

# Simulating the Manufacturing Process Chain

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## Abstract

Process simulation is routinely used in the casting and forging industries for trouble shooting and design of new products and processes. Simulation is also being used increasingly in other technologies such as machining and heat treatment. Recent emphasis has been on linking modeling tools so that the entire process chain can be simulated, with the effects of one process step on microstructure and internal condition of the product carried forward to the next process step. The goal is to improve the accuracy of each step prediction and the final performance prediction.

The DANTE software for heat treatment simulation couples metallurgical phase transformation models to a commercial finite element solver. To incorporate other mechanics such as electromagnetics and fluid dynamics, we partner with companies that use other software with these capabilities. Examples will be presented for such collaborative usage of simulation predictions.

A brief discussion of material and process data needs is included.

## Keywords

Process Simulation, Finite Element Analysis, Heat Treatment, Residual Stress, ICME

## 1 Introduction

Worldwide there are strong pushes to link process modeling methods together so that the entire manufacturing process chain and subsequent part performance can be simulated. In the US, two such efforts are the Materials Genome Initiative (MGI), spearheaded by ASM International, and Integrated Computational Materials Engineering (ICME), spearheaded by The Metallurgical Society of AIME. The objective is to model metallurgical behavior so that part performance can be accurately predicted, with performance being the material response at each step of part manufacture and during service. This requires in-depth knowledge of the individual process steps across a range of length scales, and also knowledge of the effects of prior process steps on material behavior in subsequent process steps. At DANTE Solutions, we have not yet bridged the difference in length scale between process models and microstructural models of the grain level and smaller. Right now, we are still at the finite element type of scale, relating bulk stresses and strains to metallurgical behavior, with fractions of phases describing the microstructure.

Heat treat simulation requires a combination of metallurgical models to handle phase transformations, stress and thermal mechanics models. Other physics are required to address fluid dynamics during quenching and electromagnetics during induction heating. An example of linking other physics software with heat treatment simulation follows.

## 2 Induction Hardening

The DANTE software does not include electromagnetic models needed to simulate induction heating. Instead, the results from software such as FLUX are used to facilitate induction heating with DANTE. Working with companies that are knowledgeable in using electromagnetic capable software, time-temperature predictions or time-power predictions are mapped to a DANTE heating model. Software such as FLUX simulates the electromagnetics, but phase

transformation is not considered. By running the DANTE heating model using Joule heating, with power and distribution based on the electromagnetic predictions from FLUX, austenite formation can be properly accounted for, as well as carbide dissolution during the short time at temperature. The kinetics of martensite formation can be simulated during the spray quenching step. This provides the capability for analyzing process variations such as dwell time between heating and spray quenching, the effect of scanning speed on depth of austenite formation, the effect of spray intensity on residual stress state, etc. An example application is discussed below.

### 2.1 Induction Hardening an Axle Shaft - [Li, 2013]

Induction hardening of an axle shaft made of 1541 steel was modeled. Fluxtrol performed the FLUX2D induction heating simulation. Close communication was required between companies to assist accurate use of FLUX2D results with the DANTE heating model. Figure 1 shows the dimensions of the axle shaft. Table 1 lists the induction hardening process steps. Figure 2 compares temperature distributions predicted by FLUX2D and DANTE at identical process times to show that the integration of FLUX2D results into DANTE was accurate.

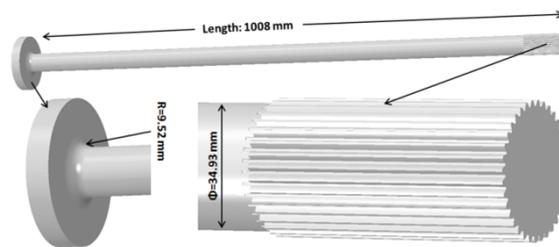


Figure 1: 1541 steel axle shaft.

