Three-Dimensional Anisotropic Thermo-Viscous- Elastic Residual Stress Model

In Moldflow 2017 R2, a three-dimensional anisotropic thermo-viscous-elastic residual stress model is developed and implemented for improving 3D shrinkage and warpage prediction. It has been shown from the validation cases that the residual stress model predicts better shrinkage, warpage and molded-in residual stresses than the generic shrinkage model.
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Introduction

Three-dimensional (3D) anisotropic thermo-viscous-elastic residual stress model is a shrinkage model to calculate initial stresses as the driving force for the shrinkage and warpage of an injection-molded plastics part in a 3D solution. In Moldflow 2017 R2, the model is developed and implemented for improving 3D shrinkage and warpage prediction.

3D Residual Stress Model

Injection molded parts are constrained in the mold during the process, and the shrinkage of the solidified layers is prevented. There are several mechanisms preventing shrinkage of the solidified layers while the part is still in the mold. Firstly, adhesion to the mold walls restrains (at least the outer skin of) the solid layers from moving, and secondly, the newly formed solid surface will be kept fixed by the stretching forces of the melt pressure. In addition, geometric constraints also play a critical role of preventing shrinkage of the solidified layers while still in the mold. In the 3D residual stress model, the part is assumed to be fully constrained in the mold, namely no part-mold detachment and no in-mold shrinkage are considered.

In-cavity residual stresses are built up during solidification. Due to the nature of constrained quenching, the residual stresses distribution is largely determined by the varying pressure history, coupled with the frozen layer growth. Though the flow-induced residual stress is critical for mechanical and optical properties, it is usually at least one order of magnitude smaller than the thermally-induced and pressure-induced residual stresses. Therefore the flow-induced residual stress is excluded from the model, i.e. only thermally-induced and pressure-induced residual stresses are considered.

In the 3D thermo-viscous-elastic residual stress model, linear elastic behavior is assumed in the solidified part and purely viscous behavior in the melt. For unfilled materials, two elastic models are used: If the mechanical property is isotropic, the isotropic material model is used. If the mechanical property is not isotropic, transversely isotropic material model is used with the frozen flow orientation as the major principal axis. For fiber-filled materials, orthotropic material model is used with the principal axes and mechanical properties obtained from the fiber simulation, and its stress-strain relationship is as follows:

\[
\Delta = \frac{1 - \nu_{xy} \nu_{yx} - \nu_{xz} \nu_{zx} - \nu_{yz} \nu_{zy} - 2 \nu_{xy} \nu_{yx} \nu_{zx}}{E_x E_y E_z} \]

\[
\begin{bmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{zz} \\
\tau_{xy} \\
\tau_{yz} \\
\tau_{zx}
\end{bmatrix} = \begin{bmatrix}
\frac{1 - \nu_{xy} \nu_{yx}}{E_x} & \frac{\nu_{xy}}{E_x} & \frac{\nu_{yx}}{E_y} & 0 & 0 & 0 \\
\frac{\nu_{xy}}{E_x} & \frac{1 - \nu_{xy} \nu_{yx}}{E_y} & \frac{\nu_{yx}}{E_y} & 0 & 0 & 0 \\
\frac{\nu_{yx}}{E_x} & \frac{\nu_{xy}}{E_y} & \frac{1 - \nu_{xy} \nu_{yx}}{E_z} & 0 & 0 & 0 \\
0 & 0 & 0 & G_{xy} & 0 & 0 \\
0 & 0 & 0 & 0 & G_{yz} & 0 \\
0 & 0 & 0 & 0 & 0 & G_{zx}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{xx} \\
\varepsilon_{yy} \\
\varepsilon_{zz} \\
\gamma_{xy} \\
\gamma_{yz} \\
\gamma_{zx}
\end{bmatrix}
\]
With these assumptions, the thermo-viscous-elastic residual stress model can be implemented in a relatively simplified way. Basically the residual stresses include the initial stresses from recorded frozen pressure at each node and the initial stresses due to isotropic or anisotropic thermal shrinkage.

\[
\begin{align*}
\{\sigma_g\} &= -[D_g][\{\varepsilon_{g0}\}] + \{\sigma_{g0}\} \\
[D_g] &= [T_e^T][D_e][T_e] \\
[\{\varepsilon_{g0}\}] &= [T_e^{-1}][\{\varepsilon_{i0}\}]
\end{align*}
\]

"g" means global coordinate system, and "T" means local coordinate system. 
\([T_e]\) is the transformation matrix from global strains to local strains. 
\([D]\) represents the stress-strain relationship matrix. 
\(\{\sigma_{g0}\}\) is the initial stress, i.e. pressure at freeze. 
\(\{\varepsilon_{g0}\}\) is the initial strain from zero pressure state or transitional temperature to room temperature.

