Heat Treatment Process Exploration with HTP Sim

Jason Meyer, Stefan Habean, Eddy Lee
DANTE Solutions, Cleveland, Ohio
Jason.Meyer@dante-solutions.com
Stefan.Habean@dante-solutions.com
Eddy.Lee@dante-solutions.com

Abstract

Heat treatment recipes consist of several processing steps developed to meet part specifications. Those in industry must have knowledge of a variety of factors that influence heat treat outcomes such as the effects of different process steps, material hardenability, and part geometry. A typical hardening process for steels involves austenitizing, quenching fast enough to create hardened martensite, and tempering to reduce brittleness. Thermochemical steps like carburizing or nitriding alter the surface chemistry of a part, affecting hardenability. Computer modeling can be used as a way to quantify the effects of heat treat by predicting profiles of temperature, carbon, hardness, and microstructure. Using Heat Treatment Process Simulator (HTP Sim), a commercial finite-element based tool developed by DANTE Solutions, four common heat treat processes are reviewed including furnace heating, carburizing, quenching, and tempering. This study focuses simulation applications to industrial challenges like optimizing process times, ensuring case depth and surface hardness, carburization recipe development, and equipment characterization for modeling.

Introduction

The heat treatment industry has significant production needs to ensure quality products are produced within a timely manner. Often, heat treaters rely on decades-old recipes, developed through test trials, to meet these part specifications. Such recipes are used over and over again because it is what has always been done, and it works. However, due to the "black box" nature of heat treating, many times it is difficult and costly to explore new recipe procedures or improve old ones. While the same parts and recipes may be used, process and material variability can affect the final results of heat treat. Today, with the increasing availability of simulation tools, these sensitivities can be accounted for in recipe design more readily. For a given recipe and part geometry, simulation provides the capability to predict the phase transformations which contribute to the final material hardness. Distortion and residual stress can also be simulated and visualized to help gain a more in-depth understanding of the dynamics of the heat treatment process. Those new to the industry also stand to benefit from process modeling, which can help them to improve their knowledge and catch up with their peers.

One challenge with finite-element modeling of the heat treatment process is the steep learning curve and relatively long processing times. Heat treatment is transient and nonlinear, requiring sophisticated material models to simulate and capture the plastic deformation and residual stresses from the phase transformations that occur. Analysts can spend weeks determining and applying proper boundary conditions, executing the models, and post-processing results. In the hands of a capable analyst, this degree of modeling can be used to investigate the sources of complex issues involving part distortion, cracking, or residual stress. behavior of a part during heat treat. However, many times, models can be simplified to reduce computational effort while still providing useful insight. HTP Sim, simplifies the complicated process of building heat treatment models, allowing virtually anyone to gain an understanding of the heat treatment process. Simple inputs of material grade, equivalent part geometry, time, temperature, and equipment keep the modeling learning curve low. For this work, HTP Sim will be used to model four main heat treatment processes: furnace heating, carburization, quenching, and tempering to show how simulation can be used to understand and improve each process. Figure 1 shows a plot of the time-temperature/carbon change at a point in a part for the four main processes defined. While this simplified model does not predict distortion and residual stress, results that can be explored with HTP Sim include temperature, hardness, phase volume fractions, carbon or nitrogen content, iron carbide weight percent, alloy precipitate volume fraction, or grain size.