Step No.	Time Period (s)	Inductor Speed (mm/s)	Power, kW	Spray Quench
1 (dwell)	9.0	0.0	26.5	No
2	1.5	15.0	23.9	No
3	105.0	8.0	35.4	Yes
4	14.7	8.0	32.0	Yes
5	60.0	8.0	0.0 (power off)	Yes

Table 1: Induction Hardening Schedule for 1541 Steel Axle Shaft.

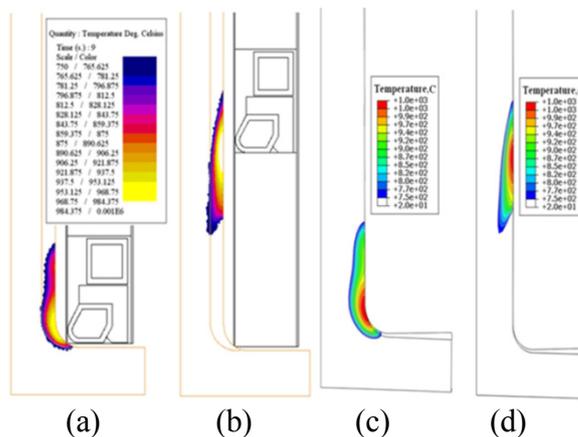


Figure 2. Temperature distributions predicted by Flux (a&b) and DANTE (c&d). Figures a & c are at the end of 9 s initial heating period, and b & d are after 16.5 s from the starting of induction heating.

There was considerable discussion about the surface heat transfer coefficient during spray quenching because no time-temperature measurements were available. Models were run using high, medium and low values for heat transfer, and stress predictions were evaluated. Based on these model results, the spray heat transfer coefficient was assigned a value of 12 kW/(m<sup>2</sup>\*K). The media being sprayed was a 6% PAG solution.

Phase transformation kinetics parameters had not been previously determined for 1541 steel, but published TTT and CCT diagrams were available. Parameters for DANTE's cooling kinetics

were determined from these diagrams. Kinetics for heating were estimated from parameters determined for other steel grades. Figure 3 shows a TTT diagram and a martensite cooling curve that were generated from the DANTE kinetics parameters used for this steel.

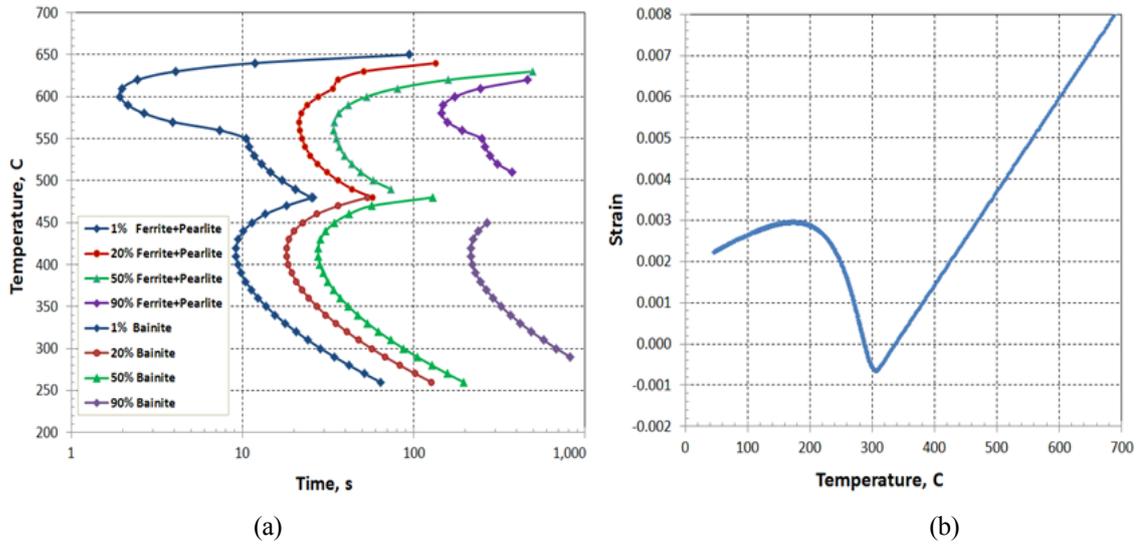


Figure 3. Phase transformation kinetics data for AISI 1541 steel. (a) Isothermal transformation curves predicted for diffusive phase formation. (b) Dilatometric predicted strain data for martensite formation from austenite during continuous cooling.

