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Incremental Thermoelastic Stress Model

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Introduction

FLOW-3D® is able to emulate elastic solids, elasto-viscoplastic materials (materials that exhibit a yielding limit, beyond which they behave like a viscous liquid), and now, thermally induced stresses during solidification of molten materials. This most recent addition to the model includes the expansion and contraction of materials due to temperature variations. The elastic stress is computed incrementally during the simulation; the elastic stress is related to the local strain (the relative displacement of the material negating solid-body translations and rotations) by the elastic modulus. New parameters needed with this model are the bulk modulus, which controls how the pressure within the solid region varies due to uniform (i.e. isotropic) expansion or contraction of the material. This expansion and contraction needs to be considered because the material is not assumed to be incompressible. Also, the thermoelastic stress model is designed to work only with ***FLOW-3D***®'s solidification model; the material at any point begins to develop elastic stress when the solid fraction reaches one. Finally, both elastic modulus and yield stress limits can either be constant or a function of the local temperature.

Approach

The goal behind development of this model was to require few changes to the existing models already incorporated into ***FLOW-3D***® so as to minimize complexity and maintain the performance of the code. Therefore, the existing model for elastic stress was only slightly modified so as to include only the deviatoric part of stress (i.e. stretching and shearing components) in the divergence of stress term in the momentum equation. The remainder of the stress (the *isotropic* part – due to uniform compression or expansion) is stored instead as the *pressure*, otherwise known as the *negative mean of the isotropic stress*. In this way, the "pressure" is computed in ***FLOW-3D***® just as it is for liquid regions. The existing logic to account for thermal expansion and bulk compressibility are also maintained and used in the incremental thermoelastic stress model.

Thermoelastic stress model

For small deformations (i.e. *Hookean* behavior), the state of stress $\boldsymbol{\tau}_E$ for an elastic solid undergoing thermal expansion (or contraction) is [1]

$$\boldsymbol{\tau}_E = \left(K - \tfrac{2}{3}G\right)e\mathbf{I} + 2G\mathbf{E} - 3\alpha K\left(\theta - \theta_0\right)\mathbf{I}\,, \qquad (1)$$

where $\mathbf{E}$ is the strain tensor, $\mathbf{I}$ is the unit isotropic tensor, G is the shear modulus, K is the bulk modulus, α is the linear thermal expansion coefficient, θ is the local temperature and θ_0 is the reference temperature. e is the *volume strain* which characterizes the isotropic expansion or contraction of the material.

Since equation 1 is a linear model, it cannot be used in situations where the magnitude of deformation is finite, which includes most simulations performed by ***FLOW-3D***®. However, an incremental model, in which the components of stress are computed incrementally over small time periods such that each incremental deformation is small enough to obey the linear assumptions, non-linear processes can be predicted. The root of this model was discussed at length in *Flow Science Technical Note 64*[2] (available at www.flow3d.com/pdfs/TN64.pdf).

To implement Eq. 1 numerically, it is convenient to separate it into its deviatoric and isotropic parts. The deviatoric part is merely

$$\boldsymbol{\tau}'_E = 2G\left(\mathbf{E} - \tfrac{1}{3}e\mathbf{I}\right). \tag{2}$$

The remaining isotropic part is then

$$p = -Ke + 3\alpha K\left(\theta - \theta_0\right), \tag{3}$$

where p is the pressure, which in elastic solids is $-\frac{1}{3}\boldsymbol{\tau}_\mathbf{E}\cdot\mathbf{I}$ in three dimensions.

In ***FLOW-3D***®, the pressure is coupled to the continuity condition, as it is in Eq. 3. Taking the time derivative of Eq. 3 and rearranging, we get

$$\frac{1}{K}\frac{dp}{dt} = -\left(\nabla\cdot\mathbf{u}\right) + 3\alpha\frac{d\theta}{dt}, \tag{4}$$

where $\frac{1}{K}$ is the *limited compressibility coefficient*, and is already used in earlier versions of ***FLOW-3D***®, and $\mathbf{u}$ is the local material velocity. Equation 4 is solved iteratively within each time cycle; the solver adjusts pressure and velocities throughout the flow domain until convergence (i.e. the residual of Equation 4 falls below a convergence criterion, ε).

