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Simulation of Thermally Induced Stress and Warpage in Injection Molded Thermoplastics

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Abstract: Thermally induced stress and the relevant warpage cause by inappropriate mold design and processing conditions are problems that confounded the overall success of injection molding. A thermorheologically simple thermo-viscoelastic two-dimension material model is used to simulate the residual stress and warpage within injection molded parts generated during the cooling stage of the injection molding cycle. The initial temperature field corresponds to the end of the filling stage. The fully time-dependent algorithm is based on the calculation of the elastic response at every time step. Numerical results are discussed with respect to temperature and pressure.

Key words: thermal residual stress; warpage; injection molding

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Introduction

Injection molding is one of the most important polymer processing methods for producing plastic parts[1]. However, there are still several problems that confound the overall success of the injection molding process, especially residual stress and warpage of parts caused by inappropriate mold design and/or processing conditions. Residual stress in injection molded parts stems from two main sources[2]: frozen-in flow induced stress and thermally induced stress. Frozen-in flow induced stress is caused by viscoelastic flow of the polymer during the filling and postfilling stages of the injection molding process. Thermally induced stress develops during cooling stage, both inside the mold and outside mold. The residual thermally induced stress is about at least one order of magnitude larger than the frozen-in flow induced stress: O(10) MPa opposed to O(1) MPa[3]. The warpage of an injection molded part can be seen as primarily due to uneven residual stress within the product. Severval numerical models have been proposed to simulate the formation for thermally induced residual stress. The Kee, Roger, and Woo (LRW) model is widely used by various researchers to predict and simulate the residual stress in different materials including polymers[4]. Compared to the research efforts on the prediction of residual stress, not as much work has been done in the area of warpage simulation and prediction. Recently, S. J. Liu uses viscoelastic phase transformation model to predict warpage[5].

In the present paper, we first explain the method that we have used for calculating the injection molded parts temperature field. Next, we examine the set of equations for solving the transient stresses, a special emphasis is put on the recurrence formulae for calculating time-dependent stress. Third, we obtain the deformation of the part based on thermoelastic model. At last, a numerical example is given.

1 Mathematical Modeling

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Biography: LI Hai-mei (1969-), female, born in Shenyang city, Liaoning province, associate professor of Zhengzhou University of Technology, Ph.D., research interests: polymer processing simulation.

1.1 Transient heat conduction analysis

As the polymer cools in mold cavity, the calculation of thermally induced residual stress first requires the transient temperature gradients to be evaluated. Since many injection molded parts are relatively thin compared to their surface area, the heat conduction equation is given as follow[6]

$$\rho C_p \frac{\partial T}{\partial t} = k \nabla^2 T . \tag{1}$$

where ρ is the density, C_p is the heat capacity, and k is the thermal conductivity of the polymer.

As initial conditions for the cooling stage, we use the final temperature field of filling. There are two ways to assign the boundary conditions for the heat conduction problem. One is to maintain a constant temperature if the mold cooling channels are relatively far away from the cavity surface compared to the thickness dimension of the cavity, while the other is to calculate by cooling analysis of mold. The temperature field is represented by means of 4 – node isoparametric shape functions. After spatial and time discretization for heat eqs. (1), we use the following scheme[7]

$$\left(\zeta[K] + \frac{[C]}{\Delta t}\right)\{T\}_t = \zeta\{R\}_t + (1-\zeta)\{R\}_{t-\Delta t} + \left\{\frac{[C]}{\Delta t} - (1-\zeta)[K]\right\}\{T\}_{t-\Delta t}, \tag{2}$$

with

$$[K] = \iint_{A_e}[B_\theta]^{\mathrm{T}} k [B_\theta]\,\mathrm{d}A + \int [N]^{\mathrm{T}}\alpha[N]\,\mathrm{d}s \;;$$

$$[C] = \iint_{A_e}[N]^{\mathrm{T}}\rho C_p[N]\,\mathrm{d}A \;;$$

$$\{R\} = \int_{\Gamma_2}[N]^{\mathrm{T}} q\,\mathrm{d}s + \int_{\Gamma_3}[N]^{\mathrm{T}}\alpha T_c\,\mathrm{d}s \;,$$

where, ζ is an adjustable parameter of time, $[k]$ contains the effects of the third temperature boundary condition and the thermal conductivity; R contains the secondary and the third temperature boundary conditions. The numerical approach assumes that the effect of the heat transfer resistance in the gaps at the mold – polymer interface can be neglected.