Predictions for temperature, austenite, hoop (circumferential) stress and radial and axial displacements at the end on the 9 second initial period are shown in Figure 4. This moment is just before scanning has started. The surface hoop stress in the fillet is neutral to low tension, with a subsurface compressive zone surrounding the austenitized layer. Centerline tension is present above the heated zone in the shaft.

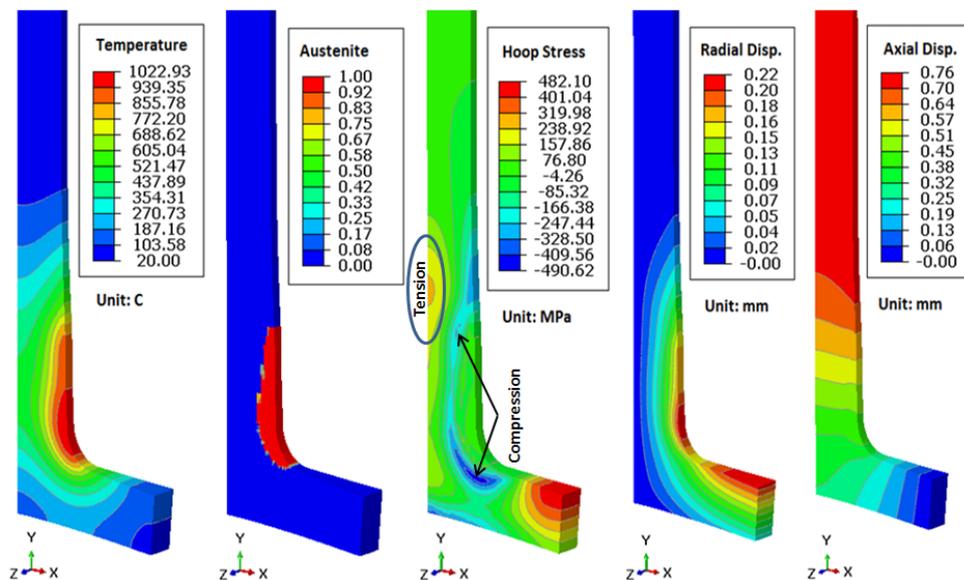


Figure 4: Predicted conditions after the initial 9 second induction heating step.

As scanning toward the splined end of the shaft takes place, the centerline tensile zone is pushed ahead of the heated section. Spray quenching does not start until 10.5 seconds into the process and the inductor head has moved 22.5 mm up the shaft. Figure 5 shows predicted conditions after 16.5 seconds into the process. The hot zone is now away from the fillet and martensite has formed at the surface of the fillet. The austenite zone is fairly extensive, occupying the shaft surface in the hot zone and sub-surface under the forming martensite. Hoop tension exists at about the case-core interface where the fillet transitions into the flange.

