ANISOTROPIC THERMO-VISCOUS-ELASTIC RESIDUAL STRESS MODEL FOR WARP SIMULATION OF INJECTION MOLDED PARTS

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Abstract

The residual stresses in injection molding process are developed due to the restriction of thermal contraction during the cooling, coupled with the frozen layer growth with the varying pressure history. The stress relaxation behavior of plastic materials also complicates the stress field. A thermo-viscoelastic model is a natural choice for predicting the residual stress in the injection molding process, but it is computationally very expensive and requires materials’ relaxation spectrum data which are not readily available in most of material databases. This study used a simplified anisotropic thermo-viscous-elastic model to calculate the residual stress development in three-dimensional simulation of injection molding process. The validation cases showed that the proposed model is able to predict the final shrinkage, warpage and molded-in residual stresses reasonably well.

Introduction

Plastic injection molding simulation provides a tool that helps manufacturers to reduce the need for costly physical prototypes, avoids potential manufacturing defects, and helps bring innovative products to market faster [1]. The truely three-dimensional solution on the solid models created by part designers is a natural choice for considering complex three-dimensional effects in the injection molding simulation [2],[3]. The residual stresses, shrinkage and warpage prediction are the key aspects of the simulation, particularly for high precision components with a tight dimension tolerance.

It is well known that the flow-induced residual stress is critical for mechanical and optical properties, but 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 normally excluded from the shrinkage and warpage simulation.

Due to the nature of constrained quenching, the thermally-induced and pressure-induced residual stresses in injection molding process are developed due to thermal contraction during the cooling, coupled with the frozen layer growth with the varying pressure history. The stress relaxation behavior of plastic materials also complicates the stress field. The thermo-viscoelastic modelling is a natural choice for predicting the residual stress in the injection molding process [4], but it is computationally very expensive and requires the relaxation spectrum data of the molding material, which are not readily available in most of material databases. This study uses a simplified anisotropic thermos-viscous-elastic model to calculate the residual stress development in three-dimensional simulation of injection molding process. The validation cases showed that the proposed model can predict the final shrinkage, warpage and molded-in residual stresses reasonably well.

Simulation Technology

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 prevents (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-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. The in-mold residual stress will relax a certain amount depending on the temperature history during cooling, and it can only be predicted by the thermo-viscoelastic model. The constitutive equation can be written as

$$\sigma_{ij}(t) = \int_{0}^{\tau} C_{ijrs} \left( \varepsilon_{ij}(t) - \varepsilon(\tau) \right) \left( \frac{\partial \varepsilon_{rs}}{\partial \tau} - \alpha_{rs} \frac{\partial T}{\partial \tau} \right) d\tau$$ (1)

Where $C_{ijrs}$ is the viscoelastic relaxation modulus, $\sigma_{ij}(t)$ is the stress tensor, $\varepsilon_{ij}$ is the strain tensor, $t$ is time, $T$ is temperature, and $\varepsilon(\tau)$ is a pseudo-time scale defined as

$$\varepsilon(\tau) = \int_{0}^{\tau} \frac{\partial \tau}{\partial \tau'} d\tau'$$ where $\alpha_{rs}$ is the time temperature shift factor that accounts for the effect of temperature on material
response. \( \alpha \) is the tensor of thermal coefficients of expansion.

The thermo-viscoelastic model requires material’s relaxation spectrum data which are not readily available for vast majority of materials. In fact, there are some complexities related to the viscoelastic data. The relaxation function may depend on the internal structures which themselves are in turn affected by processing conditions – particularly for those systems involving semi-crystalline materials and phase change. The exact relation between the internal structures and the relaxation functions is largely unknown. On the other hand, if the Deborah number (defined here as the ratio between the relaxation time of the material and cooling time) is much larger than one, the thermo-viscous-elastic model is able to give a good prediction of thermally and pressure-induced residual stress \([5], [6], [7]\) and to provide considerable simplification.

