Readme: VrHeatTreat HeatTreatDiskSetup1 Video

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The HDTV video, HeatTreatDiskSetup1, shows the procedure for setting up a heat treating project with carburization in VrHeatTreat. This 6 minute and 12 second video shows that it took exactly 6 minutes and 12 seconds to set up the project and start the analysis. This does not include the time to mesh the part.. The video shows every detail of the designers actions together with audio explanations. The file size of the video is 44 Mb. This note provides background information on what the designer was doing and why.

We recommend that the video be viewed with Adobe's Flash player. It is a free download from

`http://www.adobe.com/shockwave/download/download.cgi?P1_Prod_Version=ShockwaveFlash`

We also recommend that you use Adobe Media Player to store and manage your Flash videos.

1 Introduction to VrHeatTreat

Internally VrHeatTreat operates with pure SI units, i.e., seconds, meters, kilograms, Pascals. For example, it does not use MPa internally. Results can be visualized in different units. For example temperature can be visualized in degrees K, C or F. Stress can be visualized in MPa or Psi. Currently VrHeatTreat does not support the input of data in units other than pure SI. However, it would not be a big job to modify VrHeatTreat to allow the designer to choose they preferred units for input data. If we did, the designer would set their preferred units in the Preferences file.

VrHeatTreat stores properties of each material in the Material Library. Each material has a name, e.g., steel8620, a list of property names such as thermal conductivity and a value or function that defines that property, often as a function of temperature. The designer can visualize each property by selecting the alloy type, the property type and doing a right click of the mouse.

The designer can also add new alloy types, new property types and new property values or functions. Some companies may not want to allow designers to modify material property library. The company may want to designate one person to be responsible for modifying Material Library materials and properties. VrHeatTreat supports these options.

VrHeatTreat allows the designer to write restart files. Then the analysis can be restarted from any restart file. For the restart, process parameters could be changed. This avoids having to rerun the portion of the analysis that the designer felt was satisfactory.

Meshing in VrHeatTreat will be dealt in separate videos. VrHeatTreat has a powerful meshing capability. Our experience is that designers can make a very high quality FEM mesh for many gears with complex geometry in less than one hour.

2 Processes for Heat Treating and Carburization

In a realistic heat treat analysis, the transient temperature, microstructure, carbon composition and stress-strain must be computed. VrHeatTreat does this with the following four solvers. Much of the information in this section is for researchers who want a deeper understanding of what VrHeatTreat is doing internally. Designers have no more need to understand what VrHeatTreat is doing internally than people who watch television need know what a television set is doing internally to create its images.

These solvers can be run in a single project or as separate projects. If they are run as separate projects they can be run in parallel in the sense that microstructure can start as soon as the thermal solver has completed its first time step. Carburization can start solving a time step as soon as the thermal solver has computed the temperature for that time step that carburization requires, microstructure solver can start as soon as carburization has computed the carbon composition for that time step that the microstructure solver requires and the stress-strain solver can start to solve a time step as soon as microstructure solver has computed the microstructure that the stress solver requires for that time step. This video only shows running the analysis in a single project.

Each solver can assign its own time stepping strategy. For example, once the part has reached carburizing temperature, the thermal and the stress-strain solver can take very large time steps. If one wishes to resolve the evolution of the carburized layer with time, then one should choose short time steps at the start of carburization and increase the time step size exponentially during carburization. Also carburization need not be be solved at all until carburization starts. The video shows that this is can be done easily and quickly in VrHeatTreat.

We recommend that the temperature and microstructure be computed first and the results checked before proceeding with the carburization and stress-strain analysis. The reason is to ensure that time steps sizes have been optimized to resolve microstructure evolution and to provide accurate microstructure and temperature data that is needed for an accurate stress-strain analysis. The video shows that VrHeatTreat makes this easy to do. The 3D analysis of temperature and microstructure is very fast even with a fine mesh.

2.1 Thermal solver

This solves the equation for the conservation of energy. It requires the thermal conductivity, specific heat and specific enthalpy as a function of temperature. VrHeatTreat stores these properties in the Material Library.

The initial temperature is usually room temperature 20 C or 293 K. In heat treating the most common boundary condition is a convection boundary condition defined by a convection coefficient and the ambient temperature of the furnace or quench media. The convection coefficient can be a function of temperature. The heat treating process usually starts by putting the part in a carburizing furnace to bring the temperature up to about 900 C or 1173 K.