In general, the material deformations are large, so the value of $\mathbf{E}$ cannot be computed at each moment in time based solely on the current state. Therefore, the deviatoric part of the stress from Equation 2 must be incremented through time for each element of material involved in stress; the elastic stress at time, t, for an element of fluid is

$$\boldsymbol{\tau}'_E\left(\xi, t\right) = \int_{-\infty}^{t} 2G\dot{\mathbf{E}}'\left(\xi, t'\right)dt', \tag{5}$$

where $\boldsymbol{\xi}$ represents a material coordinate (i.e. a small, but finite volume of the material) which translates and rotates with the deforming material and $\dot{\mathbf{E}}'$ is the deviatoric part of the local strain *rate* tensor, computed from the symmetric part of the velocity gradient and divergence of velocity,

$$\dot{\mathbf{E}}' = \frac{1}{2}\left[\nabla\mathbf{u} + \left(\nabla\mathbf{u}\right)^T\right] - \nabla\cdot\mathbf{u}\,. \tag{6}$$

Written for ***FLOW-3D***®'s Eulerian (fixed grid) coordinate system, the time rate of change of Equation 5 is[3]

$$\underbrace{\left(\frac{\partial\boldsymbol{\tau}'_\mathbf{E}}{\partial t}\right)_\mathbf{x}}_{\substack{\text{Rate of change}\\ \text{at fixed point}}} + \underbrace{\mathbf{u}\cdot\nabla\boldsymbol{\tau}'_\mathbf{E}}_{\substack{\text{Advection of stress}\\ \text{as material moves}}} = \underbrace{\boldsymbol{\tau}'_\mathbf{E}\cdot\mathbf{W} + \mathbf{W}^\mathbf{T}\cdot\boldsymbol{\tau}'_\mathbf{E}}_{\substack{\text{Remove effects of rotational}\\ \text{flow in material motion}}} + \underbrace{2G\dot{\mathbf{E}}'\left(\mathbf{x}, t\right)}_{\substack{\text{Incremental generation}\\ \text{of stress}}}, \tag{7}$$

where $\boldsymbol{\tau}'_\mathbf{E}$ here is the elastic stress represented in the fixed coordinate system, $\mathbf{x}$. The first term on the right hand side prevents the formation of elastic stress due to solid-body rotation; $\mathbf{W}$ is the vorticity tensor (the *anti*symmetric part of the velocity gradient), and is

$$\mathbf{W} = \frac{1}{2}\left[\nabla\mathbf{u} - (\nabla\mathbf{u})^T\right]. \quad (8)$$

Equation 7 is the crux of the incremental stress model.

The current value of stress is a function of the past history of the fluid element. Material that enters the domain through its boundaries typically has a null state of stress; in ***FLOW-3D***®, the user can specify the boundary stress components by setting the *scalar* boundary conditions (with the *sclbc* parameter). Solidified material present at the start of the simulation also typically has a null state of stress; in ***FLOW-3D***®, this can be changed with the use of the *sclri* parameter. Furthermore, molten liquid that solidifies always has a zero initial state of stress. Material that had previously solidified, and has then re-melted, has its state of stress reset to zero.

In certain situations it may be necessary to model yielding of the solidified material. Yielding occurs wherever the magnitude of elastic stress exceeds a set value. The magnitude used is the second invariant of the deviatoric part of the stress tensor, $II_{\boldsymbol{\tau}'_E}$, commonly called the *von Mises stress*. In situations where yielding is considered, the Mises yield condition is used. This condition is

$$II_{\boldsymbol{\tau}'_{\mathbf{E}}} = \frac{Y^2}{3} \quad (9)$$

where Y is the yield stress limit, a user-specified parameter, and

$$II_{\boldsymbol{\tau}'_{\mathbf{E}}} = \frac{1}{2}\sum_{i,j} \tau'_{E,ij}\tau'_{E,ij} \quad (10)$$

is the second invariant of the strain-rate tensor.

In regions of the material where the elastic stress exceeds the yield criterion, the elastic stress is relaxed such that the condition in Equation 9 is met:

$$\tilde{\boldsymbol{\tau}}'_E = \sqrt{\frac{2Y^2}{3II_{\boldsymbol{\tau}'_E}}}\,\boldsymbol{\tau}'_E \quad (11)$$

where $\tilde{\boldsymbol{\tau}}'_E$ is the yield-limited elastic stress tensor.

Equation 7 is discretized spatially and temporally and the resulting value of the stress tensor $\tilde{\boldsymbol{\tau}}_E$ is added to the momentum equation:

$$\frac{\partial\mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = \underbrace{-\frac{1}{\rho}\nabla p}_{\text{Isotropic divergence of stress}} + \frac{1}{\rho}\left\{\underbrace{\nabla\cdot\left[\mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)\right]}_{\text{Divergence of viscous stress}} + \underbrace{\nabla\cdot\tilde{\boldsymbol{\tau}}'_E}_{\text{Divergence of elastic stress}} + \underbrace{\mathbf{F_b}}_{\text{Additional body forces}}\right\}. \quad (12)$$

Considerations at free surfaces

At free surface interfaces, the only stress imposed by the external fluid is that due to pressure, as a gas or vapor exerts negligible traction on the fluid surface. Therefore, $\mathbf{n} \cdot \tilde{\boldsymbol{\tau}}'_E = 0$ at such interfaces, and the pressure is set based on the external pressure and surface tension (if relevant). In ***FLOW-3D***®, the principal directions in which free surfaces face and the status of neighboring cells are known. From this information, the appropriate components of $\tilde{\boldsymbol{\tau}}'_E$ are set to zero at free surfaces to ensure that the aforementioned condition is met.

