Using Abaqus User Subroutines to Develop a New Finite Element Modeling Tool for Heat Treatment Simulation

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Abstract: Heat treatment processes, particularly quenching, are essential to improve mechanical properties in the production of steel castings, but they also generate residual strains and stresses and volumetric expansion due to phase transformations and microstructure changes that occur during heat treatment of a steel body. These coupled thermo-mechanical-microestructural problem involves some complex metallurgical relationships that are described by different mathematical models. In the literature surrounding this theme, numerical implementations of these models were proposed, but always considering simplifications in the mathematical relationships. The purpose of the present work is to develop a computational tool, using Abaqus and FORTRAN subroutines, for analyzing the complete problem of heat treatment distortion and thermal stresses that includes prediction of the phase transformations, microstructure and material properties. Abaqus solvers do not consider metallurgical and microestructural behavior of steel materials by themselves, but it is possible to extend the functionality of Abaqus models performing modifications or optimizations (customization) by FORTRAN subroutines. A package of subroutines were developed in order to solve the coupled problem and to calculate all the microstructures resulting from quenching (ferrite, pearlite, bainite, and martensite), depending on cooling rate. Models are developed based on time-temperature-transformation (TTT) or continuous-cooling-transformation (CCT) diagrams of different steel types by the use of FORTRAN subroutines. Model testing was conducted based on the analysis of quenching of different geometries. The numerical results provided by the model were compared with results presented in the literature and agree with them.

Keywords: Constitutive Model, Coupled Analysis, Heat Transfer, Quenching, Phase Transformation, FORTRAN subroutines, TTT/CCT Diagrams Thermal Stress, Residual Stress and Distortion

1. Introduction

Heat treatment of steels is a great usefulness stage to control residual stresses, cracking, distortion and material properties of mechanical parts and also is extensively used in industries as a procedure to relieve internal stresses, reduce fragility and improve machinability. Mathematical and computational modeling of these processes is an important tool for understand and improve the fabrication processes of a great number of parts. However, simulate these processes in finite element software implies in solve a complex coupled thermo-mechanical process, modeling solid state metallurgical transformations, the change of both thermal and mechanical properties of materials, the latent heat released during phase transformation and a lot of other complex interactions.

Quenching, in particular, is a heat treatment process generally used to control the mechanical properties of steels, whose main objective is the formation of martensite, induced by cooling the austenitized steel at a sufficiently high cooling rate, which avoid the formation of ferrite, pearlite, and bainite. The formation of each phase from austenite is associated with a specific volumetric expansion that, combined with large temperature gradients and nonuniform cooling, promotes high residual stresses.

The use of time-temperature-transformation (TTT) or continuous-cooling-transformation (CCT) diagrams can provide the prediction of the resulting microstructure-composition after heat treatment and it should be taken into account when projecting the heating and cooling sequence of the process.

Figure 1 presents a schematic of the complex thermo-mechanical-phase transformation coupling interactions.