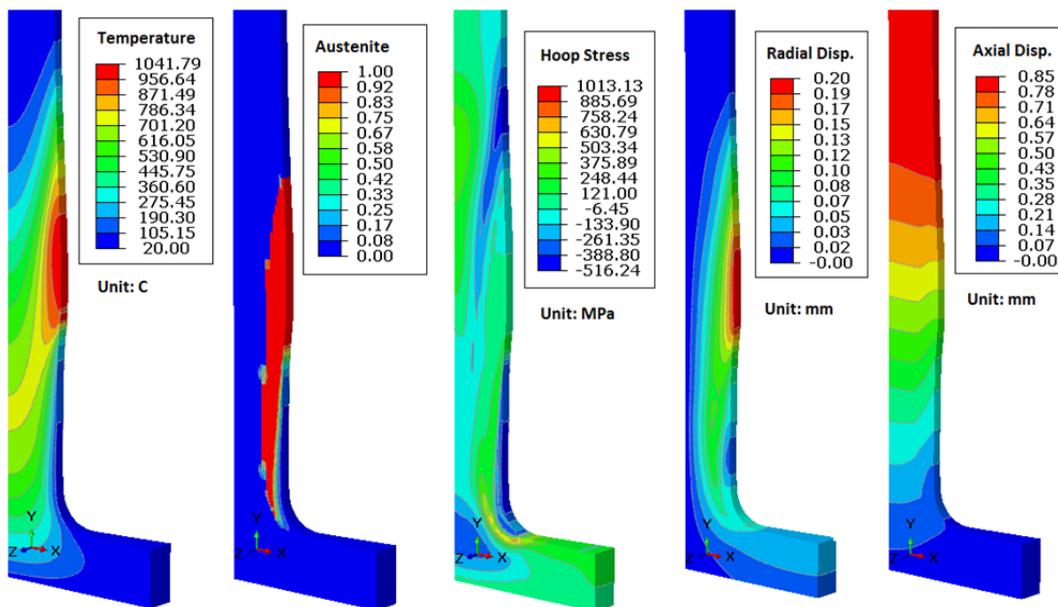


Figure 5: Predicted conditions after 16.5 seconds of the induction process.

In service, the axle shaft rotates about its axis as it transmits a torque load. A model was developed to evaluate the effect of the induction hardened state, i.e. strength, case depth, and stress state, on the shaft stress state while under a torsional load. From basic mechanics, shear stress is maximum on the surface of the shaft, and the level of shear stress increases as the torque load is increased. So, does residual compressive stress that is generated by induction hardening benefit performance of this type of shaft? Figure 6 clearly shows that residual surface compression does benefit torsion fatigue because the maximum tensile stress is reduced from 720 MPa to 150 MPa due to surface compressive stress of about -570 MPa.

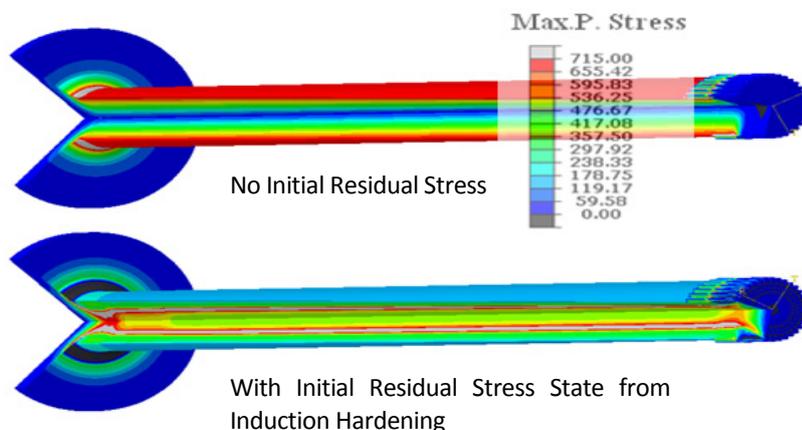


Figure 6. Maximum principal stress for a torsion load of 6,000 N\*m for the cases of no initial residual stress and the predicted residual stress state from induction hardening.

Shear stress is highest on the surface of the shaft during torsion loading and the magnitude of shear is not altered by the presence of residual compression. However, the surface stress state is shifted along the principal stress axis in that the mean stress is compressive and the maximum tensile stress is reduced. Since fatigue will be initiated from the surface, residual surface compression imparted by induction hardening will benefit torsional fatigue strength. Surface related imperfections such as inclusions, scratches, gouges and other features that act as local stress risers will have less effect.

### 3 Data Needed for Heat Treatment Models

With the emphasis on MGI, ICME, and similar directives around the world, a major need is accurate material data and process data. IFHTSE has underway the global database for quenchants initiative. For many years many individuals have stressed the need for material data and process data for heat treatment simulation, in particular Prof. Inouye and Dr. Totten. Universities around the world have government and/or industry supported efforts for such data development. However, issues exist that are difficult to overcome, such as intellectual property rights, data ownership, and cost.

