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DEVELOPMENT OF A CARBURIZING AND QUENCHING SIMULATION TOOL: NUMERICAL SIMULATIONS OF RINGS AND GEARS

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Introduction

The ability to accurately calculate temperatures, stresses and metallurgical transformations in a single calculation or in a sequence of calculations is the key to prediction of distortion, residual stress and phase distribution in quench hardened automotive parts. Successful predictions in turn rely on the adequacy of the input data to the calculational procedure. These data include mechanical and thermal properties of the alloy phases over the range of temperature and strain rates experienced during the heat treat process, the mathematical description of the transformation kinetics, and the accuracy of the heat transfer boundary conditions.

In this presentation we describe a calculational procedure using the ABAQUS⁽¹⁾ finite element code that simulates a carburizing and quench heat treat cycle for automotive gears. The calculational procedure features a numerically efficient 2-phase constitutive model, developed as part of the NCMS-Heat Treatment Distortion Prediction program, to represent transformational plasticity effects for the austenite/martensite transformation together with refined finite element meshes to capture the steep gradients in stress and composition near the gear surfaces. The calculational procedure is illustrated on carburizing and quenching of a thick ring and comparison of model predictions for distortion, phase distribution, and residual stress with experimental measurements are discussed. Included in this model study is an investigation of the sensitivity of the predictions to mesh refinement.

There are other computer codes that have been developed to simulate heat treat processes; prominent among these codes are HEARTS⁽²⁾ and TRAST⁽³⁾. The codes HEARTS and TRAST use conventional plasticity to model material behavior and they represent the stress-strain behavior as stored tables of yield stress and hardening versus composition and temperature. Our procedure represents the fundamental material behavior using physically based functional relationships in a state variable model⁽⁴⁾. In addition, our procedure employs experimentally measured phase transformation data for 5100 series steels as well as surface heat transfer coefficients measured on gears and rings that have been quenched in salt⁽⁵⁾. Finally, our numerical procedure will be demonstrated to solve complex quench hardening problems requiring the solution of thousands of nonlinear equations at each time step.

Numerical Analysis Procedure

Because of its widespread use in the automotive industry and because of its flexibility in accepting user written materials models, the ABAQUS code was selected to be the computing platform for the simulation tool. For simulating quench hardening processes, the ABAQUS code performs three separate simulations in sequence; first, a mass diffusion model of carburization that produces a carbon file; second, a thermal model of the quench that produces temperature and phase composition files; and finally, a mechanical

simulation that uses the preceding data files and calculates the evolution of stresses and the final distortion of the part. The flow of data for a quench hardening simulation is illustrated in Figure 1.

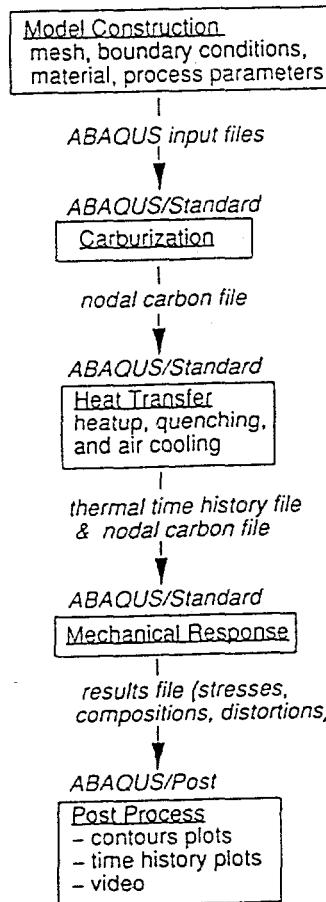


Fig. 1 - Data flow for quench hardening simulation.