Considerations at walls and solid objects

At interfaces with walls or solid objects, the fluid velocity in the cell neighboring the wall (or obstacle) and the velocity of the wall (or obstacle) are used to compute the strain rate tensor in Equation 6. A no-slip condition is always presumed. Turning off the wall shear option in ***FLOW-3D***® will not affect this. For viscoplastic flows (i.e. with a yielding condition), slip will occur where the local stress exceeds the yield stress limit.

In ***FLOW-3D***® there is an option that allows the user to control the way the material interacts at solid walls or components. The material can either adhere to walls, even as it tries to pull away, or it can pull freely away from walls; in the latter situation, wherever the local velocity adjacent to the wall is away from the wall, $\mathbf{n} \cdot \tilde{\boldsymbol{\tau}}'_E = 0$, where **n** is the unit normal vector of the wall surface. In either case, the material cannot penetrate walls.

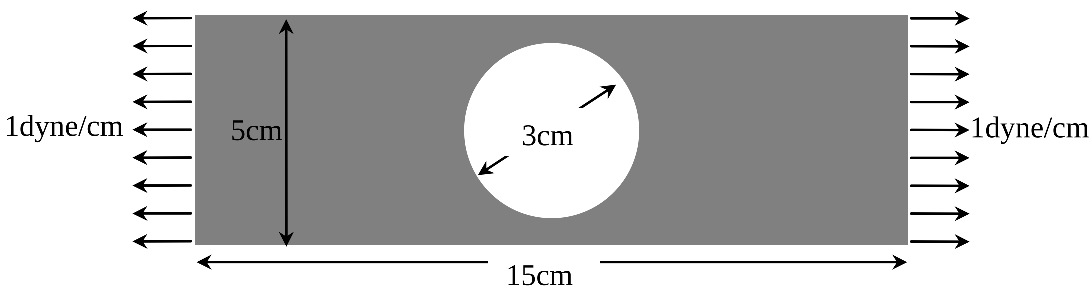

Figure 1. Setup of problem of a circular hole in a plate. The goal is to compute the maximum magnitude of elastic stress in the narrow regions of the solid adjacent to the hole.

Examples

Circular hole in plate

Figure 1 shows the setup for this test problem. We have a plate that is thin enough in the third dimension such that the stresses related to this component can be taken as zero (or, alternatively, it can be infinitely thick in this dimension such that it is a two-dimensional problem). The analytical solution to this problem is discussed by Hattel and Hansen[4]; the maximum magnitude of the stress in the narrow part adjacent to the hole is a function of the plate width and the size of the hole. Also, solutions are plotted for cases where the hole is not located at the geometric center of the width of the plate. Figure 2 shows how α, the relationship between the maximum stress magnitude (τ_{max}) and the nominal stress magnitude (τ_{nom}), is computed from the applied stress, τ_0. For this problem σ_0 is defined as 1, so the nominal stress is just the expected stress over the narrow part adjacent to the hole:

$$\tau_{nom} = \left(\frac{5}{5 - 2.5} \right) \cdot 1 = 2 \,. \tag{13}$$

From the chart in Figure 2, the value of α is 2.15 for this case (r/a=0.5; B/a=2). Therefore, the expected value of τ_{max} is **4.3**.

Figure 3 shows the steady-state (1*s* of simulation) result from ***FLOW-3D***®, with 16632 computational cells in two dimensions; the CPU time to completion was 6.5 min. What is plotted here is the total *xx*-component of elastic stress (τ'_{xx}); this includes the τ'_{xx} computed by ***FLOW-3D***® as well as the pressure. The maximum value computed by ***FLOW-3D***® is **4.28**. The error from the expected result is **0.5%**.

Solidification of Aluminum Casting of Alternator Housing

The most common application for the thermoelastic stress model is in metal casting; a complex shape is created by pouring or injecting molten metal into a mold. This mold can either be rigid so that it cannot deform due to stresses placed upon it by the cooling casting, or it can deform, as in the case of sand casting, such that the mold itself does not exert external tractions on the surface of the casting during solidification. Here, an aluminum alternator housing is cast in both types of molds, and the stresses developed within are simulated with ***FLOW-3D***®. The properties of the aluminum alloy in the simulation are detailed in Table 1. Both cases use exactly the same single-block computational mesh; approximately 500,000 cells, each of size approximately 0.2*cm*×0.2*cm*×0.2*cm*.

Density, ρ	2.642 g/cm^3
Elastic Modulus, G	2.344×10^9 $dynes/cm^2$
Thermal expansion coefficient, α	8.4×10^5 K^{-1}
Bulk modulus, K	6.56×10^{10} $dynes/cm^2$
Liquidus temperature	898 *K*
Solidus temperature	798 *K*
Latent heat of fusion	4.0×10^9 erg/g
Specific heat	1.13×10^7 $erg/(g\cdot K)$
Thermal conductivity	6.48×10^6 $erg/(s\cdot cm\cdot K)$

Table 1. Properties of aluminum alloy used in thermal stress simulation in ***FLOW-3D***® for alternator housing example (in CGS units).