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

\[
\begin{bmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{zz} \\
\tau_{xy} \\
\tau_{yz} \\
\tau_{zx}
\end{bmatrix} =
\begin{bmatrix}
1 - \nu_{xx} \nu_{yy} & \nu_{xx} + \nu_{yy} & \nu_{xx} & 0 & 0 & 0 \\
\nu_{yy} + \nu_{yy} & 1 - \nu_{yy} \nu_{yy} & \nu_{yy} & 0 & 0 & 0 \\
\nu_{xx} + \nu_{yy} & \nu_{yy} & 1 - \nu_{xx} \nu_{yy} & 0 & 0 & 0 \\
0 & 0 & 0 & G_{xy} & 0 & 0 \\
0 & 0 & 0 & 0 & G_{yz} & 0 \\
0 & 0 & 0 & 0 & 0 & G_{zx}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{xx} \\
\varepsilon_{yy} \\
\varepsilon_{zz} \\
\gamma_{xy} \\
\gamma_{yz} \\
\gamma_{zx}
\end{bmatrix}
\]

(2)

\[\Delta = \frac{1 - \nu_{xy} \nu_{yx} - \nu_{yx} \nu_{xx} - \nu_{xx} \nu_{xy} - 2 \nu_{xy} \nu_{yx}}{E_x E_y E_z} \]

(3)

The part is assumed to be fully constrained in the mold, namely no part-mold detachment and no in-mold shrinkage are considered. 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.

\[\sigma_g = - [D_g] \{\varepsilon_g0\} + \{\sigma_g0\} \]

(4)

\[D_g = [T_e^T] [D_e] [T_e] \]

(5)

\[\varepsilon_g0 = [T_e^{-1}] \{\varepsilon_{i0}\} \]

(6)

“g” means global coordinate, and “l” means local coordinate system. \([T_e]\) is the transformation matrix from global strains to local strains. \([D]\) represents the stress-strain relationship matrix. \([\sigma_0]\) is the initial stress (pressure at freeze), and \([\varepsilon_{i0}]\) is the initial strains from zero pressure state or transition 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 \(k=1,2,3,...\)

\[
\int_V C_{ijr} \Delta \varepsilon^{(k)}_{ij} \delta \varepsilon^{(k-1)}_{ij} dV + \int_V \gamma_{ij} S^{(k-1)}_{ij} \Delta \eta^{(k)}_{ij} dV = \int_V C_{ijr} \Delta \varepsilon^{(k-1)}_{ij} \delta \varepsilon^{(k-1)}_{ij} dV + \int_V C_{ijr} \Delta \varepsilon^{(k-1)}_{ij} \delta \eta^{(k-1)}_{ij} dV
\]

(7)

where \(C_{ijr}\) is the stress-strain tensor, \(\Delta \varepsilon^{(k)}_{ij}\) and \(\Delta \eta^{(k)}_{ij}\) are the linear and nonlinear incremental strain tensors for iteration \(k\), \(\delta \varepsilon^{(k)}_{ij}\) and \(\delta \eta^{(k)}_{ij}\) are the linear and nonlinear incremental strain tensors corresponding to virtual incremental displacement, \(\Delta \varepsilon^{(k)}_{ij}\) is the incremental initial strain tensor for iteration \(k\) and \(\gamma_{ij} S^{(k-1)}_{ij}\) is the second Piola-Kirchhoff stress tensor after iteration (k-1) at time \(t + \Delta t\). The anisotropic thermo-viscous-elastic residual stress model can be easily extended for thermoplastic over-molding, gas-assisted injection molding and thermoplastic microcellular injection molding processes.

