Optimum Design of Process Conditions to Minimize Residual Stress and Birefringence in Injection-Molded Parts

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ABSTRACT

In this paper, a theoretical study has been made to reduce the residual stress and birefringence in the injection-molded parts. An optimization program has been used to minimize the residual stresses and birefringence calculated from a simulation program. The thermally induced stress has been calculated using a linear viscoelasticity model. The flow stress and birefringence has been calculated using the Leonov's viscoelasticity model. This has been applied to the injection molding of a circular disc and a plate. The optimization has been done either by changing process variables while maintaining the mold temperature constant or by varying the mold-wall temperature with time. This study shows that significant reduction in residual stress and birefringence is possible through the optimization of processing conditions.

Keywords : Optimum design, Residual stress, Birefringence, Injection molding, Mold wall temperature

1. Introduction

Computer programs for the analysis of injection-molding processes are becoming more popular. Typically, these programs analyze the injection-molding process for the conditions that user specifies. However, more practical problems are concerned with finding molding conditions that satisfy some objectives, namely "inverse design problems". Such problems in injection molding include runner-balancing, mold design and determination of processing conditions for maximum productivity or quality.

Optimization technique is one of the most popular methods for solving inverse-design problems. In this approach, the goal of design is represented in terms of a mathematical objective function. The optimization technique is used to minimize (or maximize) this objective function. In injection molding, the objective function is typically either maximizing productivity (which often means minimizing the cycle time) or maximizing the quality of the product (for example, minimizing residual stress, birefringence). This technique has been used by Jong and Wang[6], Lee[8] and Kang et al. [7] to solve various inverse-design problems in injection molding. In particular, Jong and Wang[6] used an optimization technique to determine the runner dimensions which would balance the flow in each cavity connected to the runners. Lee[8] optimized process conditions and part design to minimize warpage in the injection-molded parts. Kang et al.[7] used an optimization technique to find the mold-wall-temperature history that would minimize the residual stresses in the injection molded part.

In this study, efforts have been made to minimize the residual stress or birefringence in the injection-molded part. First, this has been done by optimizing process conditions (such as fill time, melt temperature, mold temperature, packing time and packing pressure) under constant mold temperature. Next, this has been tried by optimizing the mold temperature history during each cycle of injection molding, assuming the temperature history to be a linear function of time. This study, however, is not aimed at minimizing cycle time that is longer than the normal case. In parts that require high precision molding in terms of low residual stresses or birefringence, the small increase in cycle time can be easily justified by the improved quality of the molded parts. This would include such parts as optical lenses, optical memory discs and high precision electronic parts. This study is aimed at such applications.

In the following sections, optimization methods used in this study and its application to residual stress and birefringence minimization will be presented.

2. Optimization Problem

The optimization problems studied in this paper can be stated mathematically as follows:

$$\text{Minimize}: \quad F(X) \tag{1}$$

$$\text{Subject to}: \quad X_k^l \le X_k \le X_k^u, k=1,n \tag{2}$$

Where F(X) in this study corresponds to either residual stress or birefringence and X refers to either processing conditions or mold-temperature history. Further, X_k^l and X_k^u are the lower and upper bounds on X_k whereas n denotes the number of design variables.

This problem is solved in the present study by using the "complex method". The Particular algorithm used is that due to Box[1]. The procedures involved in this algorithm are as follows[10].

Step 1 : Generate the initial set of P feasible points.

Step 2 : Carry out the reflection step: $X^m = \overline{X} + \alpha(\overline{X} - X^R)$ where $\overline{X}$ is the centroid of the set of points of X, X^m is the new point, X^R is the point which has the maximum objective value before reflection and α is a constant called reflection parameter.

Step 3 : Adjust for feasibility relative to the constraints. If the new point violates any constraint. move the point half-way toward the centroid.

Step 4 : Check for convergence. If not converged, go to step 2 and continue.

In this study, P was chosen to be 2 n and α was taken to be 1.3 as recommended in Reklaitis et al[10]. This particular algorithm has been chosen because it is rather simple to use, is rather robust and gives good engineering solutions.