As a part is lowered into a quench bath, the designer can specify the normal to the quench liquid surface, i.e., the orientation of the part as it is lowered into the quench bath and the time the part contacts the liquid and the speed at which it is lowered into the quench liquid. Then VrHeatTreat assigns the value of the convection coefficient and ambient temperature based on whether the point is in the quench bath or in the air above the quench bath.

Shortly before quenching carburization is often turned off and the temperature dropped to just above the temperature at which ferrite would start to form. There are two reasons for this. One is that it reduces the difference between the maximum and minimum temperature during quenching. This reduces distortion and the risk of cracking. The other reason relates to carburization and is discussed with the carburization solver.

2.2 Carburization solver

This solves the conservation of the mass of carbon as it diffuses into the part. The initial condition is the initial carbon composition of the part which is stored in the material library as a property of the alloy. The boundary condition during carburization is the value of the carbon on the surface of part during carburization. Mathematically, this is a Dirichlet or prescribed carbon boundary condition.

If the carbon potential is set higher than about 1.0 % carbon, there is a risk of a layer of Fe_3C forming on the surface. The vacuum carburizing process uses ‘boost-diffuse’ cycles with a carbon potential higher than 1.0 % carbon for a short period of time that might form a very thin layer of carbide. Then the diffuse step dissolves the carbide layer. VrHeatTreat currently does not support the analysis of vacuum carburizing but providing support for vacuum carburizing would not be a big job.

When carburization is stopped and the carburizing atmosphere replaced with a neutral atmosphere, the boundary condition is changed to a zero carbon flux boundary condition. This was the other reason that the temperature was dropped to just above the temperature at which ferrite would start to form just before the quench starts. It is that with carburization turned off, carbon continues to diffuse down the carbon gradient. This reduces the peak carbon on the boundary surface usually from about 0.8 or 1.0 % carbon to about 0.7 % carbon and flattens the carbon profile near the surface.

2.3 Microstructure solver

Given the initial microstructure, composition and grain size of a low alloy steel, VrHeatTreat computes the evolution of microstructure as a function of time and temperature. To do this, it contains a psuedo-Fe-C binary phase diagram, i.e., a binary phase diagram in which each of the points such as the eutectiod temperature which is about 723 C and eutectiod composition which is about 0.8 % carbon in a pure Fe-C alloy are functions of composition of Mn, Cr, Mo, W, Ni, Nb, V, As, etc. The psuedo-Fe-C binary phase diagram determines the equilibrium state for a given composition and temperature. The rate at which phases change as they move toward equilibrium is determined by integrating ordinary differential equations that contain the appropriate kinetic coefficients. The underlying theory is described in more detail in the following papers.

Watt, D.F., Coon, L., Bibby, M.J., Goldak, J.A. and Henwood, C., Modelling Microstructural Development in Weld Heat-Affected Zones, (Part A), Acta Met., vol. 36, No. 11, pp. 3029-3035, 1988

Henwood, C., Bibby, M.J., Goldak, J.A. and Watt, D.F., Coupled Transient Heat Transfer-Microstructure Weld Computations, (Part B), Acta Met., vol. 36, No. 11, pp. 3037-3046, 1988

The increase in carbon composition in the carburized layer changes the lattice parameters of austenite, bainite and martensite. It also changes the martensite start and end temperatures. The change in lattice parameters generates a strain similar to a thermal strain. The reduction in the martensite start temperature in the carburized layer means that with the right cooling rate the austenite in the interior of the part will transform to martensite before the austenite in the carburized layer. In this case, when the austenite in the carburized layer transforms to martensite, the expansion of the phase change generates the compressive stress in the carburized layer. If the quench cooling rate was too fast, the austenite in the interior would transform to martensite or bainite after the carburized layer had transformed to martensite. This would reduce the the compressive stress in the carburized layer. VrHeatTreat captures this physics.

Another important effect in the microstructure model in VrHeatTreat is that the grain growth of austenite is modelled as a function of temperature and time by integrating an ordinary differential equation at each Gauss point in the FEM mesh. Larger austenite grains reduce the grain boundary area and this reduces the number of nuclei for the transformation of austenite to ferrite and pearlite and bainite. This increases the hardenability and the probability that martensite forms. VrHeatTreat captures this physics.