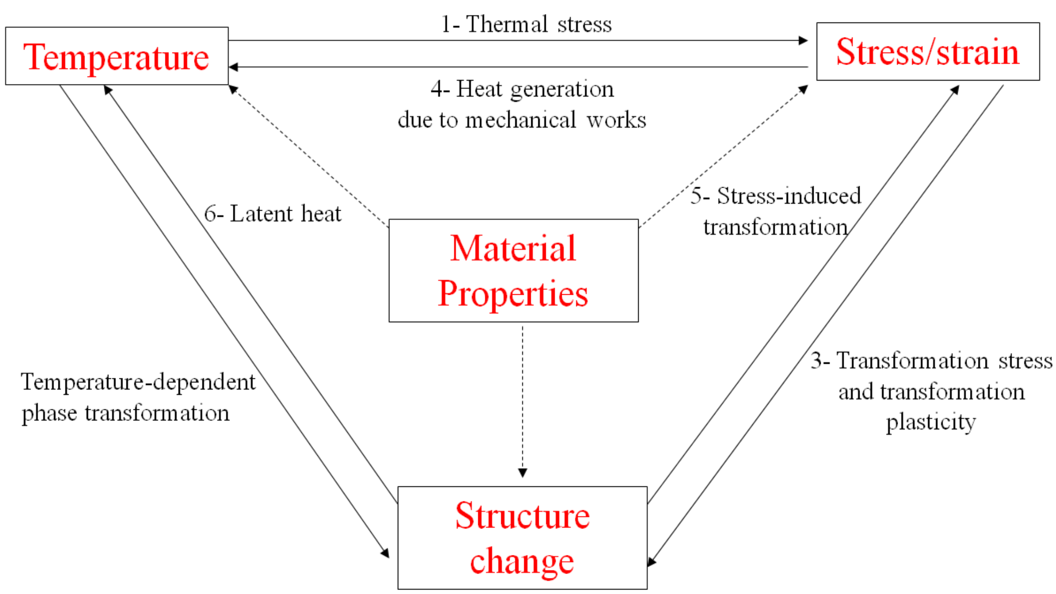

Figure 1. Schematic of the complex thermo-mechanical-phase transformation interactions

In order to correctly simulate all these interactions (thermo-mechanical and microestructural), in a wide variety of heat treatment processes, having plane, 3-D and axi-symmetrical geometries, a set of Fortran subroutines were developed to be run with Finite Element Solvers Abaqus/Standard and

Abaqus/Explicit. While the user subroutines calculate all the metallurgical phenomena, Abaqus calculates heat transfer, distortion and residual stresses after heat treatment.

The heat treatment model developed with the user subroutines considers that the transformations from austenite to ferrite, pearlite, bainite and martensite are governed by the appropriate CCT or TTT diagrams and also by Avrami's approximation:

$$y(t) = 1 - e^{-kt^n}$$

Where t is time, n is a material parameter and k is a function of temperature:

$$k = k_0 e^{-Q/RT}$$

The set of user subroutines generated for this application is described here one by one. The Abaqus Documentation user subroutines default names were maintained in order to help understanding of how they work:

USDFLD: Gives the transformed volume fraction of austenite into ferrite, pearlite, bainite and martensite.

HETVAL: Gives the heat generated by each one of the phase transformations.

UEXPAN: Gives the volumetric change by the temperature variation and by the phase transformations due to the variation of coefficient of thermal expansion.

UHARD: Gives the yield stress for the temperature and volume fractions of each phase at each integration point.

A combination in a very efficient manner of a package of developed FORTRAN user subroutines with the general Finite Element Analysis Software Abaqus is described in this work. The general scheme of this combination is given in the Figure 2.

Heat treatment processes used in different kind of mechanical parts production were investigated, from a simple cylindrical geometry, passing to a Navy C-Ring Specimen (geometry used to investigate the effects of initial microstructure and heat treatment on the residual stress, and distortion of steels) to more complex gear geometry.

Thermo, mechanical and metallurgical properties from SAE 4140 and SAE 52100 were used in the computational models.

All the results are in agreement with literature work and experimental investigation published in technical literature.

