MODELING AND MATERIAL DATA ISSUES OF INJECTION MOLDING SIMULATION

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ABSTRACT

Injection molding involves highly complex physics: fast-cooling rate, high pressure, phase change, crystallization and morphology development, fiber orientation, stress relaxation and time-varying boundary conditions during filling, packing, cooling and ejection stages. This paper discusses the modelling and material data issues in simulation of injection molding, particularly the prediction of shrinkage and warpage. Though Computer Aided Engineering (CAE) for plastic injection molding is arguably the most sophisticated and successful example in the field of process simulation, further research effort is required on the reliable and robust morphology and property prediction. On the other hand, the model calibration based on shrinkage measurement is an effective approach for improving the accuracy of shrinkage and warpage simulation.

1 INTRODUCTION

The injection molding process is a high speed, automated process that can be used to produce unfilled or discontinuous-fiber-reinforced plastic parts with very complex geometries. A typical injection molding process consists of four phases: (1) filling of the melt polymer into the relatively cool mold; (2) packing of more material into the mold under high pressure to compensate for volume contraction of the material as it cools; (3) cooling during which the material solidifies while in the mold until it is sufficiently solid, (4) ejection of the solidified product from the mold. While in the mold, the part is constrained in-plane and so stresses develop in the part during solidification. Upon ejection, the relaxation of these stresses causes instantaneous shrinkage that is usually anisotropic and non-uniform throughout the molded part. Further shrinkage may also occur during cooling after ejection. The anisotropic and non-uniform shrinkage behaviour will result in a degree of part warp.

It is well known that the relationship between injection molding process variables and shrinkage and warpage of parts is extremely complex[1,2]. The high expense of creating an injection mold and the likelihood that a problem discovered in production will result in costly retooling and lost time makes molding simulation highly valuable to industry. On the other hand, industrial demand for high dimensional stability, excellent visual appearance, and accurate fit with mating components requires that warpage simulation should be performed when designing high-precision injection molded parts. An accurate shrinkage and warpage prediction can identify where excessive shrinkage and warpage might occur and optimize part and mold design, material choice, and processing parameters to help control part deformation [1,2,3].

Since the highly complex multiphysics phenomena are involved in injection molding process, many assumptions in mathematical modeling have to be used to make simulation feasible. On the other hand, it is nearly impossible to get a full set of characterization data for a given material in the range of process variables of interest for injection molding. This paper discusses the modeling and material data issues in simulation of injection molding, particularly the prediction of shrinkage and warpage. The validation and calibration processes of injection molding simulation are also addressed.

2 GENERAL MODELLING ISSUES

The injection molding simulation establishes and solves the mathematical equations of the transport phenomena involved in the process, namely the simultaneous solution of the mass conservation equation, momentum conservation equation, energy conservation equation, and constitutive equation reflecting the material properties under the non-isothermal conditions with the correct initial conditions and boundary conditions [1,2]. The main analysis procedure is shown in Figure 1. The simulation of the filling, packing, cooling, fibre orientation, residual stress, shrinkage and warpage of injection molding process has traditionally been based on the midplane shell representation on the part-geometry. The Hele-Shaw laminar flow approximation leads to a simple equation that is readily solved using finite elements for pressure and a finite difference scheme for temperature and velocity [1]. The structural shell element based on Kirchoff or Mindlin approximation is used for the warpage analysis. However, it is not generally a simple matter to derive a midplane shell representation of the part from the three-dimensional solid model created by part designers.