Before the carbon simulation is initiated, a finite element mesh is generated, whose nodal point spacings are estimated by the desired depth of the case. For quench-hardening automotive parts such as gears, a case depth of about 1 mm is the design goal. A minimum of 5 to 6 nodal points through the case is used to catch the carbon variation. Thus, the character of the carbon variation in the part determines, in large part, the finite element mesh used to represent the quench hardening behavior. Later we discuss how the nodal point distribution affects the accuracy of results for a quench hardening simulation.

In the carbon diffusion simulation the carbon potential on the outer surface of the part is specified as well as the carbon diffusivity (as a function of temperature and carbon concentration) and the equilibrium carbon concentration. The carbon potential and temperature on the outer surface of the part are specified as a function of time according to the carburization cycle that is desired (e.g., boost or direct diffuse cycle). We have compared a one-dimensional carburization on a 5120 steel ring using ABAQUS and the MARATHON code,⁽⁶⁾ which is a one-dimensional code for simulating carbon distributions produced from specified carburization cycles. These results are shown in Figure 2, using about 15 nodal points in an approximate one mm case depth for both computer simulations. The agreement between the ABAQUS and MARATHON predictions is excellent.

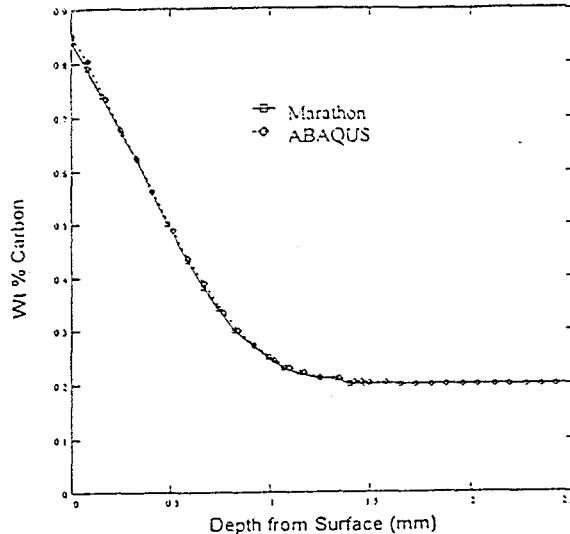


Fig. 2 - Comparison of ABAQUS and Marathon predictions of carburization of a 5120 steel ring.

In the thermal simulation (the quench) the nodal points representing the part are initialized to the furnace temperature, and the heat transfer is effected through the use of experimentally measured heat transfer coefficients and the difference between the ambient bath temperature and the part surface temperature. Initially, there are very large thermal gradients at the surface of the part (where the mesh is refined) and consequently very small temperature steps are taken. When the simulation is started the material is austenite, but as the temperature drops new phases evolve and their latent heats of

transformation are included in the heat transfer analysis; in the case of a 2-phase model, the new phase is martensite. At the end of each temperature step the temperatures are written to a file.

The heat transfer coefficients, which determine the quench behavior of the part, are a function of part geometry, position on the surface, surface temperatures and quenchant thermophysical properties. It is not yet possible to determine these coefficients directly in our numerical simulation tool. Rather, these heat transfer coefficients are determined indirectly by measuring actual surface temperatures on the outside of a part as it is quenched as described in Reference 5. These surface temperatures are then used as boundary conditions for a numerical conduction model in which heat fluxes, q , can be computed very close to where the temperature measurements were taken. The surface heat transfer coefficients, h_c , are then calculated using

$$h_c = q / (T - T_a)$$

where T is the surface temperature and T_a is the ambient temperature of the quenchant. Values of h_c as a function of temperature are then stored in a data base which serves as input for the ABAQUS quench simulation. Figure 3 illustrates heat transfer coefficients computed in this fashion for a thick ring quenched in salt from 840° C to 200° C showing the variation over inside, outside, top and bottom surfaces.