3.Residual-Stress Minimization

Large residual stresses in injection molded parts can cause several problems such as early failure of the part or severe warpage and also undesirable birefringence in case of optical products. Therefore, it is often desirable to produce injection-molded parts with minimum residual stresses. Kang et al.[7] minimized the residual stress in injection-molded parts by optimizing the mold-wall-temperature history during the cooling stage. Although significant reduction in the residual stresses can be obtained by following the mold-cooling curve obtained in this study, the cooling curve is rather complicated and can not be easily implemented experimentally. Unlike in Kang et al., in this study, the residual-stress minimization has been tried which can be more readily achieved experimentally. This has been done first for the constant-mold-wall-temperature case by optimizing the process conditions while maintaining the mold temperature constant. Secondly, the residual-stress minimization has been tried by varying the mold-wall temperature linearly with time during each cycle.

3.1 Residual-Stress Calculation

Residual-stress minimization requires accurate calculation of the residual stresses. Efforts to predict residual stresses in injection molded parts have been made by many people. such as Isayev[4], Struik[13] and Santhanam[11], making use of some earlier notable work for inorganic glass by Lee. et al.[9].

In this study, the residual-stress calculation has followed that of Santhanam[11]. The flow and temperature fields are calculated from the following set of equation(see Fig.1 for coordinate system):

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_1)}{\partial x_1} + \frac{\partial(\rho u_3)}{\partial x_3} = 0 \tag{3}$$

$$\frac{\partial}{\partial x_3}\left(\eta \frac{\partial u_1}{\partial x_3}\right) - \frac{\partial p}{\partial x_1} = 0 \tag{4}$$

$$\rho C_p\left(\frac{\partial T}{\partial t} + u_1 \frac{\partial T}{\partial x_1}\right) = \frac{\partial}{\partial x_3}\left(k \frac{\partial T}{\partial x_3}\right) + \eta \dot{\gamma}^2 \tag{5}$$

These set of equations are solved by the generalized Hele-Shaw model as in Hieber and Shen[3].

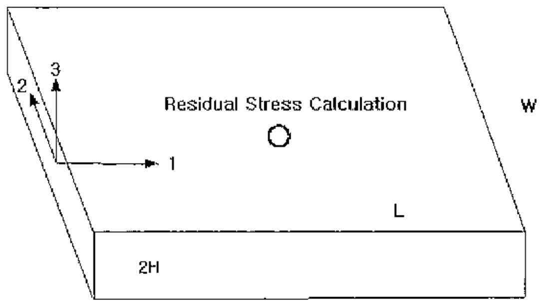


Fig. 1 Coordinate in rectangular cavity for residual stress calculation

In the residual stress calculation, thermally induced stress and flow-induced stress have been calculated separately. Thermally induced stress (or thermal stress) is the dominant form of residual stress in typical injection molding process. Thermal stress calculation is based on the assumption of a thermo-rheologically simple, linear viscoelastic model. The time-dependent material modulus at different temperatures is derived from a single master-curve of material behavior at a reference temperature. When the pressure is independent of the thickness (3) direction, the stresses can be calculated from the following equations[11].

$$\sigma=\sigma_{11}=\sigma_{22}= -[2R_1(\xi)+R_2(\xi)]p_0 + \int_0^{\xi}[R_1(\xi-\xi')-R_2(\xi-\xi')]\frac{\partial p}{\partial \xi'}d\xi' + 9K\int_0^{\xi}R_1(\xi-\xi')\frac{\partial}{\partial \xi'}(\varepsilon-\alpha_0\Theta)d\xi' \quad (6)$$

$$\sigma_{33}=-p \quad (7)$$

$$\sigma_{12}=\sigma_{23}=\sigma_{31}=0 \quad (8)$$

where σ is the stress, p is the pressure, p_0 is the pressure when the temperature passes no-flow temperature, ε is the strain whereas ξ (material time). and Θ(thermal strain) are defined as follows:

$$\xi=\int_0^t f(T)dt' \quad (9)$$

$$\Theta=\frac{1}{\alpha_0}\int_{T_0}^{t}\alpha(T')dT' \quad (10)$$

where f(T) is the shift function and α is the coefficient of thermal expansion. Moreover, R_1, R_2 are relaxation functions which depend on materials and material time and K is the bulk modulus.

