THE NUMERICAL ANALYSIS AND VALIDATION OF COMPRESSION MOLDING PROCESS

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Abstract

In this work, the simulation results from a program developed for the three-dimensional analysis of compression molding of thermoset composites were compared to the experimental results of an actual molded thermoset sample. The program predicts the flow pattern, fiber orientation, fiber length distribution, curing of the resin and mechanical properties. The comparison between simulation and experiment includes short shots and fiber orientation. Actual fiber orientation images were obtained using CT scanning. The comparison shows reasonable agreement between simulation and experiment.

Introduction

A compression molding process is illustrated in Figure 1. As can be seen from this figure, some portion of the cavity initially is filled by a charge (called "initial charge"). The initial cavity thickness is much higher than the final part thickness. The mold cavity thickness is reduced by a compressive force, forcing the resin into the unfilled portions of the cavity. The compression by the press is generally done at a controlled speed until a maximum force is reached, but may sometimes be fully force controlled. After the cavity is filled, additional press movement may be required to compensate for polymer shrinkage. This compression molding process results in more homogeneous physical properties and less molded-in stresses compared to conventional injection molding. Also, for long fiber, compression molding has an advantage in that the final fiber length will have much less breakage than that obtained from injection molding due to attrition in injection unit and feed system. Long fiber composites processed by compression molding will retain most of their original fiber length leading to enhanced mechanical properties compared to short fiber composites.

In this study, a three-dimensional compression analysis program has been developed for thermoset materials. This program can predict the flow pattern, fiber orientation, length distribution, curing and mechanical properties. Fiber content, length and orientation greatly affect the performance of the product. The three dimensional analysis is chosen instead of two dimensional analysis because it can produce more accurate results for thick parts or parts with complicated geometry. Also, the velocity and pressure in the compression direction can be calculated more accurately with three dimensional analysis. Also, the initial charge geometry can be modeled more accurately. Designers and engineers can use the results from the program developed in this study to optimize the materials and process conditions.
In the next sections, an analysis method for the compression process for flow, fiber orientation and mechanical properties calculation will be given. This will be followed by some results from a case study.

**Governing Equations for Flow and Fiber Orientation Analysis**

We need to solve the following set of equations to analyze the flow during compression molding process for thermoset materials [1]:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \textbf{v}) = 0
\]  
\[
\rho \frac{D\textbf{v}}{Dt} = -\nabla p + \nabla \cdot \tau + \rho g
\]  
\[
\rho C_p \frac{DT}{Dt} = \nabla \cdot (k\nabla T) + \eta \dot{\gamma}^2 + \beta T \frac{Dp}{Dt} + H \frac{D\alpha}{Dt}
\]  
\[
\frac{D\alpha}{Dt} = (K_1 + K_2\alpha'')(1 - \alpha)^\nu
\]

where

\[
K_1 = A_1 e^{\left(-\frac{E_1}{T}\right)} \quad K_2 = A_2 e^{\left(-\frac{E_2}{T}\right)}
\]

Equation (1) is the mass continuity equation, (2) the momentum equation and (3) the energy equation. (4) and (5) are curing kinetics equations due to Kamal [2]. In the above equations, \( \rho \) is density, \( t \) time, \( \textbf{v} \) velocity, \( p \) pressure, \( \tau \) stress tensor, \( g \) gravitational constant of the earth. Also, \( C_p \) is the heat capacity, \( T \) temperature, \( k \) thermal conductivity, \( \eta \) viscosity, \( \dot{\gamma} \) shear rate, \( \beta \) expansivity and \( H \), heat of reaction. Furthermore, \( \alpha \) is degree of cure and \( A_1, A_2, E_1, E_2, \mu, \nu \) are constants used in the curing kinetics.

A no-slip boundary condition can be applied at the fixed non-compression mold wall as in regular injection molding analysis. However, unlike in regular injection molding, a specified speed boundary condition needs to be applied at the compression mold wall when the press is moving under speed control. When the press is moving under force control, the press speed needs to be calculated based on the press force.

