [48] Thuvander, A., and Melander, A., "Prediction of Distortion and Residual Stresses of Engineering Steels Due to Heat Treatment", <u>Mater. Sci. Forum</u>, Vol.163-165, 1994, pp. 641-656.
- [49] Henriksen, M., Larson, D.B., and Van Tyne, C.J., "Modeling Distortion and Residual Stress in Carburized Steels", <u>Quenching and Distortion Control</u>, Ed. Totten, G.E. ASM International, Materials Park, Ohio, USA, 1992, pp. 213-219.
- [50] Arthur, W.R., Becker, R., and Karabin, M.E., "Experimentation and Modeling of Residual Stresses and Distortion in Quenched Rectangular Bars", <u>Conf. Proc.</u>

Heat Treating: Equipment and Processes, Schaumburg, Illinois, USA, 18-20 Apr. 1994, ASM International, Materials Park, Ohio, USA, 1994, pp. 43-50.

- [51] Inoue, T., and Arimoto, K., "Development and Implementation of CAE System "HEARTS" for Heat Treatment Simulation Based on Metallo-thermo-mechanics", <u>Journal of Materials Engineering and Performance</u>, Vol.6, No.1, 1997, pp. 51-60.
- [52] Aksel, B., Mukherjee, S., and Arthur, W.R., "A Study of Quenching: Experiment and Modelling", <u>Journal of Engineering for Industry (Transactions of the ASME)</u>, Vol.114, No.3, 1992, pp. 309-316.
- [53] Okamura, K., and Kawashima, H., "Analysis of Residual Deformation of a Gear During Quenching", <u>Conf. Proc. Thirty-Second Japan Congress on Materials</u> <u>Research, Kyoto, Japan, Dec. 1988</u>, Society of Materials Science, Kyoto, Japan, 1989, pp. 323-329.
- [54] Li, Y.Y., and Chen, Y., "Modeling Quenching to Predict Residual Stress and Microstructure Distribution", <u>Trans. Asme J. Eng. Mater. Technol.</u> Vol.110, No.4, 1988, pp. 372-379.
- [55] Nair, R.R., Natarajan, R., and Rao, U.R.K., "Analysis of Residual Stresses due to Quenching Considering Microstructural Transformations", <u>Int. J. Mach. Tool</u> <u>Design & Res.</u>, Vol.22, No.4, 1982, pp. 309-319.
- [56] Carmet, A., Debiez, S., Devaux, J., Pont, D., and Leblond, J.B., "Experimental and Numerical Study of Residual Stresses and Strains in an Electron-Beam-Welded Joint", <u>Conf. Proc. International Conference on Residual Stress. ICRS 2,</u> <u>Nancy, France, 23-25 Nov. 1988</u>, Elsevier Applied Science, Barking, Essex, UK, 1989, pp. 491-496.
- [57] Majorek, A., Scholtes, B., Muller, H., and Macherauch, E., "The Influence of Heat Transfer on the Development of Stresses, Residual Stresses and Distortions in Martensitically Hardened SAE 1045 and SAE 4140", <u>Quenching and Distortion</u> <u>Control</u>, Ed. Totten, G.E. ASM International, Materials Park, Ohio, USA, 1992, pp. 171-179.
- [58] Boyer, J.C., and Boivin, M., "Numerical Predictions of Residual Stress Relaxation in Quenched Plates", <u>Conf. Proc. Calculation of Internal Stresses in Heat</u>

Treatment of Metallic Materials, Linkoping, Sweden, 23-25 May 1984, Linkoping University, Linkoping, Sweden, 1984, pp. 97-117.