The boundary conditions used in the stress calculation are either free quenching or constrained quenching. Free quenching is the case when the part is free of constraints with respect to lateral deformation and the melt pressure is assumed to be zero throughout the cooling cycle. Constrained quenching is the case when the polymer in contact with the mold wall is restrained against lateral deformation during the cooling cycle.

If we employ an instant-freeze model and constrained-quenching boundary condition, the residual stress after ejection can be calculated from the following equation[11]

$$\sigma=(R_2^1-R_1^1)[p_g(x_3')-\frac{1}{H}p_g(x_3')dx_3'] \quad (11)$$

where R_2^1, R_1^1 are material relaxation parameters, p_g is the pressure at which the temperature at that point crosses the glass-transition temperature and H is the half-gap thickness.

The flow-stress has been calculated using the Leonov viscoelastic model. For shear flow, the model calculates the flow stress from the following equation[11] .

$$\sigma(x_3,t)=2\sum_{k=1}^{N'}\mu_k\begin{pmatrix}C_{11,k} & 0 & C_{13,k}\\ 0 & 1 & 0\\ C_{13,k} & 0 & C_{33,k}\end{pmatrix} + 2\mu s\dot{\gamma}\theta_1(T)\begin{pmatrix}0 & 0 & 1\\ 0 & 0 & 0\\ 1 & 0 & 0\end{pmatrix} \quad (12)$$

where N' is the number of modes for Leonov model, $C_{ij\,k}$ is the elastic strain tensor, s is the dimensionless rheological parameter. $\dot{\gamma}$ is the strain rate and μ_k, μ are defined as follows:

$$\mu_k=\eta_k/(2\theta_k) \quad (13)$$

$$\mu=\eta_0/(2\theta_1) \quad (14)$$

where η_k is the viscosity in k-th relaxation mode, θ_k the relaxation time in k-th relaxation mode.

The material properties needed for the flowsimulationare represented as follows. First, the compressibility of the material has been represented in terms of double-domain Tait equation which is given as follows[11] .

$$v = v_0(1 - C\ln(1 + \frac{P}{B(T)})) \quad (15)$$

$$v_0 = b_{1,l} + b_{2,l}\overline{T} \quad if \quad T > T_t \quad (16)$$

$$v_0 = b_{1,s} + b_{2,s}\overline{T} \quad if \quad T \le T_t \quad (17)$$

$$B(T) = b_{3,l}\exp(-b_{4,l}\overline{T}) \quad if \quad T > T_t \quad (18)$$

$$B(T) = b_{3,s}\exp(-b_{4,s}\overline{T}) \quad if \quad T \le T_t \quad (19)$$

$$\overline{T} = T - b_5 \quad (20)$$

The transition temperature (T_t) is obtained by the intersection of isobaric lines in the liquid and solid states. The viscosity has been fitted by the following viscosity equation based on Leonov model:

$$\eta = \eta_{0_s} + \sum_{k=1}^{N} \frac{2\eta_k}{1 + \sqrt{1 + 4\dot{\gamma}^2\theta_k^2}} \quad (21)$$

3.2 Example

The problem studied is the injection molding of a rectangular plate. The size of the plate is 10 cm long (L), 2 cm wide (W) and 0.2 cm thick (2H) (see Fig. 1).
The material used in the molding is polystyrene (Dow Styron 615). The properties of this polymer used in the simulation are as shown in Table 1[11].
The heat capacity has been assumed to be constant. The thermal conductivity has been assumed to vary linearly with temperature. In discretizing the mesh for the simulation, 15 nodes in the streamwise direction and 20 nodes in the thickness direction have been used.