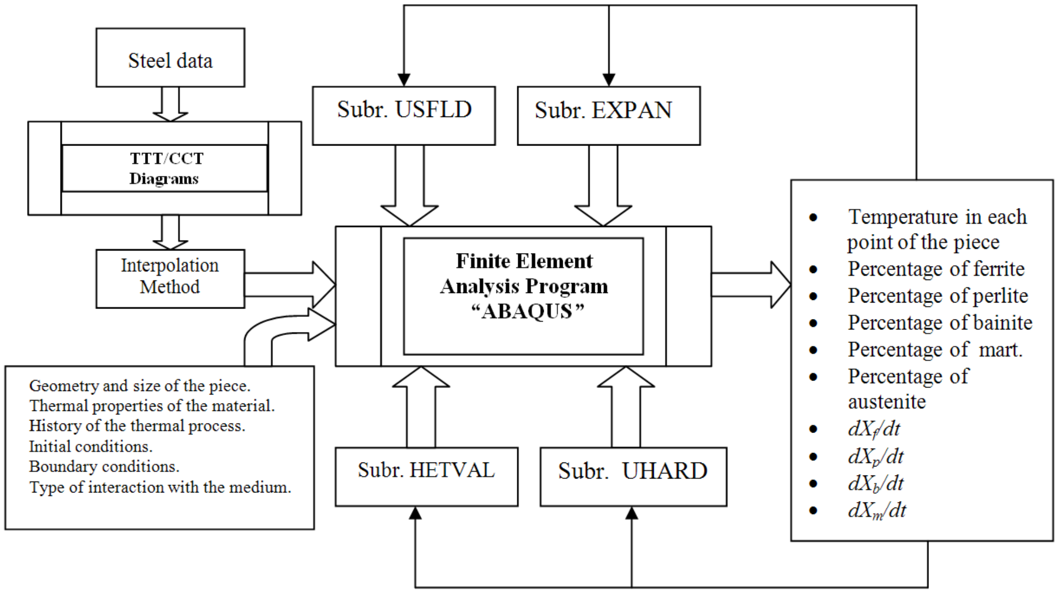

Figure 2. General scheme for modeling heat treatment process

2. Simulated Problems, Materials and Methods

In this paper, the capabilities of the set of user subroutines developed to predict phase transformations and all the metallurgical behavior will be demonstrated and discussed.

2.1 Simulated Problems

There are many heat treatment processes that could be analyzed to validate the user subroutines developed in this work. The authors have chosen examples that represent a real problem and can offer a complete understanding of how the model works. First of all, the heat treatment of a cylinder, which is a classic test problem, was considered for analyses. The solution of this problem will demonstrate the fundamental thermo-mechanical–phase transformation issues arising during heat treatment, due to thermally induced plastic deformation and the formation of multiple phases.

The second problem that was solved was the quenching of a Navy-C ring. This geometry is particularly used to analyze the effects of initial microstructure and heat treatment on the residual stress, cracking and distortion of steels.

Finally, a more complex geometry were simulated, through the quenching of a steel gear, always using Abaqus together with the set of Fortran user subroutines developed for heat treatment simulation.

2.2 Materials and Methods

In this work, heat treatment was simulated using material properties defined as functions of temperature. Table 1 indicates the thermo-physical and mechanical properties depending on temperature of AISI 4140 steel and Table 2 indicates the same for AISI 52100, as obtained from Sarmiento (1) and used in the present analysis.

Table 1. Thermo-physical and mechanical properties of AISI 4140 Steel.

Thermal conductivity		Specific heat		Young modulus		Yield stress		Coefficient of thermal explansion		Densit y
T [°C]	K [W/m.K]	T [°C]	c [J/kg.K]	T [°C]	E [Mpa]	T [°C]	σ_f MPa	T [°C]	α [10^{-6} °C^{-1}]	δ [kg/m^3]
100	42.7	100	473	205	196500	205	1641	100	12.2	7850
200	42.3	375	519	260	186000	315	1434	200	12.7	
400	37.7	575	561	315	172000	425	1138	400	13.7	
600	33.1			370	152000	370	1460	600	14.5	
				425	159000	450	834			
				480	145000	650	655			
				540	130000					
				595	115000					
				650	102000					
				705	90000					

Table 2. Thermo-physical and mechanical properties of AISI 52100 Steel.

Temperature (°C)	22	200	400	600	800	1000
Yield Strength (MPa) (0.2% offset except 22°C)	1410.17	1672.26	915.94	80.91	40.80	18.65
Tensile Strength (MPa)	NA#	2482.85	1221.36	221.46	84.06	33.14
Fracture Strength (MPa)	1866.85	2731.14	1343.50	243.61	92.47	36.45
Yield Strain (10^{-2})	0.70	1.09	1.09	0.30	0.30	0.20
Tensile Strain (10^{-2})	1.10	4.46	2.77	3.23	5.00	6.59
Fracture Strain (10^{-2})	1.10	6.97	74.35	252.18	128.37	42.64
Young's Modulus (GPa)	201.33	178.58	162.72	103.42	86.87	66.88*
Poisson's Ratio	0.277	0.269	0.255	0.342	0.396	0.490

The CCT diagrams of AISI 4140 and AISI 52100 steels used to construct the model, is exhibited in Figures 3 and 4 respectively. The information obtained from these diagrams was introduced in the FORTRAN subroutines responsible for the interpolation between temperature at every node, time and the phase transformation curve.

The thermal expansion coefficient has different values depending on what kind of phase transformations were indicated to occur by the USDFLD subroutine.