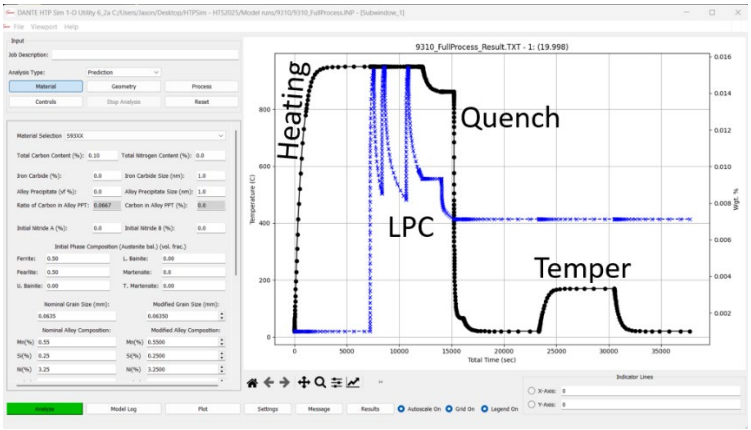

Figure 1: HTP Sim UI and Time/Temperature/Carbon plot

By simplifying the process model, simulation can be made more readily accessible to a broader audience including classrooms, captive heat treaters, and commercial heat treatment shops. Such a model can be used to determine the minimum furnace heating time required to austenitize a part, ensure that surface and case hardness are achieved, design new processes, evaluate different material grades and hardenability, or simply for teaching new users about the phase transformations that occur during heat treatment. Simulating the heat treatment process provides an understanding of the dynamic changes that occur in steel, and with that understanding, process improvements can be made.

Geometry and Equipment

Geometry

Modeling the heat treatment process using Finite Element Analysis (FEA) requires a CAD model of the geometry and extensive knowledge of meshing. Complex geometries may require large numbers of elements, increasing the required model execution time. However, simple geometries like a ring or cylinder shape can be used to approximate different geometric features in larger models. Effective use of such modeling assumptions can significantly simplify model set up and run time. The modeled geometry in HTP Sim is a ring or cylinder with infinite length, so the only user inputs required are the inner and outer diameter. Based on this input, HTP Sim automatically generates and meshes the geometry. An effectively one-dimensional and axisymmetric model is created, making it possible to evaluate and directly compare model results with experimental data like hardness profile from surface to core. This also means that more complex geometries must be simplified to a ring or cylinder with an equivalent diameter to approximate end effects which cannot be captured in this type of model. Only the ID or OD surfaces are exposed to convective heating or cooling in the surrounding environment. This simplification avoids the complicated process of importing and meshing a geometry and ensures the simulation will run very quickly compared to a full finite-element model. Most common geometries such as shafts, bearing rings, and gears have axial symmetry and can be simplified directly to a ring or cylinder shape model in the region of interest with reasonable accuracy for given process. For parts with smaller lengths, the heat transfer at the end surfaces of the part is significant. Since the model does not account for end effects, a method was developed to calculate an equivalent radius used for such geometries. The method is based on comparing the surface-area-to-volume ratio of a cylinder of part height and an infinitely long cylinder to calculate the equivalent radius. For a short part, the total surface area includes significant contributions from the top and bottom faces, whereas in a long part, the end surfaces can be neglected due to their relatively small area compared to the main body surface area. By comparing the surface-area-to-volume ratio of both geometries, the equations can be simplified down to:

$$r_{eq} = \frac{r * h}{r + h}$$

Where r_{eq} is the equivalent radius of the "infinitely" long cylinder, r is the original part cylinder radius, and h is the original part cylinder height. This equivalent long cylinder radius can be solved and used in HTP Sim models with reasonable accuracy.

Equipment

Equipment characterization is an important part of heat treatment simulation. Each piece of equipment, even if it's the same model and produced by the same manufacturer, can have different responses to the same heat treatment cycle. From the part perspective, this inherent process variability results in differences in heat transfer between the part and equipment. For modeling purposes, heat transfer coefficients (HTCs) can be used to characterize the thermal behavior of each individual equipment. These HTCs can be derived from fitting time/temperature data from experiments using thermocouple instrumented parts, or through CFD models. Once derived, the HTCs, ambient temperature, and process times are applied in the model to drive the material thermal response. Storing HTC data in an equipment database further simplifies model set up.