To deal with latent of phase change, the material enthalpy is defined as[8,9]

$$H = \int_{\Gamma f}^{T} C_p\,\mathrm{d}T = \begin{cases} C_p(T - T_f) + L & (T \geqslant T_f) \\ C_p(T - T_f) & (T < T_f) \end{cases}, \tag{3}$$

where T_f is the melt temperature, L is the latent of phase change. The thermally dependent specific heat capacity, C_p is related to the enthalpy, H according to ref. [6]

$$C_p(T) = \frac{\mathrm{d}H}{\mathrm{d}T} . \tag{4}$$

Therefore, the specific heat capacity is highly temperature dependent especially in the phase element. The numerical scheme employs the enthalpy data to obtain an apparent specific heat capacity of every element of phase change, $\langle C_p \rangle$ according to ref. [9]

$$\langle C_p \rangle \doteq \frac{\mathrm{d}H}{\mathrm{d}T} = \frac{\frac{\partial H}{\partial x}\cdot\frac{\partial T}{\partial x}}{(\partial T/\partial x)^2} + \frac{\frac{\partial H}{\partial y}\cdot\frac{\partial T}{\partial y}}{(\partial T/\partial y)^2}, \tag{5}$$

In the developments below, we assume that tie nodal temperatures are known throughout the cooling stage.

1.2 Thermally induced residual stress analysis

We assume that the cooling polymer behaves as an isotropic thermorheologically simple sold. Let $S_{i,j}$, $e_{i,j}$ denote the deviatoric components of the stress and strain tensors, respectively, while S, e denote their spherical part. The constitutive equations are given as follows[10]

$$\begin{cases} S_{i,j} = \int_0^t G_1(\zeta - \zeta')\,\mathrm{d}e_{i,j}, \\ S = \int_0^t G_2(\zeta - \zeta')\,\mathrm{d}[e(t') - e_{th}(t')] . \end{cases} \tag{6}$$

In these equations, $\zeta(t)$ is a modified time scale while e_{th} is the thermal strain to be defined below. The modified time scale $\zeta(t)$ is given by the following equation

$$\zeta(t) = \int_0^t \Phi(T)\,\mathrm{d}\tau , \tag{7}$$

with $\Phi(T)$ is the shift function, written as follows[11]

$$\lg\Phi = \frac{c_1(T - T_r)}{c_2 + T - T_r} , \tag{8}$$

in eqs. (8), c_1, c_2 are material constants, and T_r is the reference temperature.

The thermal strain e_{th} in eqs. (6) is given as

$$e_{th} = \int_{T_r}^{T} \alpha(T')\,\mathrm{d}T' , \tag{9}$$

where, α denotes the thermal dilatation coefficient, calculated by $P - V - T$ relations[11]

$$\alpha(T) = \frac{\partial \ln V(P,T)}{\partial T} \tag{10}$$

with

$$\begin{cases} V(P,T) = V(0,T)[1 - 0.0894\ln(1 + P/B(T))], \\ V(0,T) = \alpha_1 + \alpha_2 T, \\ B(T) = B_0\exp(B_1 T), \\ T_g = T_r + sP, \end{cases} \tag{11}$$

where, $a_1, a_2, B_0, B_1, T_r, s$ are material constants. If $T < T_g$, the constants of a_1, a_2, B_0, B_1 are given solid state values, otherwise given liquid state values.