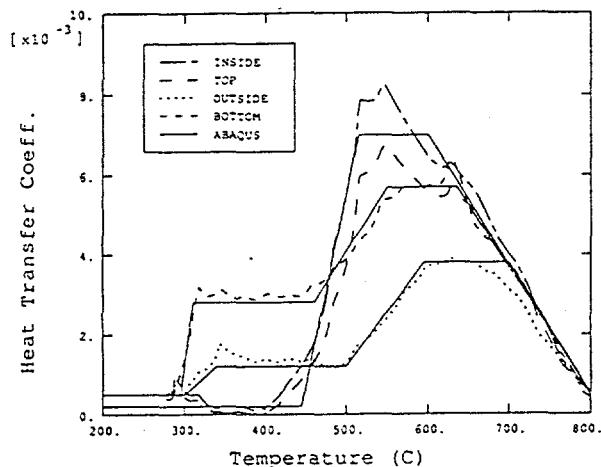


Fig. 3 - Surface heat transfer coefficients (W/mm^2) for a ring quenched in salt. The solid lines represent approximations to the experimental curves that are used in the ABAQUS simulations.

The final application of the ABAQUS code uses the carbon concentration nodal data and the nodal temperatures computed in the thermal simulation. Here the user material model that represents the mechanical behavior of the evolving phases and their transformational characteristics (e.g., the volume change associated with the austenite \rightarrow martensite transformation) is called into play. The analysis is guided by the size of time steps that were determined in the thermal analysis (based on the specified accuracy of the thermal solution), but these time steps can be further refined based on the required accuracy of the mechanical solution. This time step refinement during the mechanical analysis is always observed when phase transformations are occurring. At each specified time during the mechanical analysis, stress and distortion data are written to files for post processing.

One of the goals of our developmental effort was to make the analysis procedure available to a design or process engineer. To accomplish this, our analysis procedure employs a user interface, which allows the designer to easily construct finite element meshes of rings and gears that are refined in the case material and coarse elsewhere, to pull in material and heat transfer coefficient data bases, and to set up automatically the input files for all three ABAQUS computer simulations⁷.

Mesh Sensitivity Study

The sensitivity of numerical results to the nodal point spacing is an issue in any numerical simulation. As the distance between nodal points decreases, numerical approximations become more accurate generally, but with the accompanying penalty that computing times go up dramatically because more equations are being solved. The issue we address here is "what is the nodal point density that is required to obtain results of satisfactory (engineering) accuracy?"

We addressed the issue by simulating quench hardening of a ring that is immersed into a salt bath with its axis vertical. The ring is 10 mm thick and 10 mm high with an inner radius of 18 mm. Assuming there is no circumferential variation in heat transfer coefficients or in material properties, the analysis becomes axisymmetric. We assumed that the material was

5120 steel and that the ring was carburized to 0.85% carbon potential on all outer surfaces prior to quenching.

Figure 4 shows the four finite element meshes that were used in this study. The total number of nodal points in each mesh are 128, 338, 882, and 2312 representing about a 60 percent linear refinement of each preceding mesh. Only one-half of the ring was modeled and symmetry boundary conditions were applied along the plane perpendicular to the axis of the ring at mid-height. The ABAQUS 4-nodal point linear axisymmetric element with 4 integration points was used for the analysis.

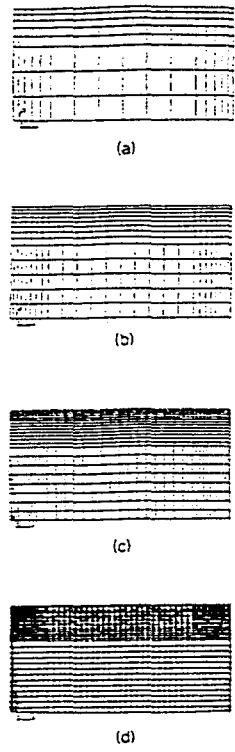


Fig. 4 - Finite element meshes for mesh sensitivity study on a carburized ring: (a) 128 nodal points, (b) 338 nodal points, (c) 882 nodal points, (d) 2312 nodal points.