Furnace Heating

Furnace Time Optimization

Furnace heating is used in a myriad of heat treatment steps for different purposes including annealing, normalizing, hardening, or tempering. This work focuses on transforming steel to austenite as part of the hardening process. An example of this process involves putting the cold parts into a hot furnace for the required soak time to allow for uniform temperature and austenitizing. The general "rule of thumb" to ensure uniform heating throughout the cross section, is to keep the part in the furnace for 1 hour per inch of section thickness. To investigate this, a furnace heating step for a 2-inch diameter cylinder is simulated. The model inputs include furnace heating at 925°C, for 2 hours using the general "rule of thumb". The furnace heating HTC used for this step is selected from the equipment database. The model results show the core of the cylinder reaches the target furnace temperature after 3300 seconds in Figure 2. After an additional 30 minutes of soaking, the part is considered fully austenitized. Using modeling, the required heating time was reduced by approximately 30% compared to the two-hour rule of thumb. Engineers can use simulations like these to better understand heating behavior to ensure proper soaking times and ultimately reduce process times and costs.

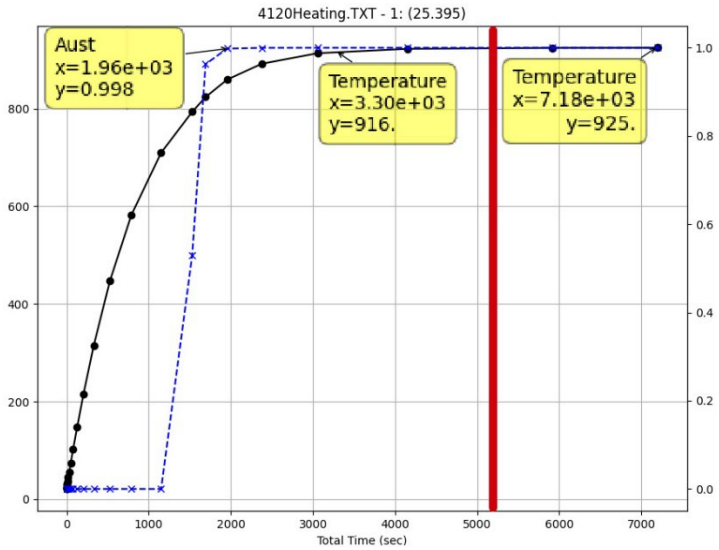

Figure 2: Predicted core temperature and austenite volume fraction in the core of a 2" diameter cylinder heated in a furnace

Another concern during furnace heating is part distortion in parts with complicated geometries. For these kinds of parts, with variable cross section thicknesses, a common practice is to use stepped heating to control the distortion to minimize the thermal gradient throughout the part. The stepped heating process starts by putting the cold part in a furnace that is below the austenite transformation temperature. After holding at this temperature to allow the part to reach thermal equilibrium, the ambient temperature in the furnace is raised to the austenite transformation temperature and held again to ensure uniform heating. Often, the temperature increases again to the soaking temperature and held for a certain amount of time. This results in a very uniform austenite transformation throughout the part reducing the distortion from heating. Figure 3 shows the time temperature comparison for a straight vs. stepped heating process, and a contour of an example bevel gear showing the uniform vertical displacement after the stepped heating process. While distortion cannot be modeled with HTP Sim, the temperature uniformity and the austenite transformation can be explored and optimized to ensure thermal equilibrium between the temperature ramps.