Although different software tools use different mathematical models for heat treatment simulation, the raw test data from which parameters are developed is the same. At least this is my belief. With such common ground, there should be a way for all to work together to achieve the common goals. The need is great, the expenses in total are staggering, but if we all participate we can make progress. The key is for everyone to have “skin in the game.”

#### 3.1. Material Data:

Main material data needs are phase transformation kinetics characterization, metallurgical issues of grain growth and second phase formation and dissolution, and mechanical and thermal property development. Comments in this section are directed towards steel alloys, but other alloy systems also require these types of tests and characterization.

##### 3.1.1. Phase Transformation Kinetics

For characterizing phase transformations, dilatometer tests are favored, where sample dimensional change is measured during heating and cooling. Important data from the dilatometer test are thermal expansion and transformation strains for each metallurgical phase. The tests can be continuous at a constant rate of temperature change, or they can be isothermal, where a temperature is quickly established and dimensional change is monitored over time. The latter test method is especially amenable to characterizing diffusive transformations such as ferrite, pearlite and bainite formation with time at temperature. Martensite characterization requires continuous cooling.

The test results include time, temperature and dimensional change. Strain is calculated from the dimensional change. The user must be aware of the nature of the test in terms of possible temperature gradients in the sample, and also of stresses induced during testing as these conditions affect the transformation temperature and rate. The initial microstructure of the sample at the start of the test also affects the formation of austenite during heating, just as the austenitizing time and temperature affect the phase transformations during cooling. [ASTM A1033, 2004] contains specifications for dilatometry testing using a machine that measures length change during heating or a machine that measures transverse dimensional changes. The data collection and the format of the data files are described.

Figure 7 shows a collection of continuous cooling curves for 1050 steel. Cooling rates of 30 C°/s or less result in diffusive phase formation, i.e. ferrite, pearlite and bainite. Cooling at 70 C/s or faster results in martensite formation. While Figure 7 does not indicate time, it is clear that the bainite formation for the 28 and 30 C/s cooling rate was incomplete and martensite formed when the temperature fell below the  $M_s$  temperature.

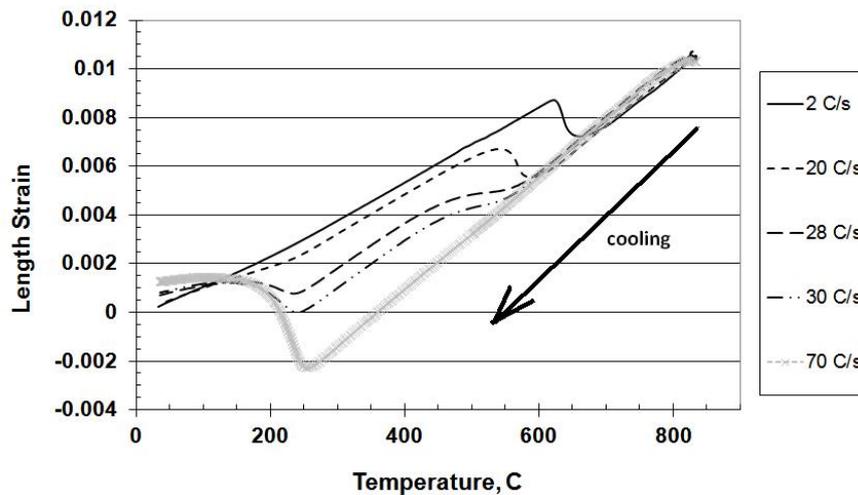


Figure 7: Dilatometry data for 1050 steel [Ferguson, 2003]

Figure 8 is a collection of austenite formation data for different initial microstructures for 5140 steel. The samples were all heated at the same heating rate, and the time-temperature data is included in the figure. The heat absorbed for transformation is evident from the slope change in the heating curves. Prior to heating the samples were austenitized and cooled to form bainite at the isothermal temperatures indicated in the figure legend. Some samples were also rapidly cooled to form martensite, indicated by the M+RA legend tag. From Figure 8 it is apparent that microstructures formed at lower temperatures transformed more readily to austenite. While no photomicrographs are offered, bainite formed at a lower temperature has a finer structure than bainite formed at a higher temperature. Martensite forms austenite the most readily because of its metastable, fine structure.