The ring finite element models were then analyzed for carburization response, thermal response to quench in a salt bath followed by a slower air cool, and mechanical response to quench in sequence. The results of these simulations with the ABAQUS code and using the material model described previously are shown in Figure 5 for the 4 finite element meshes used to represent the carburization, thermal and stress solutions. Here the residual

hoop stresses in the outer 2 mm of the ring are shown. As can be seen in Figure 5, convergence of the numerical solutions with mesh refinement is very strong and all but the coarsest mesh of 128 nodal points would give solutions of adequate accuracy.

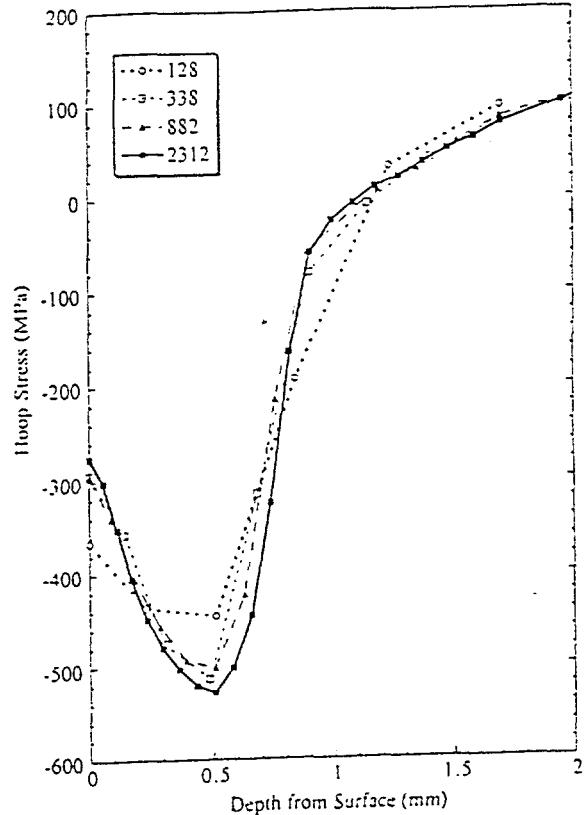


Fig. 5 - Residual stress profiles for each of the four nodal point densities.

The computer run times for the four simulations are shown in Table I below. All calculations were carried out on a Hewlett Packard workstation, HP 712/60.

Pts	Carb.(s)	Thermal(s)	Mech.(s)
128	46	239	125
338	120	556	343
882	333	1441	1022
2312	879	3932	3722

Quench Hardening of a Thick Ring in Salt

Figure 6 illustrates data taken from a quench dilatometer on a 5140 steel sample. This data was used to fix the mechanical constants in the ABAQUS 2-phase transformation model as

follows: thermal expansion coefficient for ferrite on heat up is $1.46 \times 10^{-5} /{^\circ}\text{C}$, thermal expansion coefficient for austenite on cooldown is $2.15 \times 10^{-5} /{^\circ}\text{C}$, volume strain change of ferrite to austenite transformation is -0.0075 . These data were used to determine the quench hardening behavior of a 5120 carburized thick ring at 840°C , using molten salt as the quench medium followed by an air cooling to room temperature. The ring that we modeled was assumed to be quenched in salt for 60 s with its axis vertical and thus, assuming no circumferential variation of heat transfer coefficients, carbon concentration, and material properties, the deformation is axisymmetric. Figure 7 illustrates the finite element mesh that we used to simulate the processes of carburization, quenching, and mechanical stress and distortion development. The mesh comprises 960 four-node axisymmetric elements with most of the elements in the case of the ring to resolve the steep carbon gradients there (see Fig. 2). The heat transfer coefficients for molten salt shown in Figure 3 were used in this simulation.