- [59] Hellier, A.K., Stefulj, M., McGirr, M.B., and Algie, S.H., "Computer Simulation of Residual Stresses During Quenching", <u>Conf. Proc. Quenching and Carburising:</u> <u>3rd International Seminar, Melbourne, Australia, Sept. 1991</u>, Institute of Metals and Materials Australasia, Parkville, Victoria, Australia, 1991, pp. 135-145.
- [60] Chen, X., and Meekisho, L., "Computer Simulation of Temperature and Thermal Stress Fields during Quenching Process", <u>Conf. Proc. Second International</u> <u>Conference on Quenching and the Control of Distortion, Cleveland, Ohio, USA,</u> <u>4-7 Nov. 1996</u>, Eds. Totten, G.E., Howes, M.A.H., Sjostrom, S., and Funatani, K., ASM International, Materials Park, Ohio, USA, 1996, pp. 241-247.
- [61] Buchmayr, B., and Kirkady, J.S., "A Fundamental Based Microstructural Model for the Optimization of Heat Treatment Processes", <u>Quenching and Distortion</u> <u>Control</u>, Ed. Totten, G.E. ASM International, Materials Park, Ohio, 1992, pp. 221-227.
- [62] Leblond, J.B., Mottet, G., Devaux, J., and Devaux, J.C., "Mathematical Models of Anisothermal Phase Transformations in Steels, and Predicted Plastic Behaviour", <u>Materials Science and Technology</u>, Vol.1, October 1985, pp. 815-822.
- [63] Fletcher, A.J., and Lewis, C., "Effects of free edge on thermal stresses in quenched steel plates", <u>Materials Science and Technology</u>, Vol.1, October 1985, pp. 780-785
- [64] Sjostrom, S., "Interations and constitutive models for calculating quench stresses in steel", <u>Materials Science and Technology</u>, Vol.1, October 1985, pp. 823-829.
- [65] Zienkiewicz, O.C., <u>Finite Element Method</u>, McGraw-Hill Book Company, London, 1986.
- [66] Becker, M., <u>Heat Transfer</u>, Plenum Press, New York, 1986.
- [67] Incropera, F.P., and DeWitt, D.P., <u>Fundamentals of Heat and Mass Transfer</u>, 4th ed., John Wiley & Sons, New York, 1990.
- [68] Wolf, H., <u>Heat Transfer</u>, Harper & Row, New York, 1983.
- [69] ANSYS REFERENCE MANUAL, Version 5.3, Ed. Kohnke, P., ANSYS, 1994.

- [70] <u>Atlas of Isothermal Transformation and Cooling Transformation Diagrams</u>, ASM International, Materials Park, Ohio, USA, 1977.
- [71] Agarwal, P.K., and Brimacombe, J.K., "Mathematical Model of Heat Flow and Austenite-Pearlite Transformation in Eutectoid Carbon Steel Rods for Wire", <u>Metallurgical Transactions B</u>, Vol.12B, March 1981, pp. 121-133.
- [72] Yuan, W., Chen, X., and et al., "Computer Simulation of Three Dimensional Unsteady Temperature Field During Heat Treatment", <u>Transactions of Metal Heat</u> <u>Treatment (China)</u>, Vol.12, No.2, 1991, pp. 35-42.
- [73] Koistinen, D.F., and Marburger, R.E., "A General Equation Prescribing the Extent of the Austenite-martensite Transformation in Pure Iron-carbon Alloys and Plain Carbon Steels", <u>Acta Met.</u> Vol.7, No.1, 1959, pp. 59-60.
- [74] Ankara, O.A., and West, D.R., "Some Effects of Austenitizing Conditions on Martensite Formation in an Iron--20 percent Nickel Alloy", <u>Iron Steel Inst J.</u> Vol.204, No.5, May 1966, pp. 509-511.
- [75] de Jong, M., and Rathenau, G.W., "Mechanical Properties of Iron and Some Iron Alloys While Undergoing Allotropic Transformation", <u>Acta Met.</u> Vol.7, No.4, 1959, p. 246.
- [76] Lozinsky, M., "Superhigh Plasticity of Commercial Iron under Cyclic Fluctuations of Temperature", <u>Acta Met.</u> Vol.7, No.11, November 1959, pp. 709-715.
- [77] Lozinsky, M., "Grain Boundary Adsorption and Superhigh Plasticity", <u>Acta Met.</u> Vol.9, No.7, July 1961, pp. 689-693.
- [78] Tamura, I., "Deformation-Induced Martensitic Transformation and Transformation-Induced Plasticity in Steels", <u>Met. Sci.</u> Vol.16, No.5, May 1982, pp. 245-253.
- [79] Denis, S., Simon, A., and Beck, G., "Consideration of the Behavior of a Steel With Martensite Conversion in the Calculation of Residual Stresses During Quenching", <u>Harterei-Tech. Mitt.</u> Vol.37, No.1, 1982, pp. 18-28.
- [80] Denis, S., Gautier, E., Simon, A., and Beck, G., "Stress-phase-transformation Basic Principles, Modeling, and Calculation of Internal Stresses", <u>Materials</u> <u>Science and Technology</u>, Vol.1, No.10, October 1985, pp. 805-814.