Case 1: Rigid Mold

Here, the solidification process is presumed to occur within a completely rigid mold; the boundary condition between on the solidifying metal at the mold interface is a prescribed position. However, as described above, the solidifying metal is able to pull away from the mold surface, so in some regions at the mold-metal interface, the normal component of stress is set to be zero (as stated in Equation 14). Thus, the metal cannot pull away nor deform the mold regardless of its state of stress. Figure 4 shows three-dimensional renderings of the temperature, pressure and the magnitude of elastic stress – the Mises stress. Note that in this scenario, a three-dimensional plot of displacement at the mold-metal interface does not show meaningful information because we are prescribing the displacement there. The heat transfer coefficient between the solidifying metal and the mold is 1×10^5 $erg/(s\cdot cm^2\cdot K)$.

Figure 4 shows three- and two-dimensional plots of the evolution of this simulation from 0 to 151 seconds. The plots of temperature (the color scale ranges from 425*K* to 800*K*) show the last region of the part to cool is in the vicinity of the thick mounting arm on the left. This is also the last region to solidify. The subsequent plots of pressure (the color scale here ranges from -2.5×10^8 to 0 $dynes/cm^2$) show which regions of the part are under the greatest tension. Note that pressure has the opposite scale as the stress components – large negative values indicate isotropic tension, while large positive values indicate isotropic compression. In this simulation, no region is undergoing isotropic compression because the metal is contracting during solidification and is constrained by the mold. In this simulation, the greatest tension occurs in the vicinity of the small structures of the part, and the central ring-like structure, because here the shrinkage is frustrated by the confines of the mold. Conversely, the two-dimensional plot (which is a plane just below the upper face of the bottom piece of the alternator) shows minimal tension in the flat regions because the metal here is pulling away from the mold surface, allowing relaxation of the stress. The third set of plots shows the Von Mises stress (the magnitude of the deviatoric part of elastic stress). The color scale here ranges from 0 to 2×10^8 *dynes/cm2* (by definition the Von Mises stress is always positive). Regions where the Von Mises stress is high (red) indicate locations where the metal is undergoing large amounts of shear or stretching/squeezing.

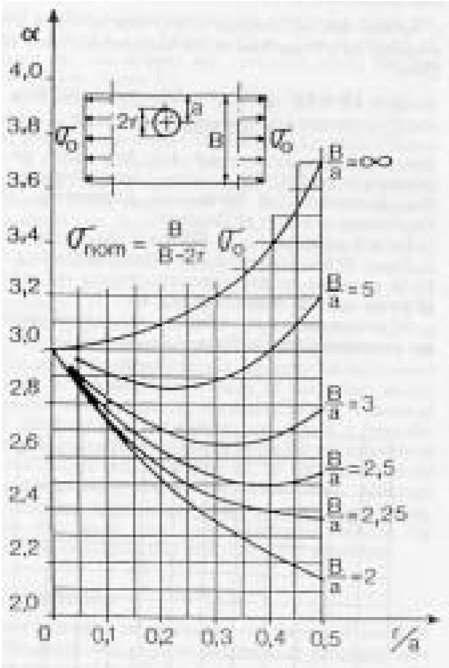

Figure 2. Chart showing geometrical shape factor as a function of the plate and hole geometry[4].

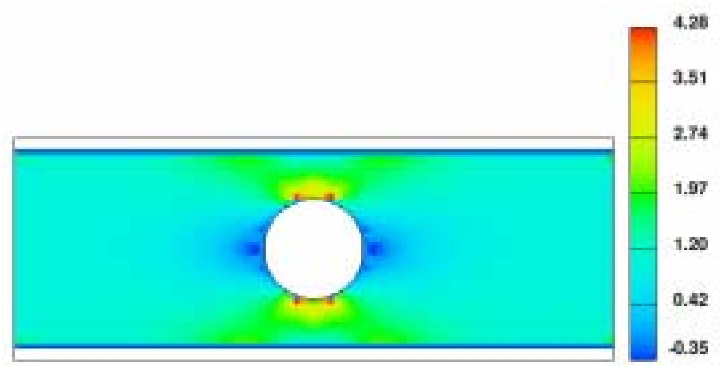

Figure 3. ***FLOW-3D***® result of hole in plate problem. The color value indicates the *xx*-component of total elastic stress; the maximum value indicated is 4.28.