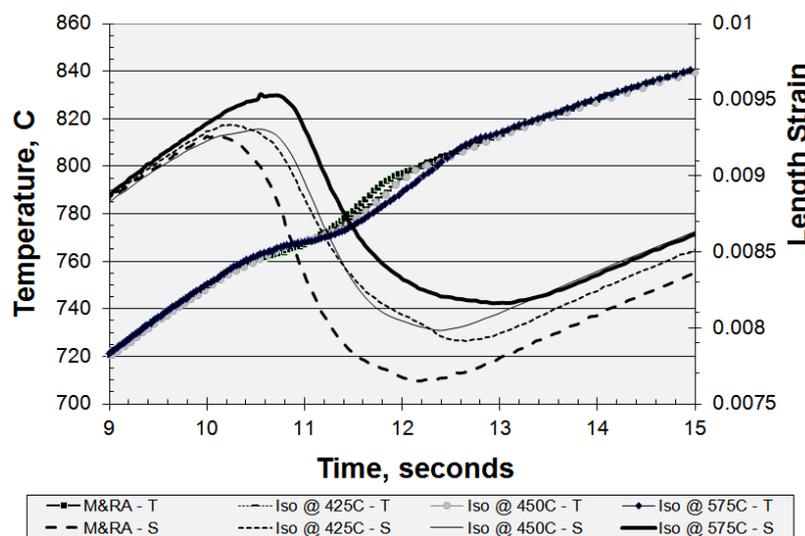


Figure 8: Dilatometry data for austenite formation for 5140 Steel.

(-T indicates temperature curve and -S indicates strain curve.) [Ferguson, 2003]

### 3.1.2. Mechanical Behavior Tests

Elastic behavior must be measured as a function of temperature for each phase. For most steels, temperature is the significant variable, with phase and alloy level being of secondary importance.

Plastic behavior is definitely a function of phase and carbon level, as well as temperature and strain rate. Temperature and strain rate controlled tests are needed to characterize steel alloys. Austenite is characterized by heating samples into the austenite phase field, rapidly cooling to a test temperature, and deforming the sample while it is austenite. The temperature range and time are of course limited. Diffusive phases are characterized by austenitizing the sample, cooling to a

test temperature, holding until austenite decomposition is completed, and then deforming the sample. Martensite is usually characterized by quenching a sample and deforming it using compression loading.

The plastic strain range of importance for heat treatment is relatively small, typically less than 5% strain. This is a nonlinear condition, however, and data collection requires patience and attention to detail. Prior to mechanical testing, the phase transformation kinetics should be known so that temperatures and times of importance are known for these tests.

### 3.1.3. Thermal Properties

Thermal conductivity, and specific heat or enthalpy should be determined by metallurgical phase and chemistry. Standard test methods exist for these determinations.

## 3.2. Process Data

To simulate heat treatment, process data are required for heating and cooling to cover the conditions that are used in production. These data normally are used as boundary conditions and step times in models, but the nature of the process may also dictate the type of analysis needed for simulation. For example, conventional gas carburization is a lengthy process. Short time events, such as the time to achieve surface equilibrium upon a change in carbon potential can usually be omitted and the carbon potential change can be treated as instantaneous without a noticeable change in accuracy of carbon profile calculation. However, the situation is different in low pressure carburization where the changes in carbon on the part surface are faster and occur more often (pulses). Low pressure carburization requires that changes in surface carbon availability be taken into account in the model for accurate prediction of the carbon profile.

Process data is difficult to make general for the simple fact that it is equipment dependent, meaning that it is unique to a particular piece of equipment and to the workload being processed. This is true for furnaces, and it is even more true for quenching systems. Nevertheless, when equipment specific data are not available, trends can be analyzed by using generic heating and cooling data.