- [81] Fletcher, A.J., and Price, R.F., "Generation of Thermal Stress and Strain During Quenching of Low-Alloy Steel Plates", <u>Metals Technology</u>, Vol.8, No.11, 1981, pp. 427-446.
- [82] Patel, J.R., Cohen, M., and Averbach, B.L., "Criterion for the Action of Applied Stress in the Martensiteic Transformation", <u>Acta Metall.</u> Vol.1, 1953, pp. 531-538.
- [83] Inoue, T., and Wang, Z., "Coupling Between Stress, Temperature, and Metallic Structures during Processes Involving Phase Transformations", <u>Materials Science</u> and Technology, Vol.1, No.10, October 1985, pp. 845-850.
- [84] Denis, S., Simon, A., and Beck, G., "Analysis of the Thermomechanical Behaviour of Steel During Martensitic Quenching and Calculation of Internal Stresses", <u>Conf. Proc. Internal Stress: Origin--Measurement--Evaluation</u> (Eigenspannungen: Entstehung--Messung--Bewertung). Vol. 1, Karlsruhe, FRG, <u>14-15 Apr. 1983</u>, Deutsche Gesellschaft fur Metallkunde, Karlsruhe, FRG, 1983, pp. 211-238.
- [85] Ferziger, J.H., <u>Numerical Methods for Engineering Application</u>, John Wiley & Sons, New York, 1981.
- [86] Chen, X., "Computer Simulation of Heat Treating Process and Computer-Aided Exploration of Optimizing Conventional Technology", <u>MS Thesis</u>, Dept. of Materials Science and Engineering, Shanghai Jiao Tong University, 1990.
- [87] Huebner, K.H., <u>The Finite Element Method for Engineers</u>, John Wiley & Sons, New York, 1975.
- [88] Noyan, I.C., and Cohen, J.B., "The Nature of the Residual Stress and Its Measurement" in <u>Residual Stress and Stress Relaxation</u>, Eds. Kula, E. and Weiss, V. Plenum Press, New York, 1982, pp. 1-17.
- [89] Chen, X., Becker, M., and Meekisho, L., "Finite Element Analysis in Moving Coordinates", ASME HTD 384, Eds. Clarksean, L., Hogan, R. and et al., 1997, pp. 91-99.
- [90] Baker, A.J., "Potential for CFD in Heat Treating", <u>Advanced Materials &</u> <u>Processes</u>, Vol.152, No.4, October 1997, pp. 44O-44T.

- [91] Garwood, D.R., Lucas, J.D., Wallis, R.A., and Ward, J., "Modeling of the Flow Distribution in an Oil Quench Tank", <u>Journal of Materials Engineering and</u> <u>Performance</u>, Vol.1, No.6, 1992, pp. 781-787.
- [92] Pritchard, J., Nurnberg, G., and Shoukri, M., "Design optimization of high pressure quench vacuum furnaces through computer modeling", <u>Industrial</u> <u>Heating</u>, Vol.62, No.9, 1995, pp. 57-60.
- [93] Pritchard, J.E., Nurnberg, G., and Shoukri, M., "Computer modeling of pressure gas quenching in vacuum furnaces", <u>Conf. Proc. Heat Treating. Proceedings of the</u> <u>16th Conference, Cincinnati, Ohio, USA, 19-21 Mar. 1996</u>, ASM International, Materials Park, Ohio, USA, 1996, pp. 399-404.
- [94] Chen, X., Meekisho, L., Zhang, J., Blicblau, A., and Doyle, D., "Computer Simulation of Velocity and Temperature Fields during Gas Quenching in Vacuum Heat Treatment Furnace", <u>Conf. Proc. 1995 Carburizing and Nitriding With Atmospheres, Cleveland, Ohio, USA, 6-8 Dec. 1995</u>, ASM International, Materials Park, Ohio, USA, 1995, pp. 385-390.
- [95] <u>Readings in Database Systems</u>, 2nd ed., Eds. Stonebraker, M., Morgan Kaufmann Publishers, San Mateo, California, 1994.
- [96] Elmasri, R., and Navathe, S.B., <u>Fundamentals of Database Systems</u>, 2nd ed., The Benjamin/Cummings Publishing Co, Inc. Redwood City, California, 1994.
- [97] <u>Readings in Object-Oriented Database Systems</u>, Eds. Zdonik, S. and Maier, D. Morgan Kaufmann Publishers, Inc. San Mateo, California, 1990.
- [98] Loomis, M.E.S., <u>Object Databases, The Essentials</u>, Addison-Wesley Publishing Company, Reading, Massachusetts, 1995.
- [99] MacKenzie, D.S., Totten, G.E., and Webster, G., "Quenching Fundamentals: Heat Transfer", <u>Conf. Proc. 2nd International Conference on Quenching and Control of</u> <u>Distortion</u>, Eds. Totten, G.E., Howes, M.A.H., Sjostrom, S., and Funatani, K., ASM International, USA, Materials Park, Ohio, 1996, pp. 329-338.
- [100] Hernandez-Morales, B., Brimacombe, J.K., Hawbolt, E.B., and Gupta, S.M.,"Determination of Quench Heat-Transfer Coefficients Using Inverse Techniques",