The residual stress at the middle streamwise location of the cavity has been used to calculate the objective function as follows.

$$F(X) = \sum_{i=1}^{N} \sigma_i^2 \quad (22)$$

where σ_i is the residual stress at the i-th layer of the given streamwise location and N is the number of layers.
The boundary condition used for the residual-stress calculation is constrained quenching.

Table 1 Properites of polystyrene used in this study

Heat capacity (J/kg-°C)	1100					
Thermal Conductivity	Temperature(°C)	0	160	300		
	Value (W/m-°C)	0.12	0.175	0.175		
Pvt	$B_{1,l}$ (m^3/Kg)	$B_{2,l}$ ($m^3/Kg\,°C$)	$B_{3,l}$ (N/m^2)	$B_{4,l}$ (1/°C)	$B_{1,s}$ (m^3/Kg)	$B_{2,s}$ ($m^3/Kg\,°C$)
	1.0071e-3	5.79e-7	2.02e+8	3.01e-3	9.892e-4	2.42e-7
	$B_{3,s}$ (N/m^2)	$B_{4,s}$ (1/°C)	B_5 (K)			
	2.26e+8	1.36e-3	423			
Others	[illegible] ($N\ sec/m^2$)	[illegible] ($N\ sec/m^2$)	[illegible] (sec)	[illegible] (sec)	S	C
	3.39e+9	1.59e+2	1.28e-1	14e-3	6.51e-4	4.8e-10

(1) Constant Mold Wall Temperature. The first part of the residual-stress-minimization study has been done by optimizing processing conditions while maintaining the mold-wall temperature constant during each cycle of the molding. The design variables used in the optimization are fill time, initial melt temperature, constant mold-wall temperature, packing pressure, packing time and cooling time (or total postfilling time).

In the optimization, we have to specify the limits of each design variable. The upper and lower bounds of each variable are shown in Table 2. These bounds are chosen based on practical considerations.

Table 2 Processing conditions for the minimization of residual stresses

	Fill time (sec)	Packing Press(MPa)	Packing Time(sec)	Postfilling Time(sec)	Melt temp (C)	Mold temp (C)
Lower Bound	0.1	15	5	20	200	25
Upper Bound	0.6	45	20	40	250	90
Initial	0.2	15	10	30	230	40
Optimal	0.163	15	8.7	20.8	244	69.7

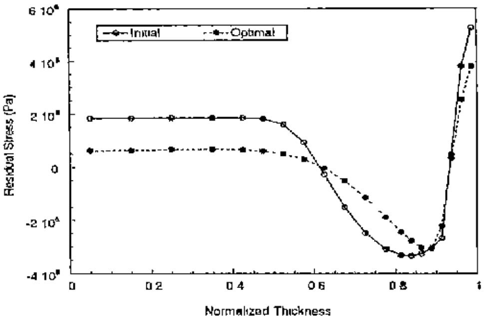


Fig. 2 Residual stress distribution in the thickness direction with initial and optimized process conditions

The optimal results have been obtained by using a residual-stress calculation based on the model outlined above. To get the optimal results, about 100 iterations of the complex method were needed(which required about 200 direct calculations of the residual stress). This takes about 10 hours of CPU time on a Silicon Graphics Indigo workstation. The optimized processing conditions are given in Table 2. In the same table, the initial process conditions in the optimization are also given. Fig. 2 shows the residual-stresses can be effected by changing processing conditions while maintaining the mold-wall temperature constant, the improvement is rather small.

(2) Variable Mold-Wall Temperature Although reduced residual stress values have been achieved in the preceding section, the improvement is not significant. In this section, an attempt to significantly reduce residual stress is made. This is done by varying the mold-wall temperature during each cycle of molding. A general cooling curve is shown in Fig. 3. This mold temperature history is chosen for ease of experimental implementation. As indicated, the mold wall is maintained at a high temperature for a while before cooling down to a lower temperature in a linear (time-wise) manner. The design variables for optimization are the initial mold temperature (T_{wi}), the initial delay time at high mold temperature(t_d) and the final time to cool down to the final mold temperature(t_f). The final mold temperature has been fixed at 40 °C. The part will be ejected at t_f. Other process conditions are the same as the initial conditions in Table 2.