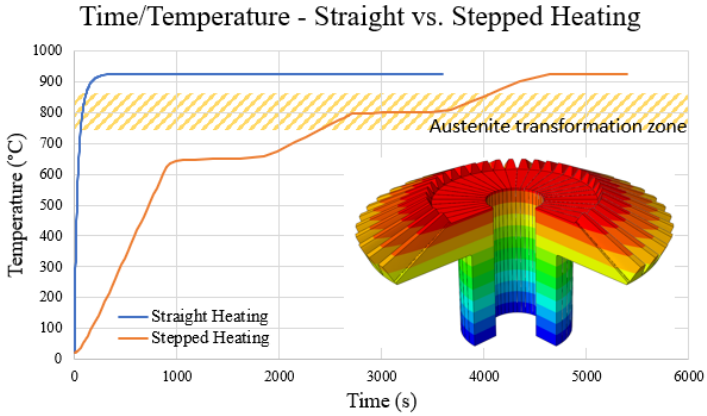

Figure 3: Time temperature plot of a stepped vs. straight heating process

Carburization

After austenitizing, the part may be carburized. Carburization is another process where simulation can provide valuable insight, specifically to predict carbon diffusion into the part to determine case depth. The purpose of carburization is to increase the hardenability near the surface of a steel part to prevent excessive wear and to form a compressive case in areas subject to bending stress cracks where fatigue failure may occur. Gas carburization is a well-controlled and well-studied process, with simple equations that can be used to estimate the case depth based on the square root of carburization time. However, for higher alloy steels, gas carburization often leads to very long processing times to achieve the required case depths. An alternative to gas carburization is low pressure carburization (LPC). This method is preferred for higher alloy steels for its reduced processing times, and surface cleanliness compared to a gas carburized surface. Either process can be included in a model to obtain the carbon profile which affects phase transformations during cooling. During LPC, the carbon carrier gas deposits a high concentration of carbon to the surface of the part during short "boost" steps. Then, the carrier gas is removed, and the deposited carbon is allowed to diffuse into the body of the part in longer "diffuse" steps. These boost and diffuse steps are repeated until the required case depth and surface carbon is achieved. If the boost step is too long, or diffusion steps are too short, alloy carbides will form, slowing diffusion and degrading fatigue performance. These alloy carbides can then coarsen with further boost steps leading to a decline in the mechanical performance of the steel. If the boost steps are too short, or diffusion too long, the processing times can be too long, and surface hardness can be diminished. Unlike gas carburization, the LPC process is not very intuitive and simple changes can result in unexpected outcomes. Simulation of the LPC process helps to determine how to achieve the required case depth and surface hardness, while reducing furnace time and mitigating alloy carbide formation. Additionally, another application for LPC simulation is to design processes to rework parts that did not achieve the required case depth. This model can be used to determine how long to reheat for diffusion, or if an additional boost step is needed for extra carbon. With the understanding gained from simulation, the LPC process can be a very effective and lean processing method.

Case Study

In work performed by Dybowski et al. at Lodz University in Poland [1], Spur gears were subject to LPC and two different quenching methods were used: oil quench and gas quench. The paper has a well described process and carbon and hardness measurements were performed and reported. This work is used to validate the LPC models and to show how even simplified models can predict the metallurgical phases, carbon distribution, and case hardness to the published data. The material used in the study was AISI 9310 and the process steps include:

- Heat up to 860°C and soak for 20 min
- Heat up to 950°C before LPC
- 3-step LPC at 950°C
    - 6/13 min (Boost/Diffuse)
    - 4/34.5 min
    - 3.5/16 min
- Precool to 860°C
- Oil quench/14 Bar quench (both 50°C)
- Cool to room temperature

These process steps were input into the model, and the simulation was executed and completed within 1 minute of CPU time. The time vs temperature/carbon results are shown in Figure 4, with the black line showing the temperature history and the blue line representing the carbon at the surface of the part. The time-temperature plot shows that the part reaches the required temperatures during each process step. The carbon plot shows the surface quickly reaches carbon saturation levels for 9310 at this temperature during the boost steps and drops down to about 0.75% carbon during each diffuse step and at the end of the process.