Quenching and Distortion Control, Ed. Totten, G.E., ASM International, Materials Park, Ohio, USA, 1992, pp. 155-164.

- Bodi, J., and Segerberg, S., "Benchmark Testing of Computer Programs for Determination of Hardening Performance", <u>Quenching and Distortion Control</u>, Ed. Totten, G.E., ASM International, Materials Park, Ohio, USA, 1992, pp. 133-139.
- [102] Bodin, J., and Segerberg, S., "Measurement and the Evaluation of Quenching Power of Quenching Media for Hardening", <u>Quenching and Distortion Control</u>, Ed. Totten, G.E., ASM International, USA, Materials Park, Ohio, 1992, pp. 1-12.
- [103] Narazaki, M., Asada, S., and Fukahara, K., "Recent Research on Cooling Power of Liguid Quenchants in Japan", <u>Conf. Proc. 2nd International Conference on Quenching and Control of Distortion</u>, Eds. Totten, G.E., Howes, M.A.H., Sojostrom, S., and Funatani, K., ASM International, USA, Materials Park, Ohio, 1996, pp. 37-46.
- [104] Beck, J.V., and Osman, A.M., "Analysis of Quenching and Heat Treating Processes Using Inverse Heat Transfer Method", <u>Quenching and Distortion</u> <u>Control</u>, Ed. Totten, G.E. ASM International, Materials Park, Ohio, USA, 1992, pp. 147-153.
- [105] Xu, X., Chen, G., Liu, C., Liu, Z., and Wu, J., "Numerical simulation of the stresses evolution during tempering of steel", <u>Heat Treatment of Metals (China)</u>, Vol.3, 1997, pp. 12-15.
- [106] Totten, G.E., Webster, G.M., Tensi, H.M., and Jarvis, L.M., "Cooling curve analysis--international and national standard development: a status report", <u>Conf.</u> <u>Proc. Second International Conference on Quenching and the Control of Distortion, Cleveland, Ohio, USA, 4-7 Nov. 1996</u>, Eds. Totten, G.E., Howes, M.A.H., Sjostrom, S., and Funatani, K., ASM International, Materials Park, Ohio, USA, 1996, pp. 585-593.
- [107] Chen X, Pan J, and et al., "Finite Difference Method for Solving Multi-Dimensional Heat Conduction and its Application in Heat Treatment", <u>Conf.</u>

Proc. International Conference on Computers in Machinery Industry, Tianjing University Press, Shanghai, PRC, 1992, pp. 625-629.