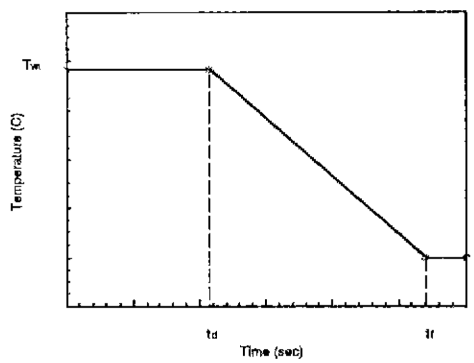
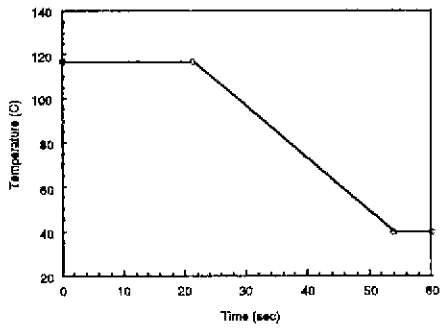
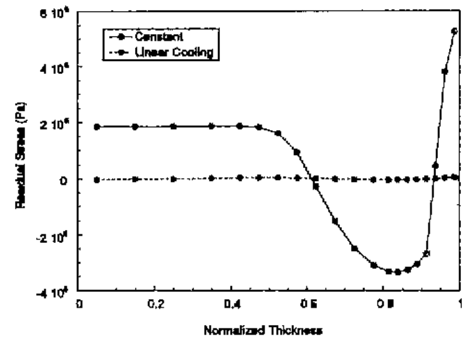


Fig. 3 General cooling curve for residual stress minimization

The optimal result is obtained in a manner similar to that in the preceding section, resulting in T_{wi} of 117°C, t_d of 21.3 seconds and t_f of 53.7 seconds. Fig. 4(a) shows this optimal cooling curve. The resulting optimization results are shown in Fig. 4 (b). This figure compares the residual stress resulting from the optimal cooling and that from the constant-mold-wall-temperature case (40 °C).



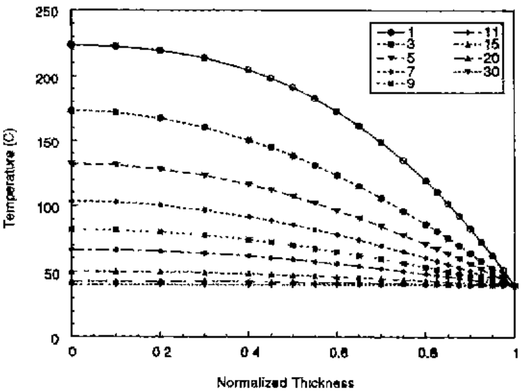
(a)



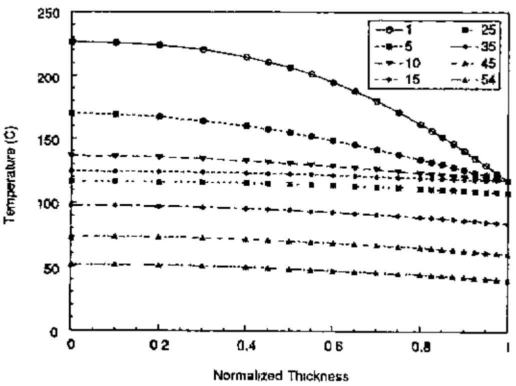
(b)

Fig. 4(a) Optimized cooling curve for residual stress minimization and
(b) Residual stress distribution in the thickness direction with constant and optimized linear cooling mold wall temperature

