Predicting the Heat-Treat Response of a Carburized Helical Gear

B. Lynn Ferguson, Andrew M. Freborg, Greg Petrus and Melvin L. Callabresi

Abstract

Using the DANTE software, a finite element simulation was developed and executed to study the response of a carburized 5120 steel helical gear to quenching in molten salt. The computer simulation included heat-up, carburization, transfer and immersion in a molten salt bath, quenching, and air cooling. The results of the simulation included carbon distribution, volume fractions and distribution of phases, dimensional change, hardness, and residual stress throughout the process. The predicted results were compared against measured results for hardness, dimensions and residual stress. The excellent agreement between predictions and measured values for this carburized 5120 steel gear provides a basis for assessing the various process parameters and their respective importance in the characteristics of not only these heat-treated parts, but of other compositions and shapes.

Introduction

Distortion of steel parts due to heat treatment is a widely known but poorly understood problem. While the general causes of part distortion are well known, in most cases the specific cause-effect relationship has not been established. The main reasons behind the lack of understanding of distortion include the many sources of distortion, the breadth of engineering disciplines that must be brought to bear on the problem, the lack of analytical tools to help dissect the problem, and the willingness of heat treaters to solve distortion problems by trial and error.

Recognizing that developing an engineering tool to address the distortion problem would require more effort and resources than any one company could devote, a collaborative project was defined that involved national laboratories, industry and academia. The project was managed by the National Center for Manufacturing Sciences, and the project team members are identified in Table 1. Besides the breadth and depth of expertise included within the project team, it is important to note that the collaborative nature of the project helped provide the substantial resources necessary to allow model development, material characterization, actual heat-treat trials, and model validation to be addressed.

A result of this collaborative effort was the development of a software tool named DANTE, which is an acronym for Distortion ANalysis for Thermal Engineering.

The DANTE Software

The DANTE software consists of a set of subroutines that describe the thermal, mechanical and metallurgical response of steel to heating and cooling. These subroutines include the Bammann-Chiesa-Johnson (BCJ) material model developed at Sandia National Laboratories in Livermore, CA; models for both diffusive and martensitic phase transformation developed at the Colorado School of Mines; and a heating-carburizing-quenching model description and methodology. These subroutines have been interfaced with the finite element solvers ABAQUS (a product of HKS Inc. of Pawtucket, RI) and KIVA (a product of Sierra Vista Technology of Albuquerque, NM).

The BCJ material model, an RD 100 award winner (Ref. 11), is based on the use of internal state variables to describe the mechanical behav-

Table 1—Heat Treat Distortion Program Participants

Industrial	Department of Energy	University
Dr. M.L. Callabresi (Consultant)	Lawrence Livermore National Laboratory	Colorado School of Mines
Deformation Control Technology Inc.	Los Alamos National Laboratory	IIT Research Institute
Eaton Corp.	Oak Ridge National Laboratory	
Ford Motor Co.	Sandia National Laboratories	
General Motors Corp.		
Torrington Co.		
The National Center for Manufacturing Sciences		

ior of individual metallurgical phases over wide ranges of temperatures, deformation levels and deformation rates. The state variables link the microscopic mechanisms active during deformation to the observed macroscopic behavior. For heat-treatment processes, where mixtures of phases are ever changing during the process, the model has been enhanced to include the effects of phase transformations, transformation-induced plasticity (TRIP), and a mixture theory that predicts the mechanical behavior of the phase mixture from the behavior of the individual phases. For details on the BCJ model as applied to heat-treat processes, see References 3 and 7.

The phase transformation predictive models have been interfaced with the BCJ material model so that the evolution of metallurgical phases is continually updated during the simulation. The phase transformation behavior of carbon and low-alloy steels has been mathematically described using a state variable method that is compatible with the BCJ model. These transformation models track the volume fraction of each metallurgical phase as functions of time and temperature. Details concerning the phase transformation models are found in References 3, 9 and 10.