Eqs.(7) to eqs.(11) fully define the set of constitutive equations for solving thermoviscoelastic problems with structural relaxation. For simplifying the system of equations, it is assumed that

$$\begin{cases} G_1(t) = 2\mu\varphi(t); \\ G_2(t) = 3\kappa\varphi(t), \end{cases} \tag{12}$$

where 2μ and 3κ denote the values of G_1, G_2 at $t = 0$, respectively. We decompose the function $\varphi(t)$ as a sum of m exponentials, i.e.

$$\varphi(t) = \sum_{k=1}^{m} g_k \exp(-t/\tau_k), \tag{13}$$

where, the τ_k are relaxation times and g_k are material constants. For each relaxation time, one may define partial stress $S_{i,j}^k$ and S^k given by equations similar to eqs.(6) with the appropriate relation functions. Using eqs.(12),(13), we get the recurrence formulae of thermoviscoelastic equations[10]

$$\begin{cases} S_{i,j}(t_{n+1}) = \sum_{k=1}^{m} Y_1^k S_{i,j}^{\ k}(t_n) + 2\mu\sum_{k=1}^{m} g_k Y_2^k \delta e_{i,j}; \\ S(t_{n+1}) = \sum_{k=1}^{m} Y_1^k S^k(t_n) + 3\kappa\sum_{k=1}^{m} g_k Y_2^k \delta(e - e_{th}), \end{cases} \tag{14}$$

where we have use the symbols

$$\begin{cases} Y_1 = \exp(-\Delta\zeta/\tau); \\ Y_2 = [1 - \exp(-\Delta\zeta/\tau)]\cdot(\tau/\Delta\zeta); \\ \delta e_{i,j} = e_{i,j}(t_{n+1}) - e_{i,j}(t_n); \\ \delta e = e(t_{n+1}) - e(t_n); \\ \delta e_{th} = e_{th}(t_{n+1}) - e_{th}(t_n), \end{cases} \tag{15}$$

Introducing the discretized constitutive eqs.(14) into the weak form of the equilibrium equations at time t, we obtain FEM scheme as following:

$$\sum_e [K]_e^{t_{n+1}} \delta u^{t_{n+1}} = \sum_e R_1 + \sum_e R_2, \tag{16}$$

$$\delta u^{t_{n+1}} = \{u\}_{t_{n+1}} - \{u\}_{t_n}, \tag{17}$$

$$[K]_e^{t_{n+1}} = \iint_A [B]^{\mathrm{T}}[D]\Big(\sum_{k=1}^{m} Y_2^{\ k} g_k\Big)[B]\,\mathrm{d}x\mathrm{d}y + \int_{\Omega_e} [B]^{\mathrm{T}}[D]\Big(\sum_{k=1}^{m} Y_2^{\ k} g_k\Big)[B]\,\mathrm{d}x\mathrm{d}y, \tag{18}$$

$$R_1 = \iint_A [B]^{\mathrm{T}}\delta\sigma_n \mathrm{d}x\mathrm{d}y + \int_{\Omega_e} -(-z)[B]^{\mathrm{T}}\cdot \delta\sigma_n \mathrm{d}x\mathrm{d}y\mathrm{d}z, \tag{19}$$

$$R_2 = \iint_A \Big(\sum_{k=1}^{m} Y_2^{\ k} g_k\Big)[B]^{\mathrm{T}}[D]\begin{Bmatrix}1\\1\\0\end{Bmatrix}\delta\varepsilon_{th}\mathrm{d}x\mathrm{d}y + \int_{\Omega_e}(-z)\Big(\sum_{k=1}^{m} Y_2^{\ k} g_k\Big)[B]^{\mathrm{T}}[D]\begin{Bmatrix}1\\1\\0\end{Bmatrix}\delta\varepsilon_{th}\cdot \mathrm{d}x\mathrm{d}y\mathrm{d}z. \tag{20}$$

The first term on the right hand of eqs.18 to 20 denotes the effect of mid-plane, and the second term denotes the effect of height direction.

To solute eqs.(16), the 4-node isoparametric shell element composed of plane element and bending element is used. By boundary conditions and FEM arithmetic we can get the restriction displacement, then get residual stress from restriction displacement. More details see ref.[12].