As the initial ferrite-pearlite or bainite microstructure transforms to austenite, there is a significant decrease in specific volume. This change in specific volume combined with thermal expansion due to heating often causes plastic deformation. For this reason, we recommend choosing time steps so that the change in the fraction gamma or austenite phase at any point does not exceed say 20 % in any time step. During quenching, the maximum change in gamma or austenite phase at any point should also not exceed say 20 % in any time step. The video shows that VrHeatTreat makes it very easy and quick for the designer to set time step sizes to do this.

2.4 Stress-strain solver

This solves the conservation of momentum with a visco-elasto-plastic stress model. VrHeatTreat uses theory and numerical algorithms for visco-plasticity theory developed by J. C. Simo and his colleagues in the late 1980s and early 1990s. For details of the theory, see J. C. Simo, Numerical Analysis of Classical Plasticity, Handbook for Numerical Analysis, Volume IV, ed. by P.G. Ciarlet and J.J. lions, Elsevier, Amsterdam (1998).

The temperature dependent material property data required for each phase include the Young's modulus, Poisson's ratio, specific volume, yield stress, isotropic and kinematic hardening modulus.

VrHeatTreat uses separate stress-strain curves or functions for each phase. We believe that this is much better than trying to contrive a stress-strain curve or function for all possible microstructures during heating and cooling.

The boundary conditions for the stress-strain solver simply remove rigid body modes. This is done by adding very weak springs to ground to all nodes in the FEM mesh of the part.

3 Stages or Steps for Heat Treating and Carburization

The designer chooses the stages in the heat treating process. The following are examples of possible stages. The designer to free to add stages. For each stage the designer specifies the start time and end time and strategy to set time step size. Also boundary conditions can be set. Boundary conditions can be functions of time. There can be no gaps in time in the stages.

1. Preheat: The part is placed in a preheat furnace.
2. Heating in the carburizing furnace.
3. Pre-quench stage in the carburizing furnace.
4. Quenching can be decomposed into three stages.
    (a) The first stage of quenching starts with the start of quench and ends when gamma or austenite phase starts to transform to martensite. The thermal contraction on cooling generates strain and stress. Note that the ambient temperature during quenching is the temperature of the quench liquid.

    (b) The next stage of quenching starts when gamma or austenite phase starts to transform to martensite and ends when the fraction austenite to martensite and bainite is largely complete. Because the volume expansion of this phase change can cause large plastic strains, short time steps are needed both to resolve the phase change and accurately solve the evolution of stress-strain.
    (c) The third stage of quenching starts when the transformation of austenite is largely complete and ends when the part is removed from the quench liquid and placed in air. Now only the thermal contraction as the martensite and bainite cools drive the evolution of stress-strain.

5. Air cool after removing the part from the quench bath.

6. Tempering furnace stage.

4 Future Work

Heat treaters use many different types of quench liquids. For each type of quench fluid the convection coefficient should be determined as a function of temperature. This could be computed fairly easily if the supplier provided a curve of the temperature of a given point of given part as a function of time. For example the time-temperature curve at a point at the center of the circular surface of the disk specimen described in the paper; Craig Zimmermann, Jonathan Hall, Dan McCurdy and Ed Jamieson, Comparison of Residual Stresses from Atmosphere and Low Pressure Carburization, Heat Treating Progress, July 2007, 41-46.

Currently VrHeatTreat deals with a single part. In reality parts are often placed in baskets and the baskets placed in a furnace or in the quench bath. As the furnace gas blows through a basket, the gas is cooled by the basket and the parts. Parts near the inlet are heated faster than parts near the outlet of the furnace gas flows. We are extending VrHeatTreat to model the fluid flow in a furnace with a basket of parts. This will require a CAD model of the furnace including specifications of the fans that drive the gas flows and a CAD model of the basket. This will also model fluid flow with vapor bubble formation as a basket of parts is lowered into a quench bath. This is expected to more accurately model the quenching process including variations in quenching for parts in different areas of the basket and for parts in different positions in a slot in a basket.

We are also working on an extension of VrHeatTreat to simulate pressure quenching of parts.