Specific material data used by these models in the simulation are determined from well known, but not often practiced, mechanical and thermal tests. The data for the BCJ material model are fit from temperature- and rate-controlled tension and compression tests. Using software developed at Sandia specifically for generation of data sets in the BCJ format (Ref. 12), true stress/true strain data for different temperatures and strain rates are determined for each material phase. The phase transformation data are derived from heating and cooling dilatometer experiments. Elastic properties and thermal properties, including latent heats of formation, were extracted from published literature and implemented within the model as functions of temperature and carbon level.

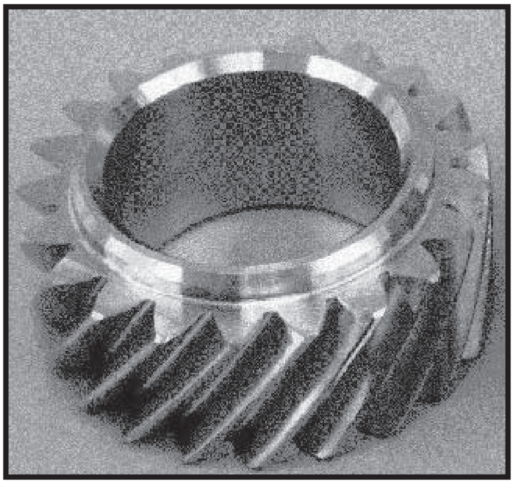

Figure 1—Carburized helical gear.

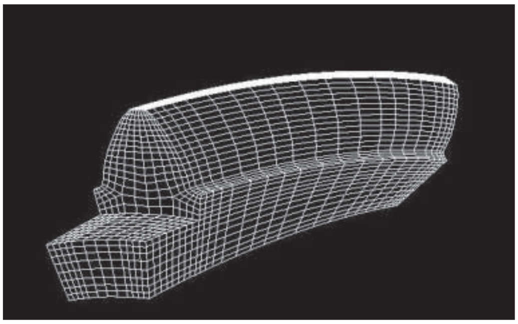

Figure 2—Mesh of single tooth.

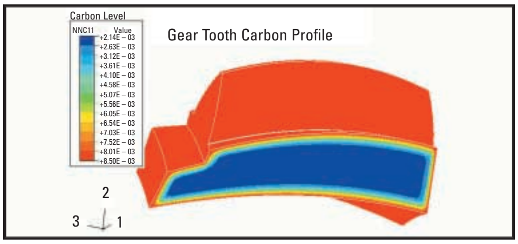

Figure 3—Carbon profile in carburized and quenched helical gear (units are weight fractions).

Heat-Treat Process Simulation

A 21-toothed helical gear, shown in Figure 1, was selected for simulation. This gear, made from 5120 steel, is typically machined from a forged blank, carburized, quenched in molten salt, washed and tempered. To simulate the response of any part, several major assumptions must first be made. For this helical gear, the assumption was made that heating and cooling conditions in the actual process were uniform around individual gears and neighboring gears did not influence the heating and cooling. This assumption allowed us to focus on a single gear tooth, as shown in Figure 2. Cyclic symmetry conditions were applied to the cut faces of the model.

The heat-treat schedule employed in the model is shown in Table 2. Heating was accomplished by applying a temperature-dependent surface heat transfer coefficient representative of typical gas-fired, continuous-throughput furnaces. A constant carbon potential of 0.85% was applied uniformly to all exterior part surfaces to provide the boundary condition for the carbon diffusion model. Quenching involved transferring the gear through air to the quench tank, immersing the gear in molten salt at a speed of 96.8 mm/s, and holding for the remainder of the time. The gear was then removed from the salt and air cooled to ambient temperature before washing. The washing step and tempering are not considered in this paper, largely because austenite

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is vice president of Deformation Control Technology. He has been working with numerous metalworking and manufacturing companies to solve their production problems. Specifically, he has concentrated on applying analytical methods to their deformation and thermal processes.