This result shows that the residual stress can be reduced by a factor of 100 by employing an optimal mold-wall-temperature history. The reason the optimal cooling curve reduces the residual stress can be understood from the temperature-distribution histories which are plotted in Fig. 5 and by using the instant-freeze model. The residual-stress calculation model from Eq. 11 shows that the residual stress is related to the pressure at the point when the temperature of a particular layer passes through the glass transition temperature. Fig. 5(a) shows the temperature-distribution histories when the mold temperature is constant at 40 °C. This figure shows that the temperature difference between layers at different gapwise locations is significant during most of the time. This means that the temperature at the various layers will pass the glass-transition temperature at much different times (the glass transition temperature of polystyrene is about 100 °C). In turn, this means that "p_g" in Eq. 11 will be less uniform in x_3, leading to larger values for the stress. On the other hand, as can be seen from Fig. 5(b), the temperature difference becomes smaller when we use the optimal mold-cooling history. Therefore, each layer will pass through the glass-transition temperature at almost the same time which in turn will lead to a smaller stress in Eq. 11, as is evidenced in Fig. 4(b).



(a)



(b)

Fig. 5 (a) Temperature distribution in the thickness direction with constant and (b) Optimized cooling mold temperature (the number inside the plot represents time in seconds)

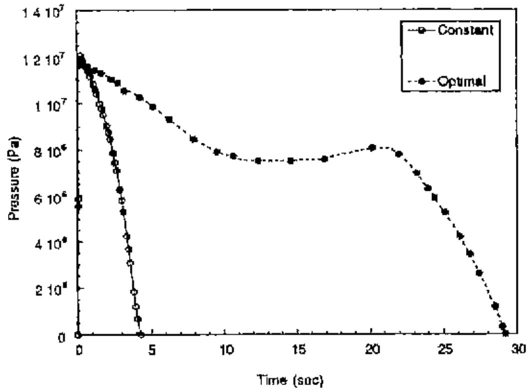


Fig. 6 Pressure history at the point where residual stress is calculated under constant mold temperature and optimal mold temperature history.

Pressure histories at the residual stress calculation point for both constant and optimal mold temperature case are plotted in Fig. 6. In constant mold temperature case, the pressure at that point reduces to zero in about 5 seconds because temperature at most layers at that point is lower than or close to the glass-transition temperature at that time. On the other hand, in the optimal mold cooling case, the pressure remains high until about 30 seconds because the mold temperature is above glass-transition temperature until that time.

4.Birefringence Minimization

The birefringence is often one of the most important properties for optical products such as optical lenses and optical memory discs. As the precision required for the optical parts gets tougher, the level of birefringence allowed becomes smaller[2]. As in Section 3, efforts have been made to minimize the birefringence in injection molded parts by optimizing either processing conditions or mold wall temperature history.

4.1 Birefringence calculation

The prediction of birefringence has been tried by Isayev and Hieber[5] and Shyu and Isayev [12]. In this study, methods used in Isayev & Hieber[5] have been used to calculate the frozen-in birefringence. The flow stress will be calculated as in the residual stress calculation. The birefringence can be calculated from the flow stress by the following equation:

$$\Delta n = C(T)[(\sigma_{11} - \sigma_{22})^2 + 4\sigma_{12}^2]^{1/2} \quad (23)$$

$$n_{22} - n_{33} = C(T)(\sigma_{22} - \sigma_{33}) \quad (24)$$

$$n_{22} - n_{33} = C(T)(\sigma_{33} - \sigma_{11}) \quad (25)$$

where C is the stress-optical coefficient. In this study, two modes have been used to represent the relaxation. Some of the material values used in the current calculation are shown in Table 1.

4.2Example

The optimization has been applied to the injection molding of a center-gated circular disc Fig. 7. The disc has 10.2 cm of diameter and 0.2 cm of thickness. The material used is polystyrene (same as in the residual stress minimization case).

The birefringence calculated at the point indicated in Fig. 7 has been used to obtain the objective function as follows.

$$F(X) = \sum_{i=1}^{N} n_i^2 \quad (26)$$

$$n_i = [(\Delta n)^2 + (n_{22} - n_{11})^2 + (n_{33} - n_{11})^2]^{1/2} \quad (27)$$

where n_i is the total birefringence at the i-th layer of the reference point and N is the number of layers.