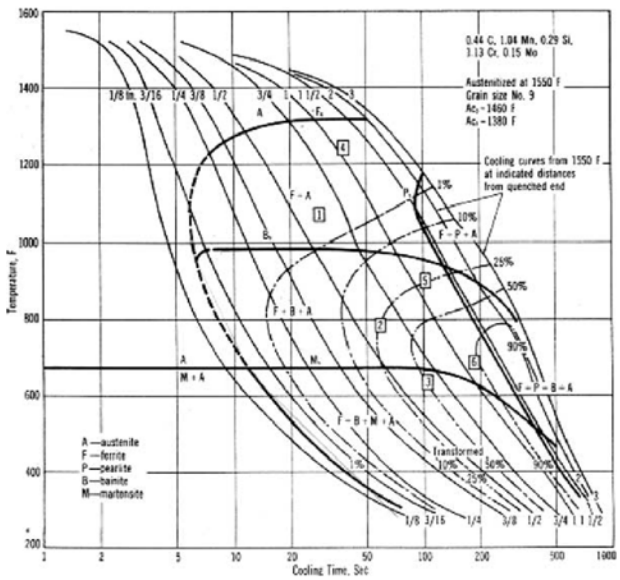

Figure 3. The continuous-cooling-transformation diagram for AISI 4140 steel used as reference to construct the model and FORTRAN subroutines

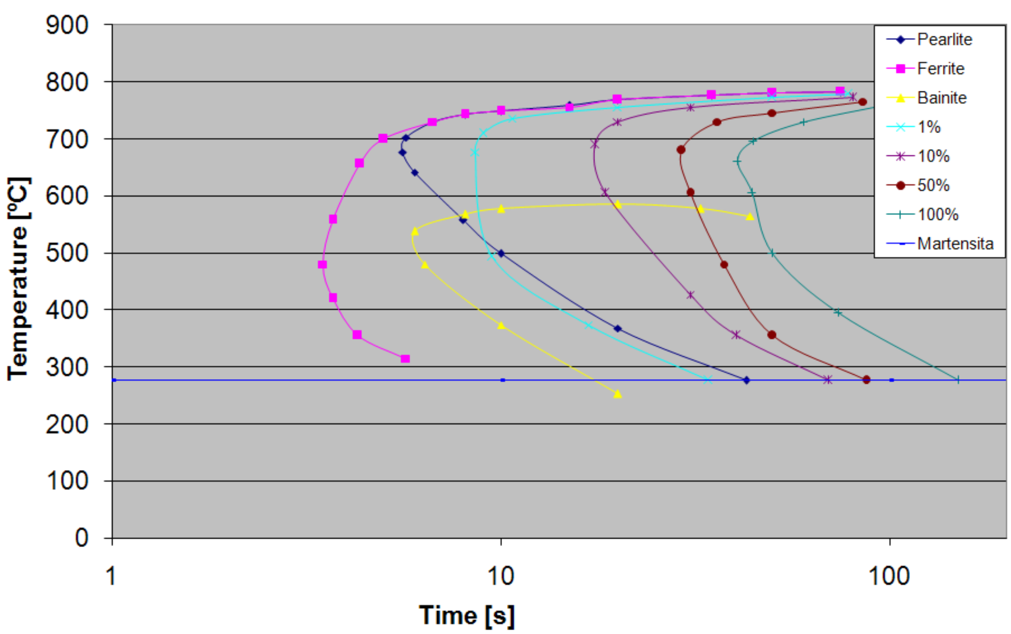

Figure 4. The continuous-cooling-transformation diagram for SAE 52100 steel used as reference to construct the model and FORTRAN subroutines

3. Results and Discussion

Abaqus CAE was used to construct the model of the cylinder the AISI 52100 steel properties were used. The cylinder with 3 cm diameter x 8 cm long was quenched according to the temperature presented in graph of Figure 5. The temperature distribution in the end of quenching is showed in the same Figure 5. Figure 6 presents the stress and volume fraction of martensite formed from austenite. According to was expected, cylinder surface is in tension while center is on compression.

For the Navy-C ring model, the finite element mesh used for these simulations was generated using Abaqus CAE. As shown in Figures 7 and 8, the mesh has 750 elements and 1116 nodes, and one-quarter symmetry is assumed for the analysis. There is a vertical plane of symmetry assumed running midway through the gap (i.e. one-half of the ring), and another plane of symmetry runs midway through the thickness (i.e. one-half the thickness. Uniform heating/cooling conditions using surface temperature dependent heat transfer coefficients as shown in Figure 7 (right) are used. AISI 4140properties were used. The measured and predicted dimensional changes were compared. The comparison between the dimensional changes agrees well for cooling conditions, as presented in Table 3.