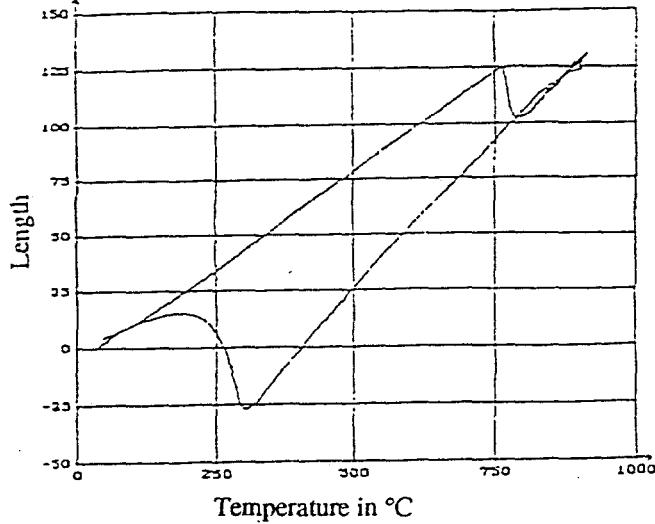


Fig. 6 - Quench dilatometer data from a 5140 steel sample.

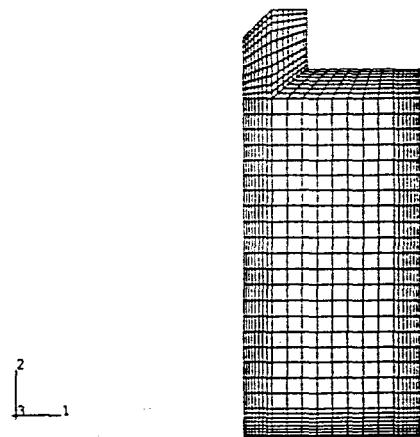


Fig. 7 - Finite element mesh for ring cross section.

We show the evolution of temperature, martensite, and hoop stress at the inner, outer and mid radii at the mid-height of the ring as well as the radial displacement due to the quench. Figure 8 shows the temperature evolution at the middle and outer radius of the ring; included for comparison is a curve showing the effect on the outer temperature of the heat associated with the austenite \rightarrow martensite transformation. It amounts to about 50°C . Figure 9 illustrates the martensite evolution during the quench at the inner and outer radii as well as at the mid-radius of the gear blank. The hoop stress evolution is shown in Figure 10, which illustrates the changing character of the hoop stress during the initial strong cooling phase, the initial austenite \rightarrow martensite transformation phase, and the final slower air cool phase. Finally, Figure 11 illustrates the distortion evolution caused by the quench; the final distortion is nil in agreement with measured values.

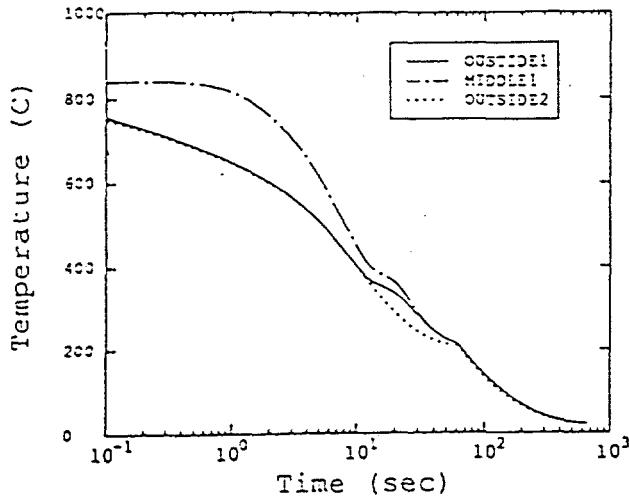


Fig. 8. - Middle and outside temperature variation of the ring during quench and air cool. Dotted curve (visible at 10s) represents outside temperature variation without latent heat.