The 3D warpage simulation is computationally expensive, even with a fast and robust parallelized algebraic multigrid preconditioned conjugate gradient (AMG-CG) equation solver in both flow and warpage analyses. The high gradient variation of velocity and temperature in gap-wise directions necessitate the use of many layers of tetrahedral elements across the part thickness in the flow simulation. Normally a good-quality anisotropic flow mesh with 10 or more layers of 4-node tetrahedral elements is used for three-dimensional flow simulation. However, Due to the shear locking problem of 4-node structural elements, they should be upgraded to second-order elements to get reliable warpage simulation results for typical thin-walled injection molded parts.
Alternative approach is to use dual mesh, in which 2 layers of 10-node tetrahedral elements are used for the warpage simulation of thin-walled parts. The Young’s modulus, Poisson’s ratios, thermal expansion coefficients of the composite material predicted from flow analysis, fiber analysis and the in-cavity residual stress calculated from anisotropic thermo-viscous-elastic residual stress model are mapped from the dense flow mesh to the coarse warpage mesh. The dual mesh approach is very effective, and recommended for the warpage simulation of typical thin-walled plastic parts[8].

**Numerical Examples**

A three-dimensional (3D) anisotropic thermo-viscous-elastic residual stress model is developed and implemented to calculate initial stresses as the driving force for the shrinkage and warpage of an injection-molded plastics part in a 3D solution. Three validation cases are presented to show the comparison between the experiment and simulation for the molded-in residual stresses, shrinkage and warpage results.

**Case 1. Rectangular Strip**

The case is a rectangular strip part, molded of an ABS material, Novodur P2X of Bayer (Figure 1). The processing condition and measurement of the residual stresses with the layer removal method were reported in detail in reference [6]. The mold cooling was slightly asymmetrical, with wall temperatures as 51.85°C/47.85°C. The simulation is run using the thermo-viscous-elastic residual stress model.

![Figure 1. Rectangular strip mold (dimensions are in mm)](image)

Figure 2 shows the calculated and measured values of the final gap-wise 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 gap-wise residual stress pattern, and good residual stress magnitudes along the thickness except in surface layers. In addition, the model also correctly predicted the slightly asymmetrical stress distribution due to the slightly asymmetrical cooling.

![Figure 2. Molded-in residual stress profile in parallel direction (unit: MPa)](image)

**Case 2. Conformal Cooling Box**

Case 2 is the conformal cooling box which was molded in Autodesk Material Laboratory, Australia. Conformal cooling channels are internal cooling channels made to a shape that follows the precise geometry of the part in the mold. Modern injection mold manufacturing technologies,
such as 3D printing, allow conformal cooling channels to be easily manufactured. Experiments were conducted on a simple 2mm thick box with conformal channels (Figure 4). The parts were produced with four combinations of the moving and fixed mold halves [9].

Figure 4. Part and combined cooling circuit

The part model is meshed into 2,285,777 tetrahedral elements, and the mold model into 3,303,544 tetrahedral elements. A sequence of “Cool(FEM) + Fill + Pack + Warp” analyses were run to predict the final box shape.

The material is PA6 with 30% glass fiber, Ultramid B3WG6 BK00564 from BASF and the Reduced Strain Closure (RSC) fiber orientation model was 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 5. In this figure, the mean deflection of four parts from experiments is plotted as 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 anisotropic thermos-viscous-elastic residual stress model (Gray 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.

Case 3. Toaster Housing

The Bayer toaster housing model is made of Pocan T &323, Lanxess, PBT with 20% glass fiber. The trial mold showed that the part is warped significantly under a certain processing condition (Figure 6). “Fill + Pack + Warp” analyses were run to predict the final warped shape, and the Moldflow Rotational Diffusion (MRD) fiber orientation model was used in the simulation.

The buckling analysis showed that the part buckled after ejection from the mold. The large deflection analysis option was activated for tracing the post-buckling response [10]. The warpage prediction from 3D anisotropic thermos-viscous-elastic residual stress model is shown in figure 7. The predicted warpage pattern is the same as that in the
trial mold. The predicted warpage magnitude is 12.22mm which is quite close to the measured deflection 13.00 mm.

Figure 7. Simulated warpage result (large deflection)

Summary

The 3D anisotropic thermo-viscous-elastic residual stress model has been developed. It does not require material’s viscoelastic data as the thermo-viscoelastic model does. It has been demonstrated in the validation cases that this simplified solution can predict the shrinkage, warpage and molded-in residual stresses reasonably well.

References