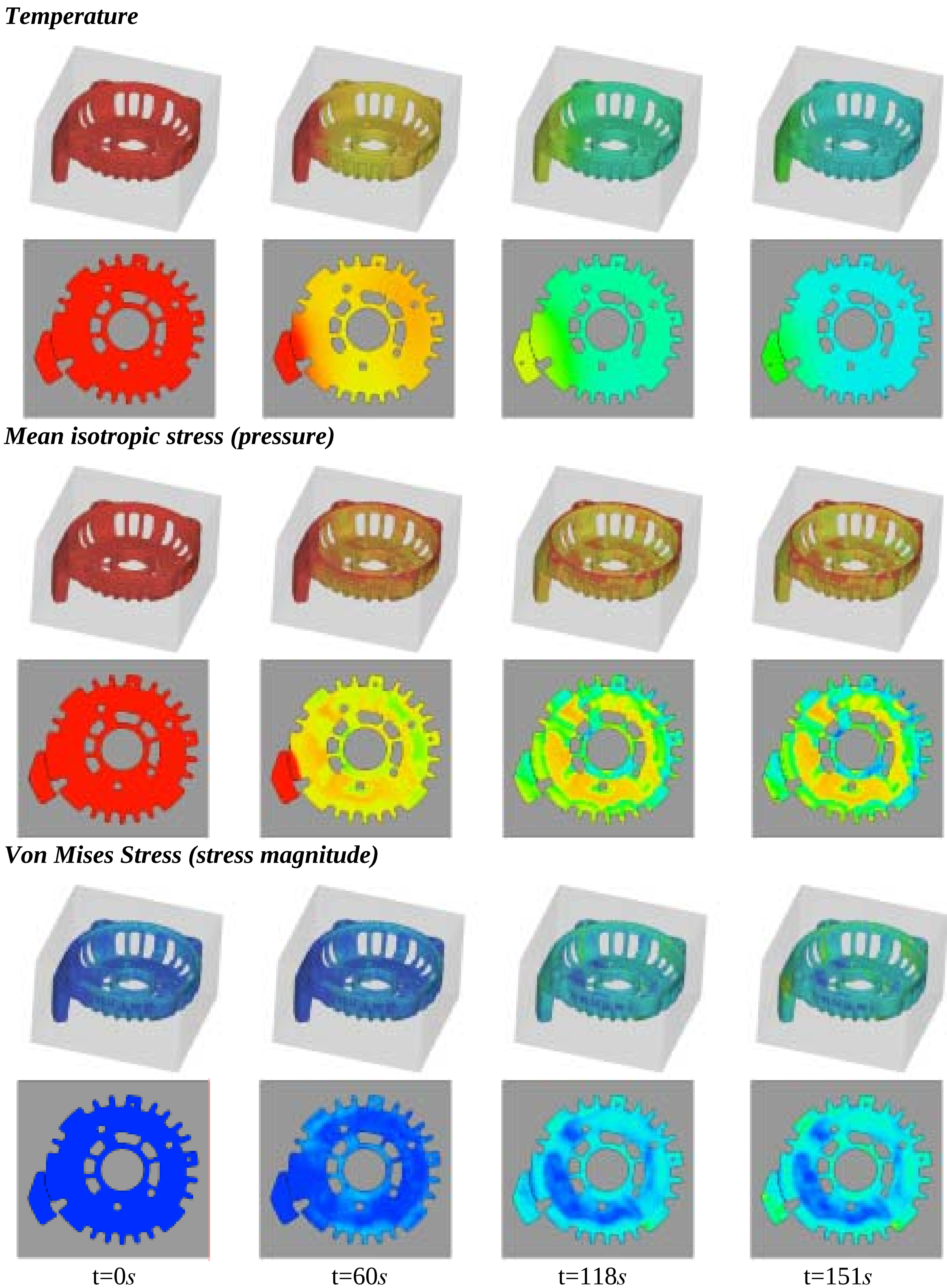

Figure 4. Results of thermal stress development during solidification of aluminum alternator housing inside a rigid mold; the solidifying metal is able to pull away from the mold interface. Both two- and three-dimensional results are shown; the 2-D results are of a horizontal plane at z=3.504*cm* below the top of the part.