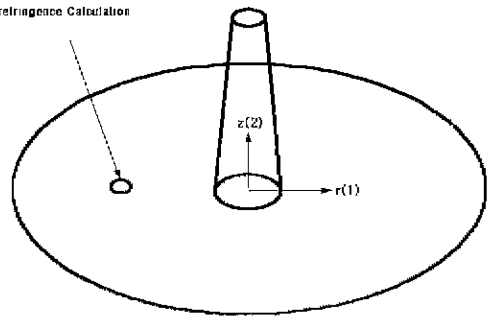


Fig. 7 Coordinate system in a disc for the calculation of birefringence

(1)Constant mold wall temperature As in the residual stress minimization case, the birefringence minimization has been tried by changing processing conditions while maintaining the mold temperature constant during the cycle. The resulting optimal process conditions as well as the upper and lower bounds and initial process conditions are shown in Table 3.

The calculated birefringence before and after optimization are compared in Fig. 8. As can be seen from this figure, the improvement in birefringence that can be achieved by process optimization under constant mold wall temperature is rather small.

Table 3 Processing conditions for birefringence minimization

	Fill time (sec)	Packing Press(MPa)	Packing Time(sec)	Postfilling Time(sec)	Melt temp (C)	Mold temp (C)
Lower Bound	0.5	27	5	20	200	25
Upper Bound	4	81	20	40	250	90
Initial	1.5	27	10	30	230	40
Optimal	1.1	28	10.3	30.1	247	49.4

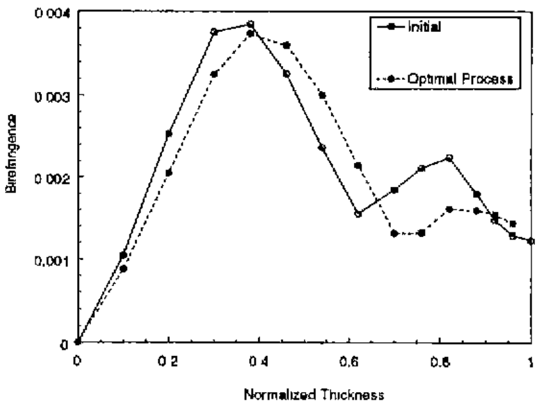
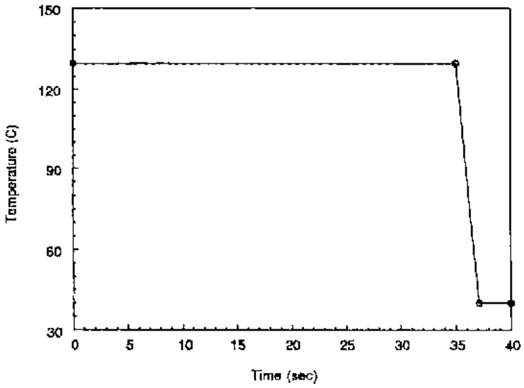
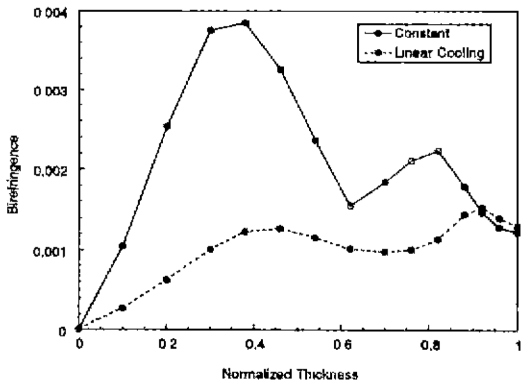


Fig. 8 Calculated birefringence with initial and optimized conditions.