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Table 2—5120 Carburization & Salt-Quench Cycle

Step	Temperature	Time	Carbon Potential
Heat-Up	20–850°C	10 mins.	–
Carburize	850–900°C, 900°C, 900–843°C, 843°C	30 mins., 3.75 hrs., 15 mins., 45 mins.	0.85%, 0.85%, 0.85%
Transfer to Quench	Air	12 secs.	–
Salt Quench	230°C	4 mins. (includes 96.8 mm/s immersion)	–
Air Cool	20°C	10 mins.	–

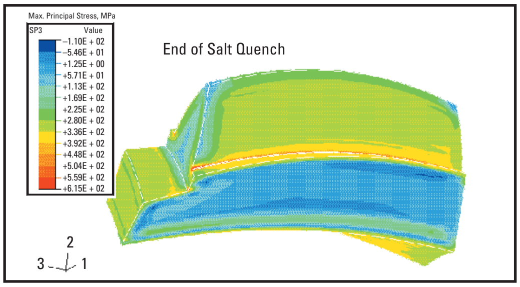


Figure 4—Maximum principal stress contour map at the end of the salt quench. Part temperature is 230°C.

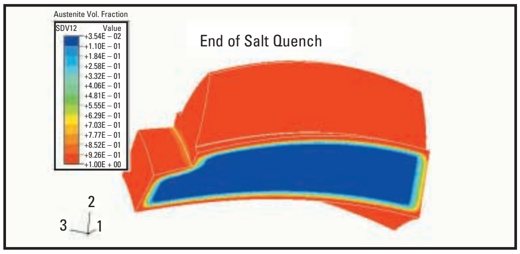


Figure 5—Austenite volume fraction at the end of the salt quench. Part temperature is 230°C.

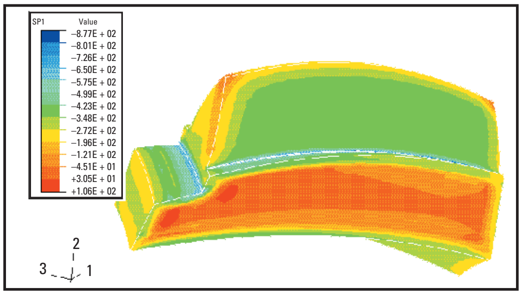
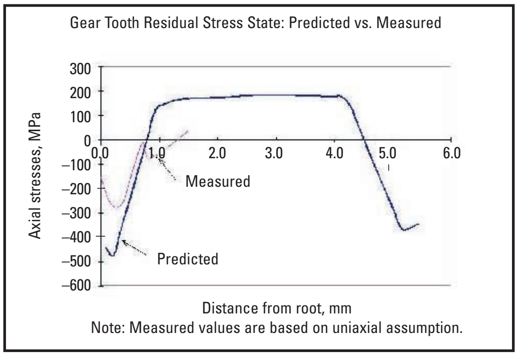


Figure 6—Minimum principal stress after salt quench and air cool. Part temperature is now 20°C.



Note: Measured values are based on uniaxial assumption.

Figure 7—Comparison of predicted stress vs. stress computed from X-ray measurements.

decomposition is completed prior to washing, and the tempering process model had not been fully implemented when the demonstration model was developed.

Model results illustrating the carburized tooth are shown in Figure 3. The main assumption in the carburizing boundary conditions was that the carbon potential was uniform around the tooth exterior and bore. The final case depth was 0.64 mm, defined as the depth at 0.4%C. Note, the carbon profile of the carburized gear was not measured; the carbon diffusion model had been validated previously where predicted profiles were found to agree with profiles determined directly by electron-beam microprobe or indirectly by microhardness measurements (Refs. 6 and 8).