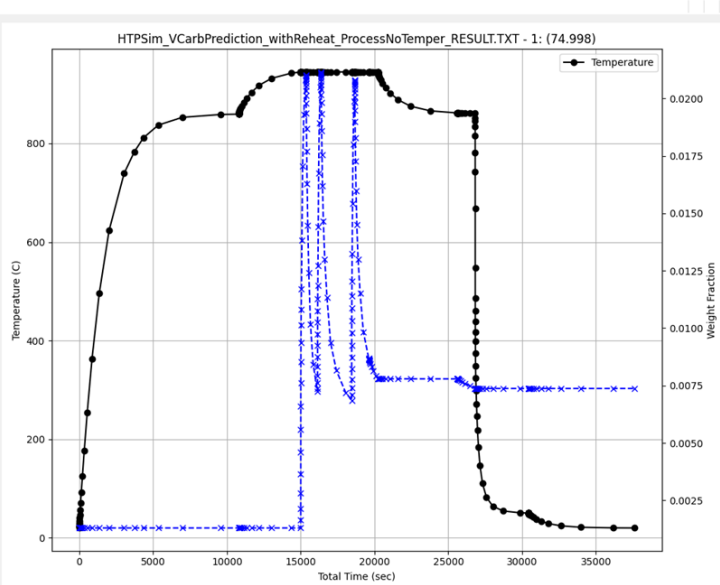

Figure 4: Time temperature/carbon plot for the 9310 hardening process

After confirming the temperature and carbon histories seemed reasonable, the carbon and hardness plot were compared to the published data. Figure 5 shows the carbon at the surface is around 0.75% for both the experimental and predicted results, and the data agrees very well through the case. The hardness plot shows the surface hardness to be about 733 HV (60 HRC). The experimental case depth (500 HV) achieved is between 0.7 and 0.8 mm from the surface agreeing well with the prediction. The simulation shows a slightly lower hardness as the values get closer to the core, but this is expected as the actual geometry is a very thin pancake gear exhibiting the end effects discussed previously. When validating simulation results with experimental data, it is important to consider the accuracy of the thermal boundary conditions and material properties used. A well-calibrated heat treat model should be able to reasonably predict the carbon and hardness profile.

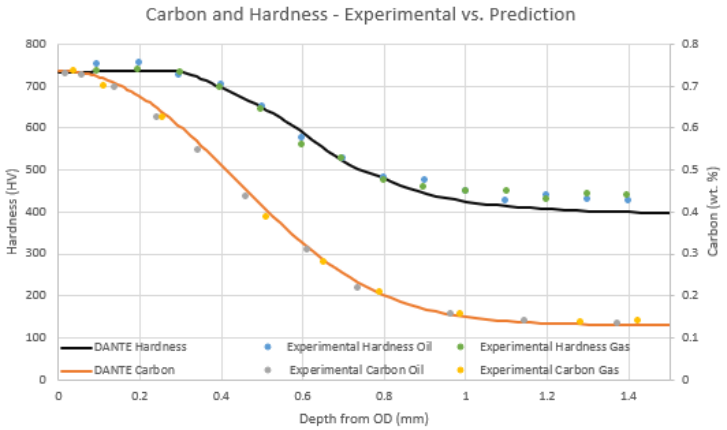

Figure 5: Carbon and hardness profiles, experimental vs. HTP Sim prediction

With the LPC model validated, different case depths can be explored by adding boost and diffuse pairs. Subsequent process steps can then be added such as quenching, deep freeze, and tempering to predict microstructure change and final hardness.

Quenching

Quenching is the most important part of the hardening process as it dictates the metallurgical phases that lead to hardening of steel. Quenching in general, for steel, is just rapid cooling of an austenitized part in oil, gas, polymer, or other fluids to achieve the required material properties. For this work, the focus is on gas and liquid quenching. There are three main phases of liquid quenching that are typically modeled, including the vapor blanket phase when the part surface is at high temperature, the nucleate boiling phase as the vapor blanket breaks down, and the convection phase as the boiling stops and convective currents in the liquid dominate. The heat transfer in each phase is captured with a temperature-dependent HTC dataset which starts off slow for the vapor blanket phase, reaches its maximum for the nucleate boiling phase, and slows down again for the convective phase. For gas quenching, the HTC can be assumed to remain constant while the ambient temperature changes. This change in temperature is mainly from the thermal load heating up the quenching gas during the initial phases of the quench, before the heat exchangers gradually cool the gas back down to room temperature as quenching continues. Liquid quenching typically has more quenching power than gas quenching and both processes can be quickly evaluated for different material grades using this model.