(2)Variable mold wall temperature. The variable mold wall temperature case has been tried using the type of cooling curve as in the residual stress minimization case. The optimal cooling curve is when the initial mold temperature is 129.8 °C, initial delay time is 35 seconds and the final cooling time is 37.1 seconds. The optimal cooling curve obtained is shown in Fig. 9(a). This cooling curve is not universal and will depend on material properties and mold geometries. Compared to residual stress minimization case, birefringence minimization requires fast cooling of the mold after initial delay time. The corresponding calculated birefringence for constant mold wall and optimal mold wall temperature history are compared in Fig. 9(b). As can be seen from Fig. 9, the birefringence has been reduced by about 3 times by employing the optimal cooling curve.



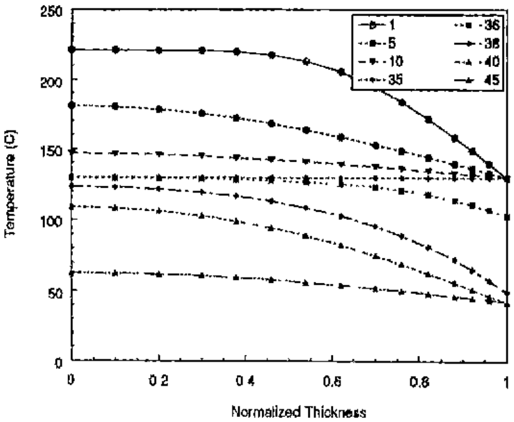
(a)



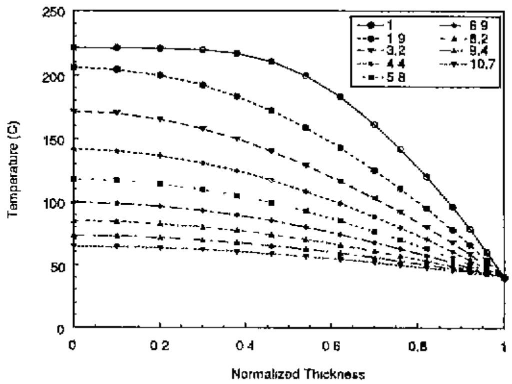
(b)

Fig. 9 (a) Optimal cooling curve and
(b) Birefringence distribution in the thickness direction with constant mold wall temperature and linear cooling of the mold wall

The temperature distribution and pressure history for constant mold temperature and optimized cases at the birefringence calculation point are plotted in Fig. 10 and Fig. 11. respectively. The reason that the optimized case reduces the birefringence can be understood this way. If we compare the temperature and pressure history at the birefringence calculation point(Fig. 10, Fig. 11) near the time when the pressure drops to zero, we can see that the temperature in the optimized case is generally higher than that of constant mold temperature case if we compare them at the same pressure level. This means that the birefringence in the optimized case has more chance to relax resulting in lower frozen-in birefringence.



(a)



(b)

Fig. 10 (a) Temperature distribution at the birefringence calculation point in the thickness direction with constant and
(b) Optimized cooling mold temperature (the number inside the plot represents time in seconds)

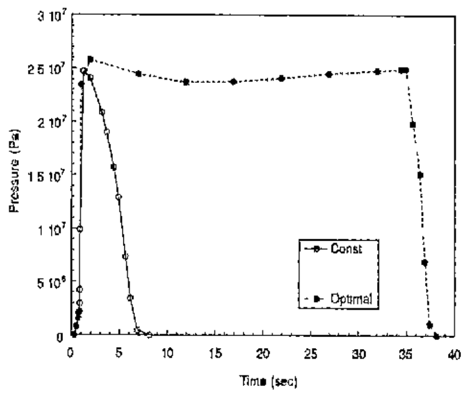


Fig. 11 Pressure history at the point where residual stress is calculated under constant mold temperature and optimal mold temperature history

Conclusion

Following conclusions can be drawn from this study.

(1) The complex method yielded optimization results at reasonable computational cost for the problems in this study.
(2) The residual stress and birefringence in the injection molded parts can be reduced moderately by setting the process conditions such as fill time, mold temperature, packing pressure and packing time at opticamal condution
(3)Significant reduction in residual stress and birefringence during each cycle of injection molding. Varying mold wall temperature is technically challenging at this moment, but has a good potential to reduce the residual stress and/or birefringence significantly when implemented properly.

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