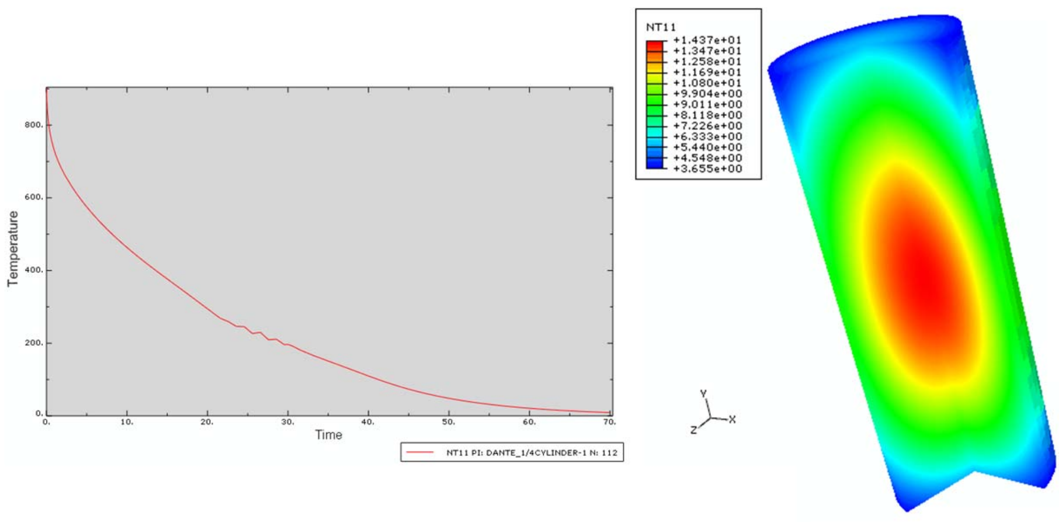

Figure 5. Temperature variation at the surface of the cylinder quenched (left) and temperature field after the heat treatment end (right)

For the gear finite element model the AISI 52100 material properties was also utilized. A vertical plane of symmetry was again assumed running midway through the radius (i.e. one-half of the gear), and another plane of symmetry runs midway through the thickness (i.e. one-half the thickness. Uniform heating/cooling conditions using surface temperature dependent heat transfer coefficients was used. Figures 9 and 10 present the results for stress and volume fraction of martensite, respectively

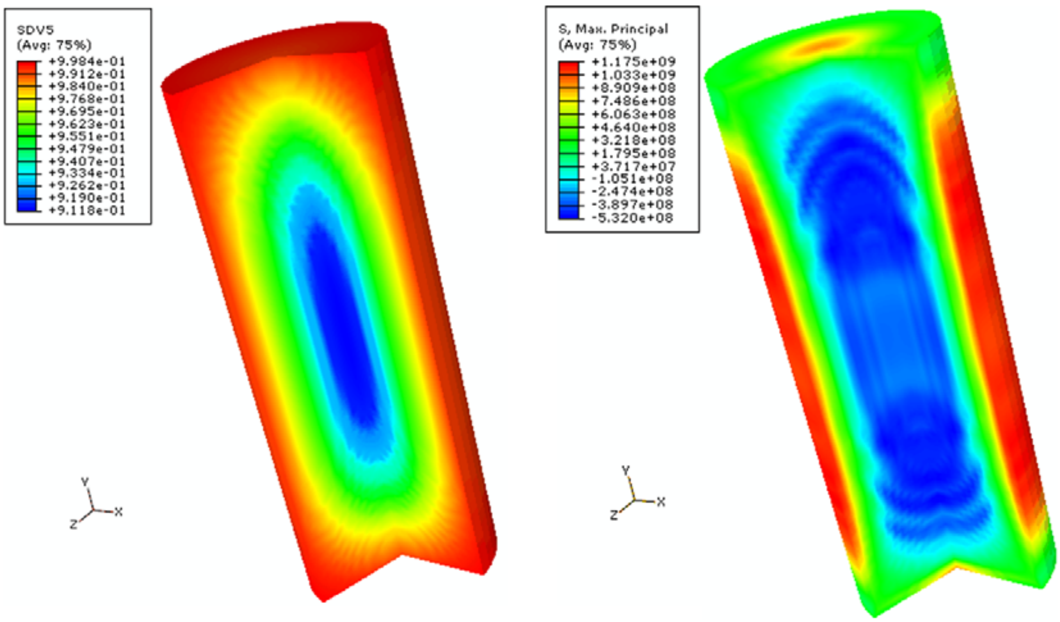

Figure 6. Volume Fraction of martensite (left) and stress field at the end of quenching (right)