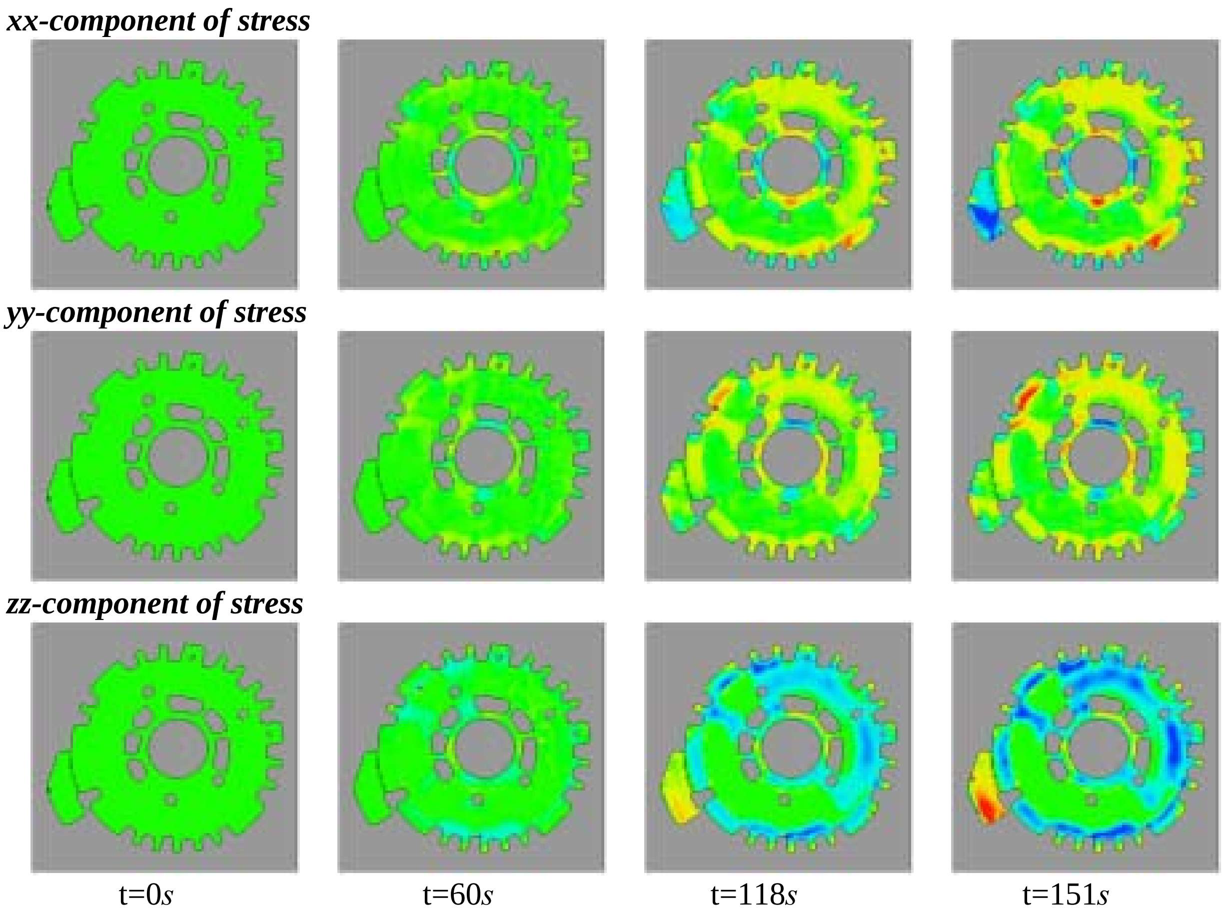

Figure 5. Results for rigid mold showing stretching (or squeezing) along each of the three Cartesian directions. Red and blue indicate regions being stretched and squeezed, respectively. Green regions are relaxed. The plots are of a horizontal plane at z=3.504*cm* below the top of the part. In these plots, x to the right, y is to the top, and z is out of the page.

Figure 5 shows two-dimensional plots of the stretching (or squeezing) along each Cartesian direction. The color scale varies from -5×10^{5}*dynes/cm*^{2} (blue) to 5×10^{5}*dynes/cm*^{2} (red). In both the x- and y-directions, the greatest areas of concern (red) are near the junctions of the ventilation gaps with the solid body of the alternator housing. It is here that the shrinkage is frustrated by the mold geometry. Conversely, in the z-direction, the metal is under compression at these junctions, much as when a metal rod is stretched axially, there is compression in the radial direction due to volume conservation. However, there is significant stretching in the z-direction in the mounting arm at left because this is a large block of metal and the last to cool, causing the total amount of shrinkage to be great, and last to solidify metal is constrained not only by the mold, but by the previously solidified metal surrounding it.

Case 2: Air cooled or sand mold

In this scenario, the boundary condition at the surface of the solidifying casting is presumed to be

$$\mathbf{n}\cdot\boldsymbol{\tau}_{\mathbf{E}}=\mathbf{0}. \qquad (14)$$

so that it is able to deform and translate at will. This condition is approximate for the case of sand casting, where the stress exerted by the sand is small relative to that within the solidifying metal, and is true for the case of open-air solidification, where the casting is ejected from a mold and allowed to cool surrounded by air. The heat transfer coefficient to the surroundings used for this simulation is assumed to be 1×10^{5} erg/(s $\cdot$cm$^2\cdot$K).