The fiber orientation is calculated for long fibers using the anisotropic rotary diffusion model combined with the reduced strain closure model (ARD-RSC) as in [3].

\[
\frac{dA}{dt} = (W \cdot A - A \cdot W) + \xi (D \cdot A + A \cdot D - 2[A + (1 - \kappa)(L - M : A)] : D)
\]
\[
+ \dot{\gamma}^2 (2[C - (1 - \kappa)M : C] - 2\kappa(trC)A - 5(C \cdot A + A \cdot C) + 10[A + (1 - \kappa)(L - M : A)] : C)
\]
\[
C = b_1 I + b_2 A + b_3 A^2 + b_4 \frac{D}{\dot{\gamma}} + b_5 \frac{D^2}{\dot{\gamma}^2}
\]

In the above equations, \( A \) is the second-order orientation tensor, \( \textbf{A} \) fourth-order orientation tensor,
C rotary diffusion tensor, W vorticity tensor, D rate-of-deformation tensor. Also, L, M are fourth-order tensors, \( \kappa \) RSC factor, \( \xi \) particle shape parameter, and \( b_1, b_2, b_3, b_4, b_5 \) are constants for anisotropic rotary diffusion.

The fiber length distribution is calculated using a fiber-breakage model as in [4]. In this study, fiber migration or curvature of the fiber is not considered.

### Mechanical Properties Calculation

When fibers are fully aligned and have the uniform length, the stiffness of the composite is calculated as [5]

\[
H^*(l/d) = H_m + c_f(H_f - H_m); A_f
\]  
(8)

or

\[
H^*(l/d) = [(1 - c_f)H_m + c_fH_f; T]; [(1 - c_f)I + c_fT]^{-1}
\]  
(9)

where \( c_f \), \( l \), and \( d \) are the fiber volume fraction, length, and diameter, respectively. \( H^*, H_m, \) and \( H_f \) are the stiffness tensors of the unidirectional (UD) composite, matrix, and fiber, respectively. \( A_f \) is the fiber strain-concentration tensor, and is computed with a selected micromechanical model. The Eshelby-Mori-Tanaka approach [6, 7] gives

\[
A_f = T; [(1 - c_f)I + c_fT]^{-1}
\]  
(10)

with

\[
T = [I + S; H_m^{-1}; (H_f - H_m)]^{-1}
\]  
(11)

where \( S \) is the Eshelby tensor and \( I \) is the fourth-order identity tensor.

Due to the fiber breakage during the process, the fiber length is not uniform and the distribution can be described with the probability density function \( P(l) \). The stiffness of the composite is

\[
H = \frac{\int_0^\infty H^*(l/d)P(l)dl}{\int_0^\infty P(l)dl}
\]  
(12)

The stiffness tensor \( H^*(l/d) \) must be calculated for each length segment \( l_i \), which requires a lot of computation. To simplify the computation, the average fiber length by weight, \( \bar{l} \), is used in Equation (8) or (9) to calculate the stiffness, i.e.

\[
H = H^*(\bar{l}/d)
\]  
(13)

Then the averaging technique [8] is employed to calculate the composite stiffness averaged over the fiber orientation distribution.

The imperfect fiber/matrix interface model by Qu [9] is employed for the expression of the stiffness tensor for a unidirectional composite that contains partially debonded fiber/matrix interfaces. The Eshelby-Mori-Tanaka formulation (9) for the unidirectional composite is modified as
where the fourth-order tensor $\mathbf{T}$ is determined from Equation (11) in terms of the modified Eshelby tensor $\mathbf{S}^*$ given as

$$\mathbf{S}^* = \mathbf{S} + (1 - \mathbf{S}) : \mathbf{N} : \mathbf{H}_m; (1 - \mathbf{S})$$

in which the fourth-order tensor $\mathbf{N}$ is given by

$$\mathbf{N} = \beta r (\mathbf{P} - \mathbf{Q})$$

where $r$ is the radius of the fiber. $\beta$ represents the compliance in the tangential direction of the interface, and can be expressed in terms of the matrix elastic modulus as $\beta = \beta^* / E_m$. $\beta = 0$ corresponds to a perfect fiber/matrix interface while a very high value of $\beta$ represents complete debonding. Components of the fourth-order tensors $\mathbf{P}$ and $\mathbf{Q}$ for ellipsoidal inclusion are provided by Qu [9].