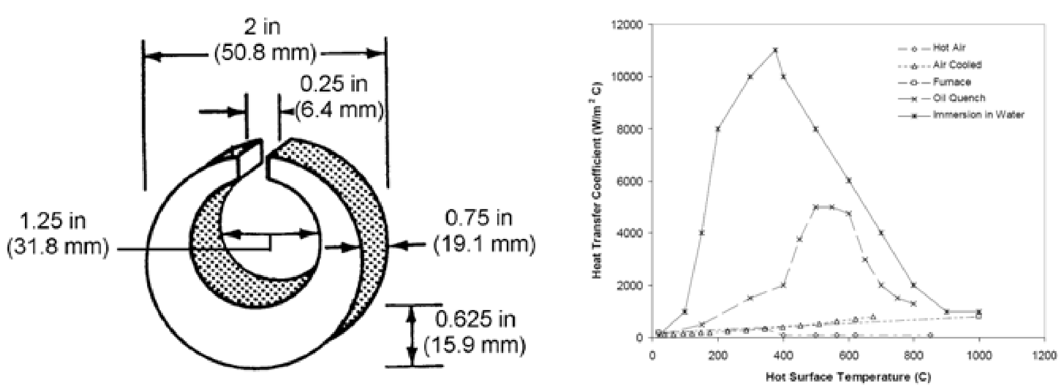

Figure 7. Geometry parameters (left) and temperature boundary condition (right) for the Navy -C Ring analyses

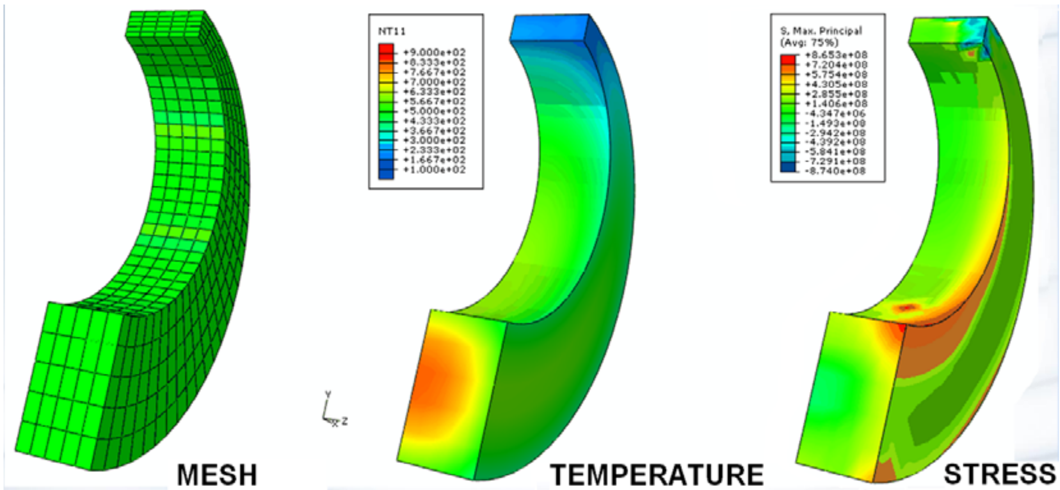

Figure 8. Result for the Navy-C Ring geometry

Table 3. Comparison between measured and calculated geometric changes

	Dimensional Change (mm)	
	Gap Opening	Outside Diameter
Measured	0,04064	0,01524
Simulated in the Present Work	0,04486	0,0636
Simulated by a Commercial Package of sub-routines	0,56	0,18