1.3 Warpage analysis

The analysis is based on thermal linear elastic model. The equilibrium equation for every time step, with R_T representing the thermal load and R_0 representing the thermally induced residual stress load is as follows[13]

$$\sum_e [K]_e \delta u = \sum_e R_T - \sum_e R_0, \tag{21}$$

$$[K_e] = \int_{\Omega e}[B]^{\mathrm{T}}[D][B]\mathrm{d}x\mathrm{d}y + \int_{\Omega e} z^2[B]^{\mathrm{T}}[D][B]\mathrm{d}x\mathrm{d}y\mathrm{d}z, \tag{22}$$

$$[R_T] = \int_{\Omega e}[B]^{\mathrm{T}}[D]\{\varepsilon_0\}\mathrm{d}x\mathrm{d}y + \int_{\Omega e} -z[B]^{\mathrm{T}}[D]\{\varepsilon_0\}\mathrm{d}x\mathrm{d}y\mathrm{d}z, \tag{23}$$

$$[R_0] = \int_{\Omega e}[B]^{\mathrm{T}}[D]\{\sigma_0\}\mathrm{d}x\mathrm{d}y + \int_{\Omega e} -z[B]^{\mathrm{T}}[D]\{\sigma_0\}\mathrm{d}x\mathrm{d}y\mathrm{d}z, \tag{24}$$

In warpage analysis, the thermal residual stress, $\{\sigma_0\}$ is calculated by residual stress analysis, treated as initial load of structural analysis. The thermal laod is obtained from temperature filed data.

2 Numerical Example

We consider the simple case of a disk plate with large lateral dimensions as compared to it is thickness. The material constants data in eqs.(13) for polystyrene are same as ref. [14]. The material constants of shift function in eqs. (8) and $P-V-T$ data in eqs. (11) can be found in ref. [11]. The mold and polymer material data for thermal analysis are given in ref. [15]. The initial temperatures conditions are $T(0) = 230$ ℃ and the boundary conditions of mold are taken to be T_{c1} and T_{c2}, $T_{c2} = T_{c1} + \Delta T$. $T_{c1} = 30$ ℃ and $T_{c1} = 50$ ℃, The processing conditions for numerical experiments are shown in table 1.

Table 1 Processing conditions for numerical experiments

ΔT/℃	44.4	33.3	22.2	11.1	0
P/MPa	0/2/4	–	0/2/4	–	0/2/4

Thermal analysis results of prediction temperature and residual stress can be seen ref. [12]. From the results, we know that when the cooling is asymmetric, the side in contact with the warmer mold plate exhibits lower levels of compressive stress than the cooler side, resulting in warpage toward the former. As the temperature imbalance increase, the core region does not exhibit as significant a change in stress level as the outer layer, resulting in a higher imbalance moment. Also we know that faster cooling rate ($T_{c1} = 30$ ℃) has higher stress level. As the pressure increase, the magnitude of the residual stress shows slightly decreasing trends.

The calculated curvatures of the PS part are shown in table 2 based on warpage analysis, which are in agreement with published experimental data[15].

Table 2 Calculated curvatures of the PS part

P/MPa	44.4 ℃	22.2 ℃
0	0.429	0.215
2	0.401	0.201
4	0.378	0.189

The results show that the temperature asymmetry is of principal importance in determining the deformities of the molded part. Secondary effects can be discerned due to change in holding pressure below a high - threshold level.

3 Conclusions

For the injection molding part studied in this article, temperature imbalance is found to be the primary factor determining warpage whereas the holding pressure below a certain threshold was of secondary importance. The theoretical schemes provide valid estimates of the curvature of the warpage part and also capture the trend in the variation with applied temperature asymmetry.

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注塑件成型尺寸质量预测的数值方法

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摘　要: 不均匀的热残余应力及其变形是注塑成型加工中常见的工程问题之一. 应用热流变简单材料的二维热粘弹本构方程得到的递推公式, 数值模拟了成型中的热残余应力及其翘曲变形, 并用数值实验讨论了温度、压力对注塑件残余应力及变形的影响, 发现温度变化不均匀是注塑件翘曲变形的最主要原因, 其影响远大于压力的作用, 与工程实验的结论一致.

关键词: 热残余应力; 翘曲; 注塑件