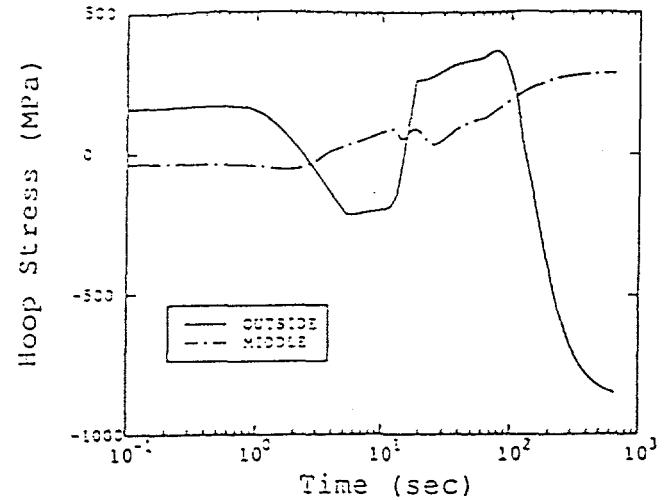


Fig. 10 - Hoop stress evolution in the middle and outside of the thick ring. Note the changing character - tensile to compressive to tensile, to final compressive - of the hoop stress in the case material.

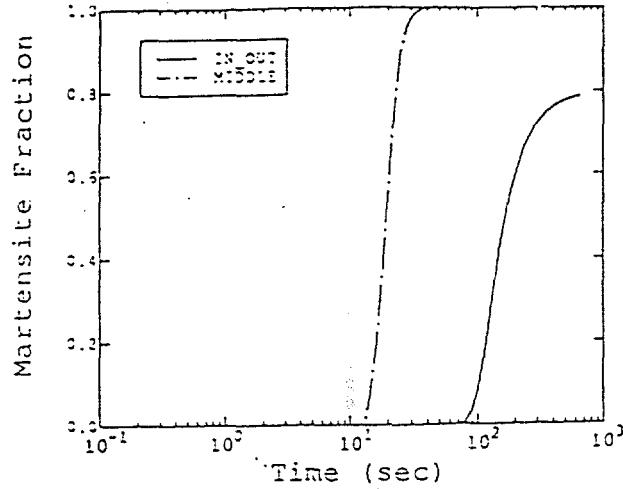


Fig. 9 - Martensite evolution on the inner and outer surfaces of the thick ring and in the middle of ring.

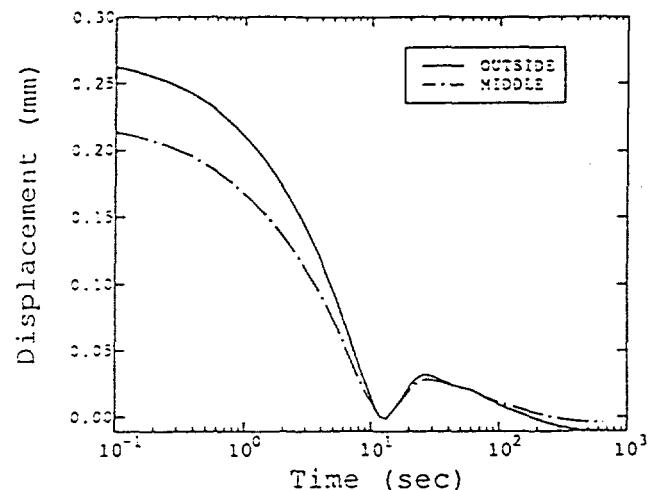


Fig. 11 - Radial displacement (distortion) of the thick ring as a function of time in salt quench and air cool.

Residual stress distributions in these 5120 quench hardened rings had been measured using x-ray techniques as well as by the crack compliance method⁽⁸⁾. The data from the crack compliance method, shown as a function of depth measured from the outer surface, are shown in Fig. 12 together with the predicted residual hoop stress distribution from our numerical simulations. The disagreement between measured and numerically predicted values is currently under study. A likely source of the disagreement is our use of a 2-phase model to represent the 5120 behavior in a situation where a high ferrite contribution is known to be present.