Quench Exploration

Simulating the quenching process provides valuable insight on the dynamic phase transformations that occur during the process. Several aspects of quenching that can be investigated by modeling include sensitivity to quench agitation, different

quenching temperatures, or different quenchant media. One example is to explore the material response of AISI 9310 to liquid and gas quenching. Currently, 9310 is liquid quenched to ensure core properties are met. A 6 BAR gas quench is proposed to provide cleaner parts after heat treatment, and control distortion. First, a model was developed using the current oil quench process, and the modeling results are compared to experimental data for core hardness, between 40 and 43 HRC. The gas quench model was developed using a constant HTC of 800 W/m^2*k, and a variable ambient temperature starting off at 400°C that ramps down to room temperature after the first 300 seconds of quenching. After executing the model, the predicted core hardness of the one-inch cross section cylinder is about 35 HRC, as shown in the blue line in Figure 6.

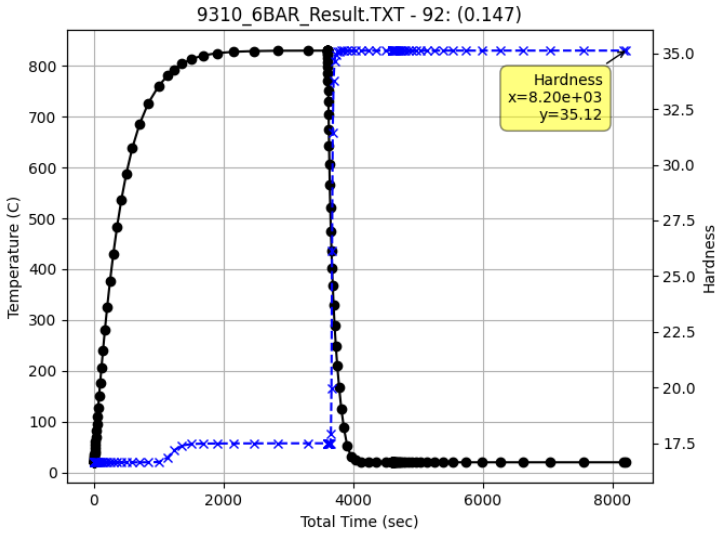

Figure 6: Time vs Temperature/Hardness for gas quenched 9310

This exploration quickly showed that the core hardness of the one-inch cross section suffers due to the reduced quenching power of gas quenching compared to the oil quench baseline. The phase volume fractions in the core after quenching for both processes are shown in Table 1. The oil quenched model predicts about 96% martensite in the core. The gas quenched model predicts only 51% martensite with the balance in upper and lower bainite, which results in a lower surface hardness.

Table 1: Phase volume fractions after oil and gas quenching

Quenchant	Austenite	U bainite	L bainite	Martensite
6 BAR	0.00	0.19	0.30	0.51
Oil	0.01	0.00	0.03	0.96

This difference is due to the slower cooling rate of the gas quench, captured through the difference in HTCs between the processes. The effect of gas quenching pressure on core hardness can be investigated further to determine if microstructure and hardness similar to oil quenching can be achieved.

Tempering

Tempering is a heat treatment process used to improve ductility and toughness after quenching and is usually done in a furnace at lower temperatures well below austenitizing. After quenching, steel is very hard and brittle due to the as-quenched martensite phase. During tempering, the carbon trapped in the as-quenched martensite exits the BCT structure, making tempered martensite to be more ductile. Tempering at higher temperatures and longer times will allow the carbon to form iron carbides and coarsen, further softening the steel. Thus, the tempering process can be tailored to achieve the required hardness by adjusting the time or temperature. Tempering kinetics are built into the DANTE material database, so exploring different required hardness after tempering is as simple as defining the process time and temperature. Two models were developed to look at the effects of tempering temperature on the core hardness of AISI 4120. The model steps consist of furnace heating, oil quenching, cooling to room temperature, a 200°C temper or a 350°C temper, and finally another step to cool back to room temperature. Figure 7 shows the results of the 200°C (a) tempering model and the 350°C (b) tempering model. The results show the core hardness of the 200°C tempering model is about 40 HRC, while the 350°C model shows about 36 HRC. This model can be used to determine different tempering times and temperatures for achieving desired core hardness in a part.