Figure 4 shows a contour map of maximum principal stress at the end of the salt quench. The case is in residual tension of approximately 300 MPa, with the direction of this stress being along the length of the tooth. The part temperature at this point in the process is 230ºC, which is above the martensitic temperature of the carburized case. As indicated in Figure 5, the high carbon case is still fully austenitic at this point, while the low carbon core of the part has transformed to a mixture of ferrite-pearlite (up to 7%), bainite (up to 35%) and martensite (remainder).

Figure 6 shows a contour map of minimum principal stress after cooling the quenched gear to room temperature. The case now exhibits residual compression of approximately 400 MPa along the tooth face and 500 MPa in the root. For comparison, Figure 7 illustrates the predicted versus measured surface and near-surface stresses, with the measured values determined from X-ray diffraction patterns taken along the direction of the root valley. These values were measured for martensite and were not corrected for multiaxial effects. Qualitative agreement between the measured and predicted values seems reasonable, but the differences between the two still require further examination. At this time, there is not sufficient basis to comment definitively on the accuracy of the measurements derived from X-ray analysis and the comparison with predicted values.

Previous validation studies that focused on simpler ring shapes have shown a similar difference between predicted and measured surface stresses but virtually identical values for stress through the case and into the core (Ref. 8). A slight amount of surface decarburization and oxidation may have a significant impact on the localized measured surface stress state.

The helical gear model indicates that at the end of the final air cool, the case is transformed to martensite with about 25% retained austenite, as shown in Figure 8. The retained austenite level in the model matches the amount observed in the carburized case of gears at this point in the process. The volume fractions for the phases were also corroborated by qualitative matches of predicted phase volume fractions versus metallographic observations.

The hardness model in DANTE is based on a simple rule of mixtures, where the hardness of each individual phase is calculated and the combined hardness is then based on the summation of the phase fraction times its respective hardness. Martensite hardness is based on carbon level, and the hardness of the diffusive phases of ferrite, pearlite and bainite are functions of the temperature of phase formation in addition to carbon level. Martensite and lower bainite therefore are dominant phases in parts with high hardness, while retained austenite, ferrite and pearlite reduce hardness. The predicted hardness of the gear tooth model is plotted in Figure 9, with the high carbon case being the high hardness region as expected.

Figure 10 shows a bar graph describing the radial displacements of the four corner bore nodes for the evaluated gear tooth section at the end of each process step. After heat-up, the part expansion is evident by the radial expansion of all four bore points. As carburization progresses during the next process step, the bore shrinks slightly as carbon diffuses into the austenitic lattice. The part then thermally contracts as it slightly cools during transfer to the quench. The bar marked "Immerse" is actually at 5 seconds into the salt quench after immersion has been accomplished during the first 0.3 seconds. Transformation of the austenite is still negligible at this time, while thermal contraction is pronounced. After completion of the salt quench, the core of the tooth has now transformed to martensite and bainite, with the result being a reversal in radial movement as the bore grows with the formation of these phases. The final air cooling produces a thermal shrinkage, with the bottom radius being approximately 12 microns smaller and the top radius being 10 microns larger than original size.

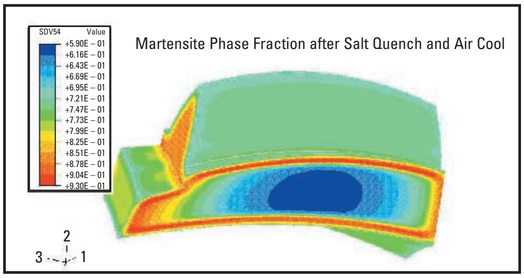


Figure 8—Volume fraction of martensite after salt quench and air cooling to 20°C.

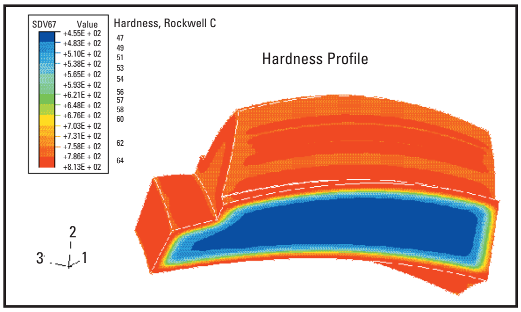


Figure 9—Predicted hardness contours in gear tooth after quenching and air cooling to room temperature.