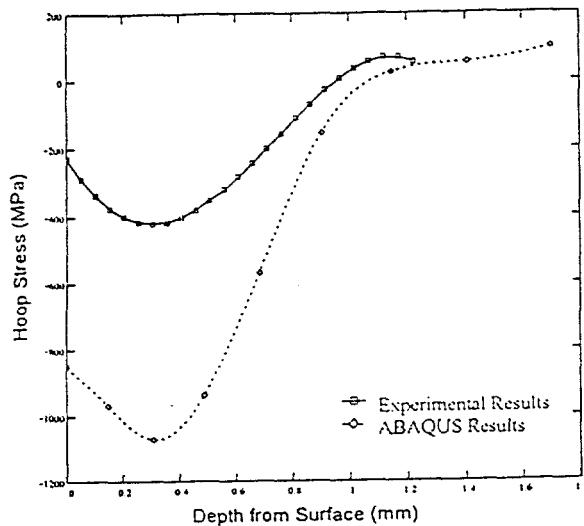


Fig. 12 - Experimental and numerically predicted (ABAQUS) residual hoop stresses near the outer surface of the thick ring.

Conclusions

The numerical simulation tool that we have described here is sufficiently robust to solve heat treat distortion problems for parts with complex geometries. The simulation capability rests on an efficient state variable material model that accounts for the stress changes of the austenite \rightarrow martensite phase transformation and the ability to construct finite element meshes with a high density of nodal prints in the case regions characterized by steep gradients in temperature, composition, and stress. Numerical predictions for distortion agree well with experimentally measured values. Finally, computer run times are consistent with current work station capabilities.

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REFERENCES

1. Hibbit, Karlsson & Sorensen, Inc., ABAQUS/Standard Users Manual, Volumes 1, 2, Pawtucket, RI, 1995.
2. Inoue, T. K. Arimoto, "Metallo-Thermal-Mechanical Simulation of Quenching Process-Theory and Implementation" of Computer Code 'HEARTS'." Quenching and Distortion Control Conference Proceedings, ASM International, pp 205-12 (1992)
3. Jarvstat, N. and S. Sjostrom, "Current Status of TRAST: a Material Model Subroutine System for Calculation of Quench Stresses in Steel," ABAQUS Users' Conference and Proceedings, pp 273-87 (1993).
4. Bammann, D., V.C. Prantil, A.A. Kumar, J.F. Lathrop, D.A. Mosher, M. Lusk, H.J. Jou, G. Krauss, W.H. Elliott, Jr., M. Callebresi, D. Nikkel, "Development of a Carburizing Quenching Simulation Tool: A Material Model for Low Carbon Steels Undergoing Phase Transformations," Quenching and Distortion Control Conference Proceedings, ASM International, 1996.
5. Shick, D., D. Chenoweth, N. Palle, C. Mack, W.T. Lee, W. Elliott, J. Park, H. Walton, M. Howes and W. Copple, "Development of Carburizing and Quenching Simulation Tool: Determination of Heat Transfer Boundary Conditions in Salt," Quenching and Distortion Control

- Conference Proceedings, AMS International, 1996.
6. McCurdy, D.W., "Software Simulation of Atmospheric Carburizing and Hardening," in Carburizing, Processing and Performance, G. Krauss editor, ASM International, 1989.
7. Dowling, W.E. Jr., T. Pattok, B.L. Ferguson, D. Shick, Y.H. Gu, M. Howes, "Development of a Carburizing and Quenching Simulation Tool: Program Overview," 2nd International
- Conference on Quenching and Control of Distortion Proceedings, ASM International (1996).
8. Cheng, W., I. Finnie, M. Gremaud, and M.B. Prime, "Measurement of Near Surface Residual Stresses Using Electric Discharge Wire Machining," ASME Journal of Engineering Materials and Technology, Vol. 116, No. 1, pp. 1-7 1994.

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