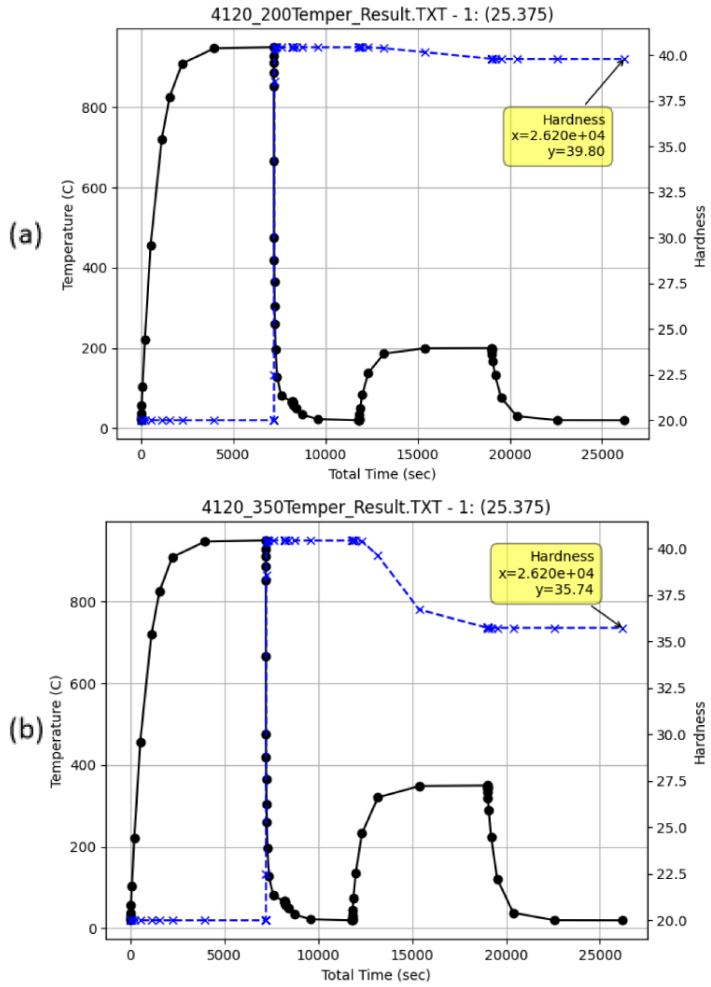

Figure 7: Time vs Temperature/Hardness for 200°C (a), and 350°C (b) tempered 4120

Conclusions

In this work, four common heat treat processes were investigated using a simplified numerical model: furnace heating, carburizing, quenching, and tempering. A transient, 1D, FEA-based model capable of predicting temperature, carbon, phase volume fractions, and hardness for a simple ring or cylinder shape was used to analyze each process. While models that include the entire geometry of a part can also predict distortion and residual stress, this simplified model has the advantage of fast run time and easier setup. This makes process modeling more accessible for determining process parameters, improving recipes, or evaluating different material grades for a given process. In addition, similar inputs like time, temperature, heat transfer coefficients, material grade, and inner/outer diameter are used to define the model. By simulating furnace heating, the minimum soak time needed to ensure that a part is fully austenitized through its cross-section was calculated. Likewise, the minimum time to reach thermal equilibrium can also be calculated for other furnace heating operations like annealing or normalizing. Carburization processes, especially low-pressure carburization schedules, can be developed more easily with the aid of computer modeling to achieve desired target surface carbon and effective case depth. Simulating quench hardening and tempering steps helps to understand the effect of quench severity and material hardenability on the phases and hardness profiles formed from surface to core. Finally, experimental data such as thermocouple time-temperature history, LECO carbon measurements, hardness data, or microstructure analysis can all be directly compared to predicted results, helping to fine tune the heat treat model. Simulating the heat treatment process provides an understanding of the dynamic changes that occur in steel, allowing for process and part improvements to be made.

References

[1] Dybowski, K., Sawicki, J., Kula, P., Januszewicz, B., Atraszkiewicz, R., & Lipa, S. (2016). The effect of the quenching method on the deformations size of gear wheels after vacuum carburizing. Archives of Metallurgy and Materials, 61(2), 1057–1062. https://doi.org/10.1515/amm-2016-0178