Once the mold boundary constraints are released, warpage and molded-in residual stress results are calculated. As all variables refer to the initial configuration at time zero in the solution scheme, the incremental initial strains or stresses can be naturally implemented. The following equilibrium equation is solved iteratively at time \( t + \Delta t \), for iteration \( k=1,2,3,... \)

\[
\int_V C_{ijrs} \Delta e_{ij}^{(k)} \delta \Delta e_{ij}^{(k-1)} dV + \int_V t+\Delta t S_{ij}^{(k-1)} \delta \Delta h_{ij}^{(k)} dV = \\
- \int_V t+\Delta t S_{ij}^{(k-1)} \delta \Delta e_{ij}^{(k-1)} dV + \int_V C_{ijrs} \Delta e_{rs}^{in(k)} \delta \Delta e_{ij}^{(k-1)} dV
\]

where \( C_{ijrs} \) is the stress-strain tensor, \( \Delta e_{ij}^{(k)} \) and \( \Delta h_{ij}^{(k)} \) are the linear and nonlinear incremental strain tensors for iteration \( k \), \( \delta \Delta e_{ij}^{(k)} \) and \( \delta \Delta h_{ij}^{(k)} \) are the linear and nonlinear incremental strain tensors corresponding to virtual incremental displacement, \( \Delta e_{rs}^{in(k)} \) is the incremental initial strain tensor for iteration \( k \), and \( t+\Delta t S_{ij}^{(k-1)} \) is the second Piola-Kirchhoff stress tensor after iteration (k-1) at time \( t + \Delta t \).

The 3D thermo-viscous-elastic residual stress model currently supports all thermoplastics processes, including thermoplastic injection molding, thermoplastic overmolding, gas-assisted injection molding and thermoplastic microcellular injection molding. It does not support thermosets processes in AMI2017 R2.

**Running 3D Residual Stress Analysis in Moldflow 2017 R2**

The 3D anisotropic thermo-viscous-elastic residual stress model is termed as “uncorrected residual stress model” in the UI option for 3D shrinkage model, which is available in the “Shrinkage Properties” tab under the “Thermoplastics material” dialogue as shown below. The user can use this option to switch between the generic shrinkage model and the uncorrected residual stress model. The default option in AMI2017R2 is Generic Shrinkage model.
An analysis sequence that includes “Fill+Pack+Warp” or “Cool+Fill+Pack+Warp” analyses for a 3D process should be selected. If this model is selected and run, two messages will be shown in the analysis log, one under the flow section: “Residual stress calculation: ON”; and the other shown in the warp section: “Residual stress model is used.”

New Results with 3D Residual Stress Model

The following results are generated with the 3D uncorrected residual stress model:

1. “Pressure at Freeze”: shows the pressure value when the node solidifies during the flow analysis. It is closely related to the pressure and temperature history in the flow analysis. It can be used as an indicator of nodal shrinkage variance. High nodal value of “Pressure at freeze” suggests less shrinkage at the node.

Figure 1. “Pressure at freeze” result
2. “Stress tensor (warp)”: is a tensor plot at the element level that shows the molded-in residual stress (after deformation) in the part;

![Stress tensor (warp) plot](image)

**Figure 2. Molded-in residual stress result**

3. “Strain tensor (warp)”: is a tensor plot at the element level that shows the strain status after deformation;

![Strain tensor (warp) plot](image)

**Figure 3. Strain tensor result**
4. "Maximum shear stress (warp)" shows the maximum shear stress value resulted in the part after deformation;

![Figure 4. Maximum shear stress result](image)

5. "Stress, Mises-Hencky (warp)" shows the Mises-Hencky stress value resulted in the part after deformation;

![Figure 5. Mises-Hencky Stress result](image)
Warpage Validation

3D anisotropic thermo-viscous-elastic residual stress model has been extensively verified and validated through many real-world cases. Simulation results of three injection-molded parts are presented in this report to illustrate its performance.