### 3.2.1. Heat Transfer Coefficients During Quenching

At the present time, the best method for determining surface heat transfer coefficients during quenching is from measured time-temperature-location data using thermocouples. Ideally, the actual part being modeled is used, but generic shapes may also be used. The conditions should be as close as possible to production conditions, meaning the rack and workload should match production. With sufficient numbers of thermocouples that are located strategically in the part, a mapping of heat transfer coefficients can be determined using one of the many available calculation methods. However, in the majority of simulation cases such testing is not done for a variety of reasons. This is where computation fluid mechanics (CFD) is proving to be a valuable tool.

CFD provides a method for predicting the flow field of the quenchant around the racked parts. From the local velocity field, surface heat transfer coefficients can be estimated.[Mackenzie, 2007] [Banka, 2008] Limitations is CFD accuracy, such as boiling phenomena, are being addressed but at the present time, use of heat transfer coefficients calculated by CFD analysis requires user intervention. The meaning here is that the CFD results provide a good guideline for modification and application of heat transfer values that are based on experience or extrapolation from other cases.

Companies have been collecting data for many years now on liquid quench media using a variety of probes to measure temperatures during the cooling process. These devices provide a great method for calibrating the quench media, checking batch to batch consistency, and maintaining the quenchant in use. But, except for the Liscic-Nanmac probe [Liscic, 2009], they do not adequately characterize the quenching system, and that was not their intent. The quench system

requires parts or part like objects to be used, and the measurements must be made in the system being modeled. Work presented in [Ferguson, 2012] discusses a quench probe used to determine heat transfer during intensive quenching of cylindrical shapes in a closed system that was used to quench single parts. The same probe was used to determine heat transfer in water tanks with still and agitated water. The interesting findings were:

- the heat transfer along the length of the cylinder was uniform during intensive quenching;
- the values of heat transfer coefficients for flow rates of 4.2 and 6m/s were constant at 22 and 25 kW/(m<sup>2</sup>\*C) respectively during the intensive quenching process once full water flow was achieved;
- the top of the cylinder being intensively quenched had a lower heat transfer coefficient of 10 kW/(m<sup>2</sup>\*C) in both cases; and
- both still and agitated water had heat transfer coefficients that changed during quenching, with film boiling and final convective cooling having low values, and nucleate boiling producing coefficients of about 12 kW/(m<sup>2</sup>\*C).

Figure 9 compares the heat transfer coefficients determined for the intensive and water immersion conditions.

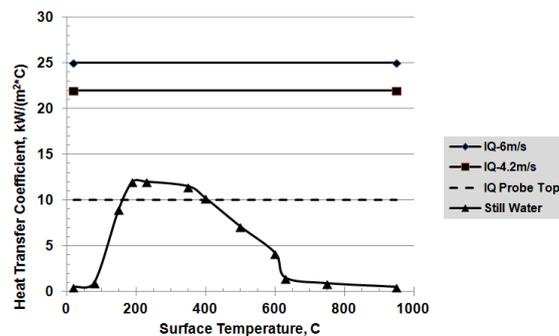


Figure 9: Surface heat transfer coefficients determined from experimentally measured time-temperature data.

#### 4 Summary

Heat treatment is an important step in the manufacturing process chain as this process has major impact on material properties and final part performance. In the move toward improving part performance by optimizing the entire manufacturing process, it must be considered. For carburized steel parts, the beneficial residual compressive stress imparted aids part performance in addition to the benefit of the hard, wear resistant case. This is also generally true for case hardened parts using flame or induction hardening. Often in simulations of a part in service, this benefit of heat treatment is ignored.

Heat treatment is a complicated science in that it spans many technical fields. This means that simulations can be complex and require multiple mechanics to be invoked. An example was given for electromagnetics used for induction hardening. Mention was made of coupling CFD analysis with thermal and stress mechanics to improve heat transfer accuracy.

For improved modeling accuracy, material and process data must be accurate and have high fidelity to the process and equipment being used. To model the process chain, significant amounts of data are required to feed the wide variety of models and methods applied.

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