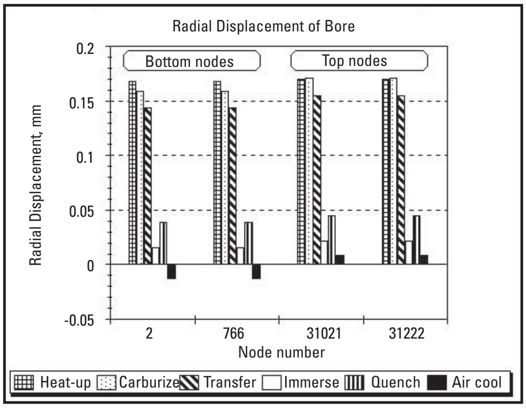


Figure 10—Predicted bore displacement during heat treatment.

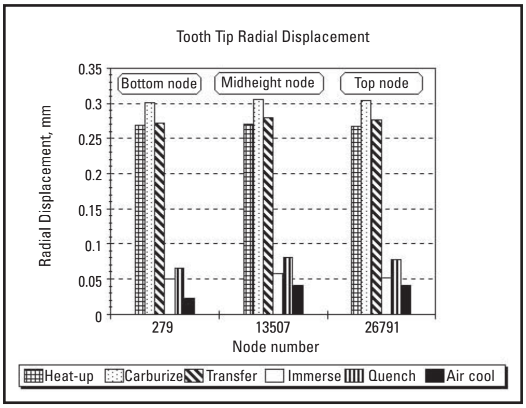


Figure 11—Predicted tooth tip displacement during heat treatment.

The chart shown in Figure 11 is similar to Figure 10, except that Figure 11 tracks the radial movement of the tooth tip. The tooth tip moves outward during heating and carburizing. However, more significant is radial growth and barreling of the tooth that is shown at the end of the final air cool. The bottom node has grown the least at approximately 25 microns, the midheight node has grown more than 40 microns, and the top node of the tooth has grown just less than 40 microns. While these radial growths may seem small, they

ABOUT DANTE

A software tool called Distortion ANalysis for Thermal Engineering (DANTE) was recently developed by a team of specialists to analyze part-distortion problems. Because of the many sources of distortion, the variety of engineering disciplines required to analyze the problem, the lack of analytical tools to solve the problem and the tendency of heat treaters to use trial and error for distortion problems, the DANTE tool was created to look deeper into the issue.

Benefits

The immediate benefit from using DANTE is prediction of dimensional change, residual stress state, and part hardness. These predictions provide direct insight into the effects of steel chemistry, part shape and process on these values; and a method for comparing processes, green shapes and steel grades can therefore be achieved. This knowledge, when applied, provides a means of reducing costs and time associated with distortion-corrective steps, through reduced straightening, reduced machining of hardened parts, and possible substitution of free quenching for press- or fixtured-quenching processes.

As an example, high-pressure gas quenching following vacuum carburizing is becoming a popular process substitution for conventional gas carburizing followed by immersion quenching in oil. The DANTE simulation tool provides a valuable means of comparing these processes. Also, processes such as induction hardening, which is done as an in-line process on individual parts, can be compared against batch-quenching processes. Thus DANTE provides a powerful means of assessing potential process developments prior to initiating potentially expensive plant trials.

Simulation using DANTE can improve part quality through:

- More uniform carburized case, which can minimize machining after hardening;
- Achievement of deeper levels of surface compression and improved fatigue life through improved understanding and control of the heat-treat process;
- Optimal design of part geometry and required fixturing to maximize heat-treatment response and minimize undesirable distortion.

DANTE provides technical insight into the heat-treat process, which is a benefit by itself; but when skillfully applied, it can result in design- and production-cost reduction and improved part quality.