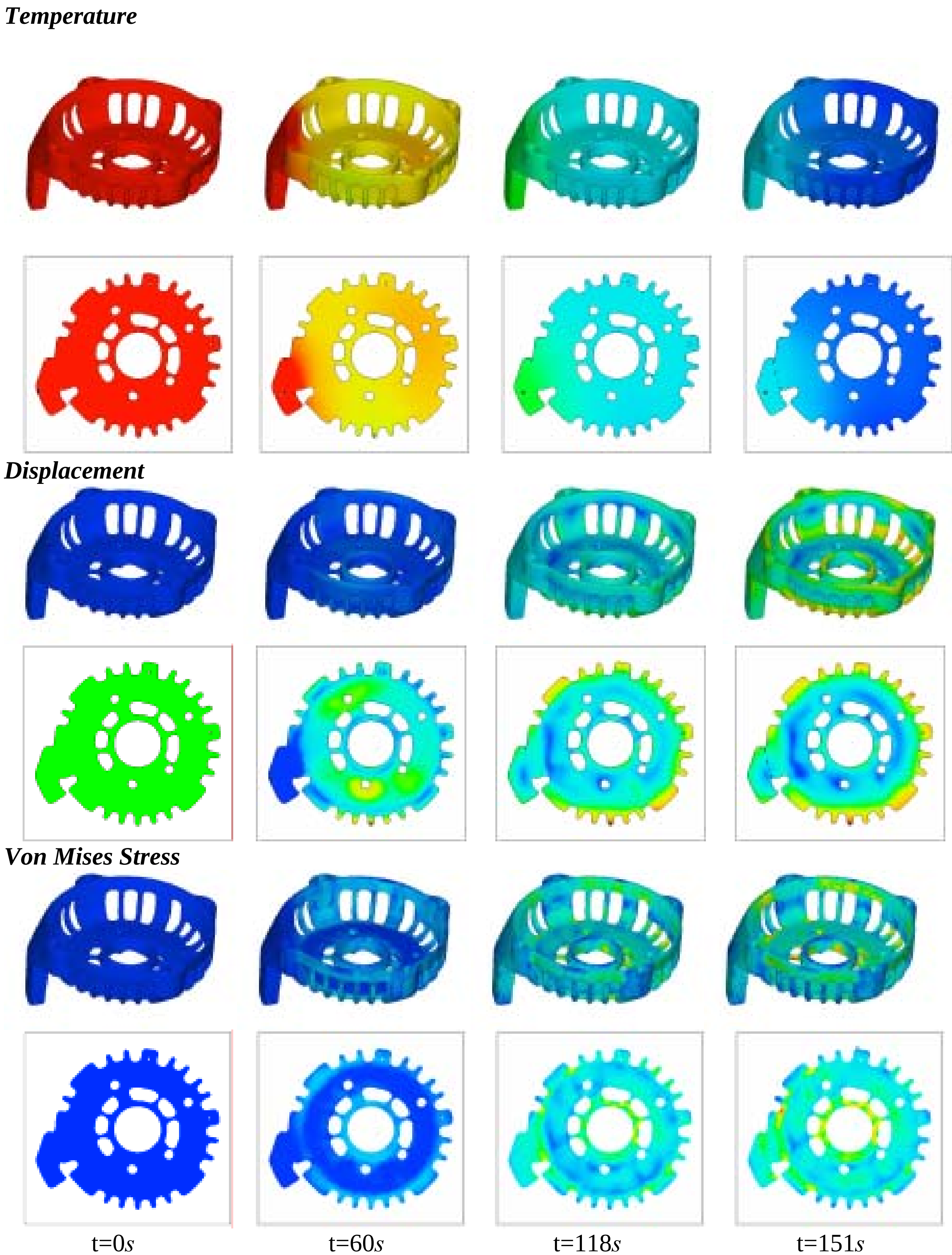

Figure 6. Results of thermal stress development during unconstrained solidification of aluminum alternator housing; the surface of the solidifying metal is able to deform and translate freely. Both two- and three-dimensional results are shown; the 2-D results are of a horizontal plane at z=3.504*cm* below the top of the part.