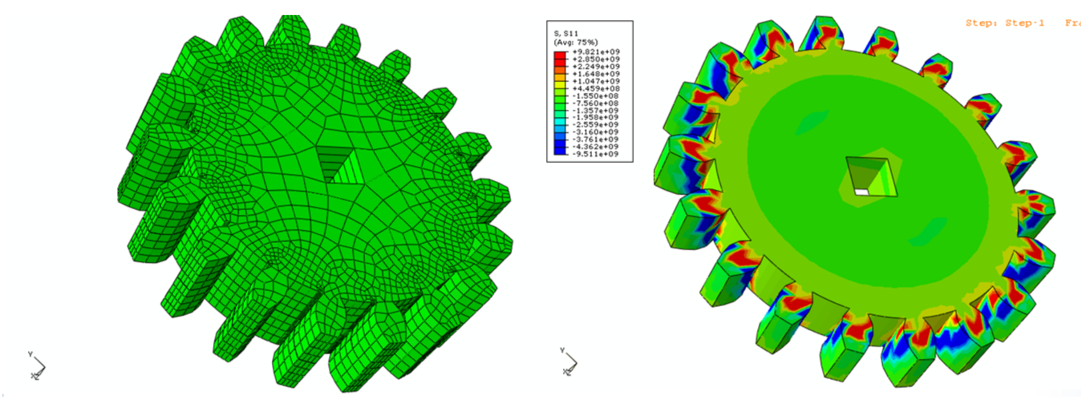

Figure 9. Finite Element Mesh for the gear model (left) and stress field at the end of quenching (right)

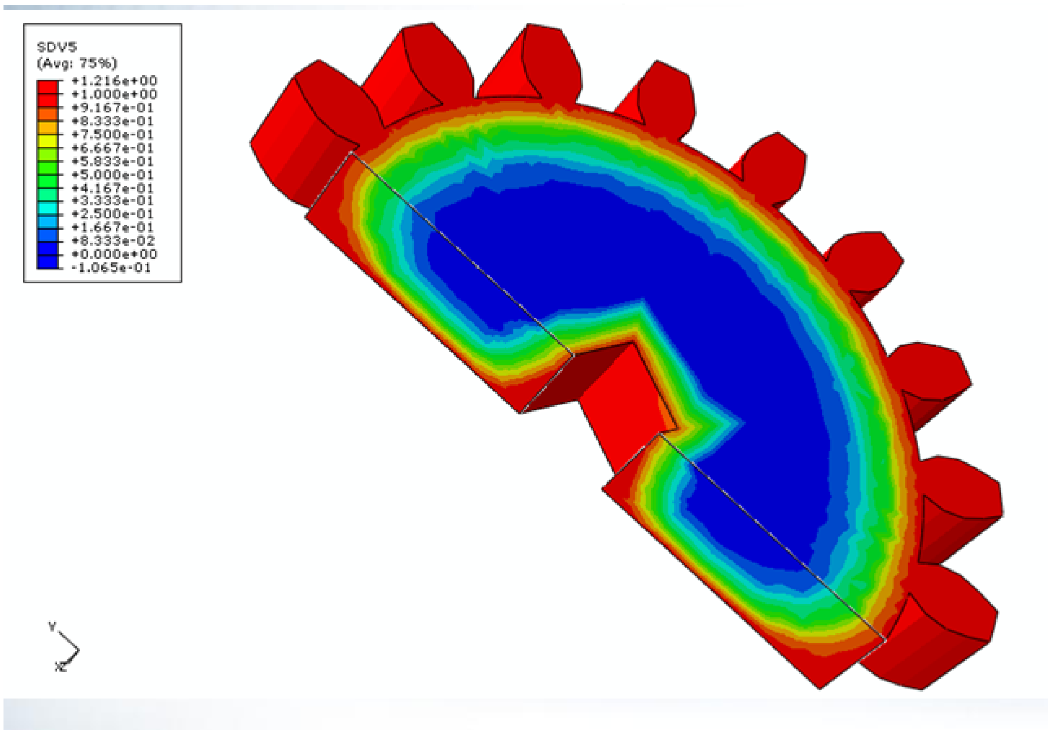

Figure 10. Volume Fraction of martensite in gear geometry

4. Conclusions

The present work gives an overview of the problem of heat treatment stress and distortion. Simulations were performed and are presented here to demonstrate that the user subroutines developed to simulate phase transformations in heat treatment generate results for predicting heat treatment stress and distortion. The predictions were shown to agree in a relative sense with some previously made measurements of heat treatment distortion presented in literature. The stress also agree with literature (2-6).

Experimental measurement of temperatures and distortions during heat treatment, and (possibly) residual stresses, will be made in the future as part of both experiments on test piece castings, and on production case study castings, to validate and improve the software predictions.

5. References

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