Theory

During heat treatment, dimensional changes occur due to thermal expansion and contraction, phase transformation, and internal stress. Dimensional change cannot be prohibited during heat treatment, but it can be taken into account during design. However, unanticipated dimensional change, termed distortion, is a major problem in heat-treat processes and costs the industry millions of dollars each year. DANTE predicts the phases and distribution of phases, internal stress state, and final hardness of the steel part.

DANTE's Material Model: DANTE includes a multiphase material model based on the Bammann-Chiesa-Johnson (BCJ) internal state variable model to address heat treatment of steel. This material model was recognized as a RD 100 award winner in 2000.

The internal state variable model characterizes the internal state of a phase, where the state variable relates to the microscale physical state of the phase. Evolution equations describe how the state variables change with temperature, rate of deformation, and deformation level. State variables included in the BCJ model are static- and rate-dependent, yielding as functions of temperature and alloy content, and hardening balanced by recovery mechanisms. The constants that define the state variables are derived from conventional temperature- and rate-controlled tension and compression tests.

DANTE's Phase Transformation Kinetics Models: The steel transformation models in DANTE include austenite formation during heating, and austenite decomposition to ferrite/pearlite, bainite and/or martensite during quenching. At present, low-temperature tempering of martensite is also addressed. The kinetics model is driven by phase transformation data obtained from dilatometry.

DANTE's Carburizing Model: DANTE includes carburization as a mass diffusion model where the diffusivity of carbon in iron is controlled as a function of carbon content and temperature. The effects of selected alloy elements, such as chromium, on carbon diffusivity are also included. The surface carbon potential may be specified as a constant value, or it may be defined as a function of time and temperature based on particular furnace performance data. The carburization model can be used to simulate conventional gas carburizing, as well as vacuum carburizing.

Material Data: During the initial collaborative project, the mechanical, thermal and phase transformation behavior of the 5100 series of low alloy steel was developed in detail. Phase transformation kinetics data and mechanical behavior data were later developed for some other grades of alloy steels, including 8620, 9310, and 4320 steel. During a subsequent U.S. Army-sponsored Small Business Innovative Research (SBIR) program, comprehensive material data were developed for the high alloy gear steel Pyrowear 53 (a trademarked and patented alloy produced by Carpenter Technology Inc.), which is used in gear transmission applications for military helicopters.

Quench Media Data: Part of the processing data available with DANTE are heat-transfer tables for selected oils, salts, water (immersion and spray), and gases.

Software Packages

DANTE exists in two versions. The DANTE/ABAQUS version requires that users have a valid license for ABAQUS/Standard and ABAQUS CAE for pre- and post-processing of results. The DANTE subroutines are distributed as object code that is linked to ABAQUS at run time. This version of DANTE runs on any platform on which ABAQUS runs, including Windows NT and UNIX workstations. Models may be either 2-D or 3-D in nature and element types include quadrilateral, hexahedron, wedge, and tetrahedron elements.

The second version of DANTE is called DANTE/KIVA and has the same capabilities as the ABAQUS version, but instead the software couples with the KIVA special purpose finite element solver. KIVA solves coupled mechanics problems involving carbon diffusion and transient thermal-stress process steps, but is limited to hexahedral elements at this time. KIVA's primary advantage over the DANTE/ABAQUS package is much faster solution times for 3-D problems. KIVA relies on existing pre- and post-processing software such as ABAQUS CAE or PATRAN for model-building and graphical display of results.

About DANTE

The DANTE software package is available for licensing from Deformation Control Technology Inc. A product of a collaborative industry-government laboratory-university consortium, DANTE consists of several components, each with separate ownership but covered by commercial licensing of the software. The material model was developed by Sandia National Laboratories of Livermore, CA, and is owned by Sandia. The phase transformation kinetics models were developed by the Colorado School of Mines under contract to the National Center for Manufacturing Sciences, and NCMS is the owner. DCT is responsible for maintaining, marketing, distributing and training. For more information, contact DCT at (440) 234-8477. ⚙

are highly significant from a design and application standpoint because they use up most of the allowable dimensional variation in the gear tooth.