**An Example Case**

In the example, the software developed in this study is used to simulate the molding of a panel. Figure 2 shows the geometry of the part. Figure 3 shows the simulation model for the initial charge and the part. In this figure, the green area is the final shape of the part to be molded, and the gray area is the initial charge. The length of the part is about 800 mm, the width is 200 mm and the typical thickness of the final part is about 4 mm. The finite-element mesh has approximately 1,585,000 tetrahedral elements and 276,000 nodes.

The following process conditions are used in this example. The initial melt temperature is 45°C, and the mold temperature is 149°C. The nominal fill time is about 12 second. The maximum press force (compression tonnage) is 300 tons and press compression time is 20 seconds. The compression is switched to force control when 99% of the cavity is filled. After that, the press force is maintained at the switch-over value for 10 seconds. The press open distance is 27 mm. The press moves at a controlled speed until switch over to force control. The initial press speed is at 3.5 mm/sec, but it drops with time as shown in Figure 4(a). Figure 4(b) shows press displacement versus time. After switch over to force control, the press moves at a constant press force. The total filling and post-filling time is about 40 seconds. The polymer used is a sheet molding compound (SMC) from Premix (Premi-Glas 1286). This is a composite material with 34% glass fiber by weight (with initial fiber length of 12 mm).

The simulation results and comparison with experiment are shown in Figures 5 - 13.

Figure 5 shows the pressure distribution in the cavity at two different times during filling. As the initial charge lies near the center of the cavity, the pressure is highest near the center of the cavity. Figure 6 shows the degree of cure distribution near the end of molding.

Figure 7 and Figure 8 show the short shot images from the actual molding experiment and simulation. Figure 7 is at time of 5.6 seconds during filling, and Figure 8 is at time of 8.3 second during filling. For Figure 7, the material inside the circular areas at the left and right ends of the part has been removed from the experimental short shots (and so is not shown in the experimental image). Although
there are some differences between simulation and experiment, overall, the agreement is reasonable. The difference could be due to the initial charge placement. Since the initial charge is cut and placed in the mold manually, the shape and location of the initial charge can be somewhat different from those used in the simulation. The other potential causes of difference include the effects of fiber orientation on flow (which is neglected in the current study).

Figure 9 is the CT (Computed Tomography) scan images of the part which show the fiber orientation. Figure 9 (a) and (b) are images at different layers. Figure 10 shows the fiber orientation (first principal value) obtained from simulation. In this plot, the direction of the long bar represents the direction of the first principal value of orientation. If the value is high (close to 1), it means that more of the fibers are aligned in the first principal direction. Comparison between Figure 9 and 10 indicate that there are some correlations between the fiber orientation obtained from the experiment and that predicted by the simulation.

Figure 11 shows the fiber length distribution obtained from the simulation. As can be seen from this figure, the fiber length at the end of molding is 11 mm or longer in most regions (with minimum length around 10 mm) which are close to the initial length (12 mm). This indicates that there is not much fiber breakage for this case. Experiment confirms that the fiber length after the molding is almost the same as that before the molding. Figure 12 shows the calculated tensile modulus in the first principal direction. Figure 13 is the calculated Poisson's ratio. In these calculations, the fiber length obtained in Figure 11 is used. Since there is not much fiber breakage, the mechanical properties are expected to be similar to those with initial fiber length for this case.

Conclusion

The results from the simulation program developed in this study show that the simulation results for filling pattern and fiber orientation match reasonably well with the experiment.

References

Figure 1: The schematic of the compression molding.

Figure 2: A geometry model for the part used in the current study.

Figure 3: A simulation model which shows the part (green) and the initial charge (gray).
Figure 4: (a) Compression speed versus time and (b) press displacement versus time.
Figure 5: Pressure distribution in the cavity during filling at 5.6 second (a) and 11.5 second (b) (in MPa).

Figure 6: Degree of cure distribution in the part at the end of molding.
Figure 7: Short shots from experiment (a) and simulation (b) at 5.6 seconds during filling.
Figure 8: Short shots from experiment (a) and simulation (b) at 8.3 seconds during filling.
Figure 9: CT scan images that show the fiber orientation near the right end. Figures (a) and (b) are at different layers.
Figure 10: Calculated fiber orientation results (first principal value); (a) magnified view near the right end and (b) overall view.
Figure 11: Fiber-length distribution in the cavity (in mm).

Figure 12: Calculated tensile modulus in the first principal direction (in MPa).

Figure 13: Calculated Poisson’s ratio ($\nu_{12}$).