- [108] Hu, M., Pan, J., Tain, D., and Zhang, W., "Computer simulating of the threedimensional temperature field of quenching process with suddenly changed surface condition", <u>Conf. Proc. Second International Conference on Quenching</u> <u>and the Control of Distortion, Cleveland, Ohio, USA, 4-7 Nov. 1996</u>, Eds. Totten, G.E., Howes, M.A.H., Sjostrom, S., and Funatani, K., ASM International, Materials Park, Ohio, USA, 1996, pp. 63-67.
- [109] Liscic, B., "Possibilities for the Calculation, Measurement and Control of the Temperature Change During Quenching", <u>Neue Hutte</u>, Vol.28, No.11, 1983, pp. 405-411.
- [110] Chen, J., and Wang, H., "The Computer Simulation on Heat Transfer of Thickwall Tube during Quenching", <u>Transactions of Metal Heat Treatment (China)</u>, Vol.18, No.1, 1997, pp. 38-44.
- [111] Hodgson, P.D., Browne, K.M., Gibbs, R.K., Pham, T.T., and Collinson, D.C.,
 "The Mathematical Modeling of Temperature and Microstructure During Spray Cooling", <u>Quenching and Distortion Control</u>, Ed. Totten, G.E. ASM International, Materials Park, Ohio, USA, 1992, pp. 41-49.
- [112] Lainer, K., and Tensi, H.M., "Heat Transfer Coefficient and Heat Flux Density Distribution, Influenced by the Wetting Behavior of Hollow Cylinders", <u>Conf.</u> <u>Proc. Second International Conference on Quenching and the Control of</u> <u>Distortion, Cleveland, Ohio, USA, 4-7 Nov. 1996</u>, Eds. Totten, G.E., Howes, M.A.H., Sjostrom, S., and Funatani, K., ASM International, Materials Park, Ohio, USA, 1996, pp. 93-100.
- [113] Beck, J.V., <u>Inverse Heat Conduction</u>, <u>Ill-posed Problems</u>, Wiley-Interscience, New York, 1985.
- [114] Iyer, K.A., "Quantitative Characterization of Thermophisical Properties in Computational Heat Transfer", MS thesis, Dept. of Materials Science and Engineering, Oregon Graduate Institute of Science and Technology, 1993.

- [115] Walton, H., "Dimensional Changes During Hardening and Tempering of Through-Hardened Bearing Steels", <u>Quenching and Distortion Control</u>, Ed. Totten, G.E., ASM International, Materials Park, Ohio, USA, 1992, pp. 265-273.
- [116] Leblond, J.B., and Devaux, J., "A New Kinetic Model for Anisothermal Metallurgical Transformations in Steels Including Effect of Austenite Grain Size", <u>Acta Metall.</u> Vol.32, No.1, 1984, pp. 137-146.
- [117] Carmet, A., Debiez, S., Leblond, J.B., Deveaux, J., and Pons, D., "Numerical Determination of the Stresses and Residual Deformations in an Electron Beam Welded Joint", <u>Soudage Tech. Connexes</u>, Vol.43, No.9-10, 1989, pp. 55-62.
- [118] Leblond, J.B., Mottet, G., and Devaux, J.C., "A Theoretical and Numerical Approach to the Plastic Behaviour of Steels during Phase Transformations. I. Derivation of General Relations", <u>J. Mech. Phys. Solids</u>, Vol.34, No.4, 1986, pp. 395-409.
- [119] Leblond, J.B., Mottet, G., Devaux, J., and Devaux, J.C., "Mathematical Models for Description of Anisothermal Phase Transformations in Steels and Their Consequences on the Plastic Behavior", <u>Conf. Proc. Calculation of Internal Stresses in Heat Treatment of Metallic Materials, Linkoping, Sweden, 23-25 May 1984</u>, Vol. 1, Linkoping University, Kurssekretariatet, Linkoping, Sweden, 1984, pp. 191-220.
- [120] SYSWELD+ REFERENCE MANUAL, Version 1.0, FRAMASOFT+CSI, 1990.
- [121] Brooks, C.R., <u>Principles of the Heat Treatment of Plain Carbon and Low Alloy</u> Steels, ASM International, Materials Park, Ohio, USA, 1996, p. 32.
- [122] Pan J, Private Communication.[Unpublished], Dept. of Materials Science and Engineering, Shanghai Jiao Tong University, Shanghai, PRC, 1998.
- [123] Conf. Proc. 2nd Internationa Conference on Quenching and Control of Distortion, <u>Cleveland, Ohio, USA, 4-7 Nov. 1996</u>, Eds. Totten, G.E., Howes, M.A.H., Sjostrom, S., and Funatani, K., ASM International, Materials Park, Ohio, USA, 1996.

[124] Reti, T., and Felde, I., Unpublished Research and Discussions on Data Smoothing for Quenching Probe Test. [Unpublished], Banki Donat Polytechnic, Budapest, Hungary, 1998.

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