Summary

A simulation of the carburizing and quench hardening of a 5120 helical gear has been conducted using the DANTE heat-treatment simulation software package. Agreement between predicted values and measurements for phase volume fractions and distribution of phases, and residual stress state was excellent. The predicted dimensional changes associated with the heat treatment of this type of gear were also in agreement with experience. However, a more robust system for accurately comparing model results with typical gear measurements and properties (such as surface residual stress) is still required for a realistic judgement of model performance and accuracy. This work is in progress.

Additional work also continues in refining the experimentally measured phase transformation kinetics, characterization of additional steels, and characterization of other quench processes.

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References

1. Dowling, W., et al. "Development of a Carburizing and Quenching Simulation Tool: Program Overview," *2nd International Conference on Quenching and Control of Distortion*, edited by G.E. Totten, M. Howes, S. Sjostrom, K. Funatani, ASMI, Cleveland, pp. 349–355, November 1996.
2. Shick, D., et al. "Development of a Carburizing and Quenching Simulation Tool: Determination of Heat Transfer Boundary Conditions in Salt," *2nd International Conference on Quenching and Control of Distortion*, edited by G.E. Totten, M. Howes, S. Sjostrom, K. Funatani, ASMI, Cleveland, pp. 357–366, November 1996.
3. Bammann, D., et al. "Development of a Carburizing and Quenching Simulation Tool: A Material Model for Carburizing Steels Undergoing Phase Transformations," *2nd International Conference on Quenching and Control of Distortion*, edited by G.E. Totten, M. Howes, S. Sjostrom, K. Funatani, ASMI, Cleveland, pp. 367–375, November 1996.
4. Anderson, C. "Development of a Carburizing and Quenching Simulation Tool: Numerical Simulations of the Rings and Gears," *2nd International Conference on Quenching and Control of Distortion*, edited by G.E. Totten, M. Howes, S. Sjostrom, K. Funatani, ASMI, Cleveland, pp. 377–383, November 1996.
5. Mgbokwere, C., et al. "Modeling the Heat Treatment Behavior of a Transmission Ring Gear Blank," *3rd International Conference on Quenching and Control of Distortion*, edited by G.E. Totten, B. Liscic, H.M. Tensi, ASMI, Prague, pp. 355–364, March 1999.
6. Ferguson, B.L., G.J. Petrus, and T. Pattok, "A Software Tool to Simulate Quenching of Alloy Steels," *3rd International Conference on Quenching and Control of Distortion*, edited by G.E. Totten, B. Liscic, H.M. Tensi, ASMI, Prague, pp. 188–200, March 1999.
7. Prantil, V.C., et al. "Simulating Distortion and Residual Stresses in Carburized Thin Strips," submitted to *ASME Journal of Engineering Materials and Technology*.
8. Ferguson, B.L., A.M. Freborg and G.J. Petrus, "Software Simulates Quenching," *Advanced Materials & Processes*, pp. H31–H36, August 2000.
9. Lusk, M.T., and Y-K Lee, "A Global Material Model for Simulating the Transformation Kinetics of Low Alloy Steels," *7th International Seminar on Heat Treatment and Surface Engineering of Light Alloys*, IFHT, Budapest, pp. 273–282, September 1999.
10. Lusk, M.T., et al. "An Internal State Variable Model for the Low Temperature Tempering of Low Alloy Steels," *1st International Conference on Thermal Process Modeling and Computer Simulation*, Shanghai Jiaotong University, 2000.
11. "Material Modeling Predicts Failures," *Research & Development*, September 2000.
12. J.F. Lathrop, "BFIT—A Program to Analyze and Fit the Sandia Plasticity (BAMMANN) Model Parameters to Experimental Data," SNL Report, September 1995.