Case 1: Moldflow Conformal Cooling Box

3D printing of molds has enabled the production of complex cooling systems that conform to the shape of the part. Experiments were conducted on a simple 2mm thick box with conformal channels (Figure 6). The parts were produced with four combinations of the moving and fixed mold halves.

![Figure 6. Part and combined cooling circuit](image)

A sequence of “Cool(FEM)+Fill + Pack + Warp” analyses were run to predict the final box shape. The material is Ultramid B3WG6 BK00564 from BASF, and the RSC fiber orientation model is chosen for the analysis. The simulation and measured results were compared. The larger inward deflection at the longer wall section is plotted for each condition in Figure 7. In this figure, the mean deflection of the four parts from experiments is shown as the height of the blue column, with error bars denoting the 95% confidence interval based on its variation.
As expected, the largest deflection occurs when the moving half that forms the inside of the box is hotter than the fixed half. Conversely, the smallest deflection occurs when the temperatures are reversed, i.e. inside is cooler than the outside. When both mold halves are at the same temperature (80 or 95°C) the deflections are at similar levels.

It can be seen that the predicted deflections using the 3D residual stress model (Green columns) are within the measured deflections 95% confidence interval for each mold temperature condition. The predicted warpage also follows the trend that the amount of deflection is driven by the temperature difference between the mold halves. Generic shrinkage model predicted right warpage shapes as well, while its magnitude accuracy is not as good as what the 3D residual stress model predicted.

**Case 2: Rhodia Box**

Rhodia box model is a typical thin-walled part with an average wall thickness of 1.5 mm (by courtesy of Rhodia Engineering Plastics of France). The processing conditions are listed in Table 1. Figures 8 and 9 shows the predicted warpage shape using the generic shrinkage model and residual stress model respectively. Both models predicted the right warpage pattern. The predicted long edge deflection from both models are smaller than the measured value 0.6mm, with 0.390mm from the generic shrinkage model and 0.485 mm from the residual stress model, which suggests that the 3D residual stress model predicted a better warpage magnitude.
Table 1. Processing condition for Rhodia box model

<table>
<thead>
<tr>
<th>Material Type</th>
<th>Technyl A218 V30 Natural, Rhodia Engineering Plastics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mold temperature</td>
<td>80.0 Degree C</td>
</tr>
<tr>
<td>Melt Temperature</td>
<td>290.0 Degree C</td>
</tr>
<tr>
<td>Injection Time</td>
<td>0.8 Seconds</td>
</tr>
<tr>
<td>Packing Profile</td>
<td>77.77 MPa for 5 Seconds</td>
</tr>
<tr>
<td>Total Cooling Time</td>
<td>4.0 Seconds</td>
</tr>
<tr>
<td>Circuit Coolant Temperature</td>
<td>65 Degree C</td>
</tr>
</tbody>
</table>

Figure 8. Simulated warpage result using generic shrinkage model
Case 3. Rectangular Strip

The last case is a rectangular strip part, molded of an ABS material, Novodur P2X of Bayer (Figure 10). The processing condition and measurement of the residual stresses with the layer removal method were reported in detail in reference [3]. The mold cooling was slightly asymmetrical, with wall temperatures as 325K/321K.
Figures 11 and 12 show the calculated and measured values of the final gapwise molded-in residual stress profile distribution at a position between P2 and P3, where the stress measurement bars were cut out. It can be seen that the 3D residual stress model predicted the right gapwise residual stress pattern, and good residual stress magnitudes along the thickness except surface layers. In addition, the model also correctly predicted the slightly asymmetrical stress distribution due to the slightly asymmetrical cooling. Please note that molded-in residual stress results are available only when the uncorrected residual stress is selected for the 3D shrinkage model option in AMI2017 R2.

Figure 11. Molded-in residual stress profile in parallel direction

Figure 12. Molded-in residual stress profile in perpendicular direction
Concluding Remarks

The 3D anisotropic thermo-viscous-elastic residual stress model has been developed to improve shrinkage and warpage prediction. It has been shown from the validation cases that this solution performs better than the existing generic shrinkage model, and predicts better shrinkage, warpage and molded-in residual stresses.

References