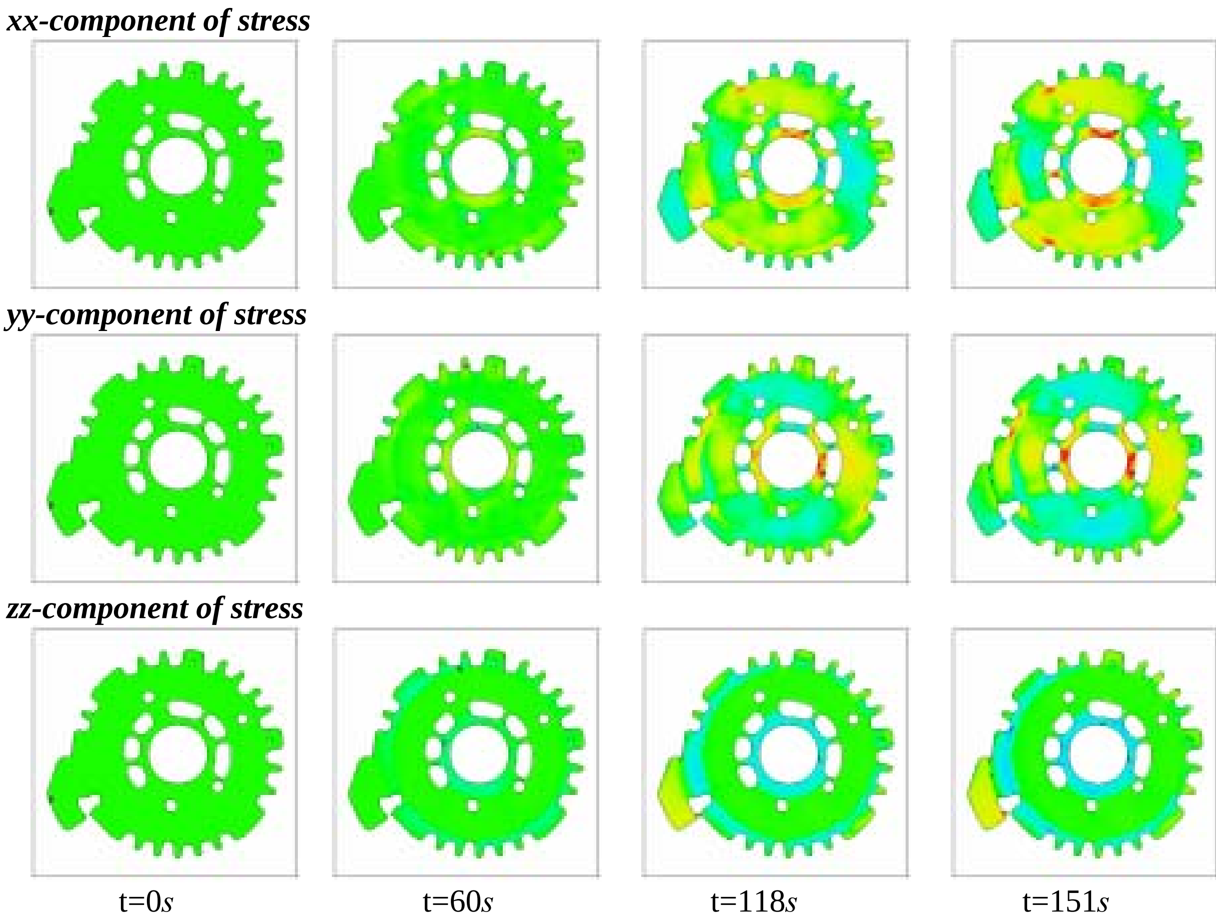

Figure 7. Results for unconstrained solidification showing stretching (or squeezing) along each of the three Cartesian directions. Red and blue indicate regions being stretched and squeezed, respectively. Green regions are relaxed. The plots are of a horizontal plane at z=3.504*cm* below the top of the part. In these plots, x to the right, y is to the top, and z is out of the page.

Figure 6 shows three- and two-dimensional plots of the evolution of this simulation from 0 to 151 seconds. The plots of temperature (the color scale ranges from 425*K* to 800*K*) show that, once again, the last region of the part to cool is within thick mounting arm shown to the left. When compared to the case where the part is cast within a solid mold, the cooling rate is somewhat quicker. The plots of displacement magnitude (color scale ranges from 0 to 0.39*mm*), not shown for the rigid mold casting (because the displacement is largely prescribed), show the greatest deformation occurs in the thin structures. This makes sense, because it is here that the material is least confined, allowing deformation and the relaxation of the elastic stress. As would be predicted, the magnitude of elastic stress (the Von Mises stress) shows the lowest stress in these structures, with the greatest magnitude resulting in the ring-like structures where shrinkage is confined by geometry. The color scale for the Von Mises stress here is 0 $dynes/cm^2$ (blue) to $-2.5\times10^8 dynes/cm^2$ (red).

Figure 7 shows two-dimensional plots of the normal components of elastic stress. Both the x- and y-direction plots show significant residual tension in the ring structure at the bottom of the housing, as well as the ring-like upper region of the part. The circular geometry of these structures, when confined by the remainder of the part, limits the deformation, thus causing frustrated shrinkage. In the z-direction, the only region of significant residual stress is in the thick mounting arm, where the large volume of material shrinks at different rates. Note, however, that the residual stress is far smaller than that which occurred during solidification within the rigid mold.

Remarks

A fully three-dimensional, transient model to simulate the effects of shrinkage during solidification of molten materials has been included into ***FLOW-3D***®. Such shrinkage is an important consideration during the casting of metals, as the stresses that develop during the solidification phase may remain at the completion of the casting as residual stresses. These residual stresses can compromise the integrity of the part or worse, result in cracks or structural defects that render the part worthless. ***FLOW-3D***® can now, with an accurate rendition of the geometry and material properties, predict the regions of the part with the greatest residual stress, as well as the type and orientation of this stress. This information allows engineers to modify the geometry, process and/or material properties to alleviate these residual stresses.

References

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4. Hattel, J.H. and P.N. Hansen, A control volume-based finite difference method for solving the equilibrium equation in terms of displacements. *Appl. Math. Modelling*, **19**, 210-243, 1995.