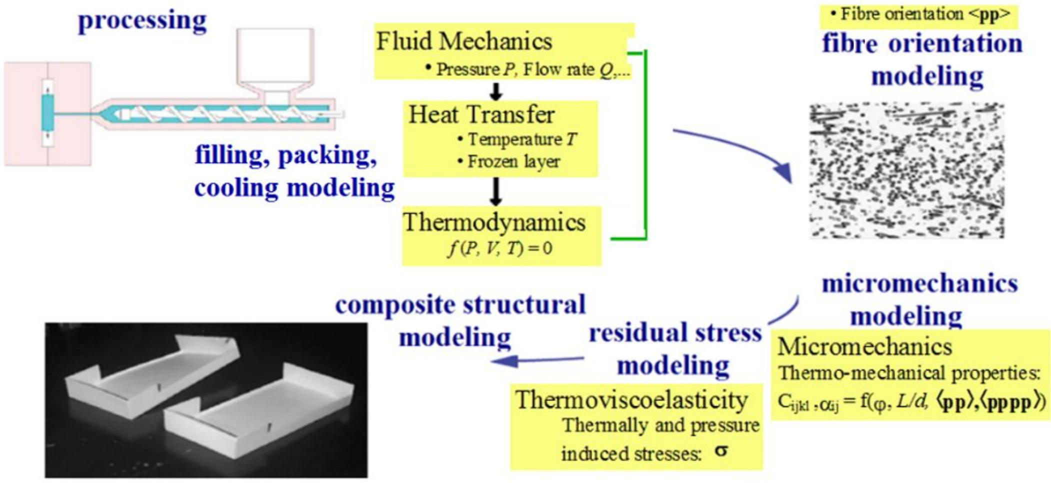


Figure 1. Major Steps of Injection Molding Simulation

A technique called Dual Domain Finite Element Analysis has been developed, which allows simulations directly on a surface mesh on the exterior of the solid models [4,5,6]. The technique has proved robust and has been extended to filling, packing, cooling and warpage analysis of thin-walled injection molded components. Dual domain Finite Element Analysis is basically a shell finite element solution, and still uses the Hele-Shaw approximation in filling and packing analysis and Kirchoff or Mindlin approximation in warpage analysis. These approximations are not suitable when the geometry or fluid behavior has complex three-dimensional features,which cannot be well approximated by 2.5D shells. For example, the corner effect simulation in the warpage analysis requires the consideration of a 3D flow effect, 3D heat transfer effect and 3D fiber orientation effect at corners. The anisotropic shrinkage induced spring-forward/spring-back effect at corners (so-called corner-effect) is not naturally considered in the shell solution [7], and special treatment has been developed for eliminating the limitation. The full 3D solution is a natural choice for considering these effects [8,9,10,11,12].

For some complex injection overmolding cases, a 3D analysis could be the only feasible solution. Injection over-molding has become a popular fabrication process in recent years. Many industries use over molding to produce a wide range of fabricated parts. In injection over-molding, a polymer melt is injected over a solid metal or polymer insert to form the fabricated part. Injection overmolding of thermoplastic over a continuous fiber reinforced composite is one of the new manufacturing approaches for automotive light-weighting which is emerging as a potential way to increase vehicle fuel economy. It not only takes advantage of excellent strength and stiffness properties of continuous fiber reinforced composite, but also has the advantage of forming complex and intricate functional shapes with the injection molding process. In two shot sequential over-molding, the first component is injected into a closed cavity. The mold or cores then move to create a new cavity with the first component as an insert for the second shot of a different polymer. To fully consider the complex insert and multi-shot effects, a full three-dimensional finite element solution is the best choice [13,14,15].

However, the high gradient variation of velocity and temperature in gap-wise directions and the limitation of maximum element aspect ratio necessitate the use of many elements across the part thickness. Consequently, the number of elements for 3D analysis becomes very large, and leads to high demands of computing time and resources. A fast and robust parallelized algebraic multigrid preconditioned conjugate gradient (AMG-CG) equation solver has been developed for flow and warpage analyses. A fast and parallelized eigen-solver has also been developed, which combines an algebraic multigrid preconditioned conjugate gradient (AMG-CG) equation solver with a subspace eigenvalue iteration algorithm, making the large-scale 3D buckling analysis feasible for the warpage simulation in industrial applications [16].

A good-quality anisotropic flow mesh with 10 or more layers of 4-node tetrahedral elements is normally required 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 the 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 [17].

Simulation has generally assumed that the mold cavity does not change during processing. Pressure in the melt can reach very large values during the injection molding process. By effect of such a cavity pressure, injection molds are exposed to a high mechanical loading that induces a deformation. In spite of the rigidity of the mold components, this deformation along the thickness direction can be significant, especially when very high pressure levels are reached [18]. The mold deformation could have a significant effect on the pressure decay during packing, and therefore have significant impact on shrinkage and warpage prediction [19, 20]. Another issue is the core-shift which is caused by an uneven distribution of melt flow around a core pin during injection molding. In turn, core shift affects the melt flow pattern as it changes the boundary conditions of the flow. Prediction of core shift is important because it causes variations in the wall thickness of thin-walled parts. The mold deformation and core-shift effects can be predicted by mold filling and packing simulation coupled with elastic analysis of mold and core components, though the modeling efforts and computational time will be significantly increased [21].

3 MATERIAL DATA ISSUES IN SHRINKAGE AND WARPAGE SIMULATION

Injection molding process involves highly complex physics: fast-cooling rate, high pressure, phase change, crystallization and morphology development, fiber orientation, stress relaxation and time-varying boundary conditions during filling, packing, cooling and ejection stages. Many assumptions have to be used to make the simulation feasible. These assumptions fall into two categories: the physical modeling assumptions and the data assumptions. The quality of the physics modeling depends on the fidelity and comprehensiveness of physical detail embodied in the mathematical model representing the relevant physics taking place in the system of interest. The data assumptions are about the input data for the material and the parameter values for the mathematical models.

Shrinkage and warpage is arguably the most important problem to be tackled by injection molding simulation. 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[22,23,24]. 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 constitutive behaviour of the material is described by the following equation:

$$\sigma_{ij} = \begin{cases} \int_{-\infty}^{t} C_{ijkl}(\xi(t)-\xi(t'))\dfrac{\partial \varepsilon_{kl}}{\partial t'}dt' - \int_{-\infty}^{t} \beta_{ij}(\xi(t)-\xi(t'))dT(t'), & T \le T_s; \\ -p\delta_{ij} + \eta(p,T,\dot{\gamma})\left(\dfrac{\partial v_i}{\partial x_j} + \dfrac{\partial v_j}{\partial x_i}\right), & T > T_s. \end{cases}$$

where T_s is the solidification temperature, a critical criteria to determine the point of liquid-solid phase change. This model assumes that the material behaves like a linear viscoelastic solid below the solidification temperature, and like a generalized Newtonian fluid at a temperature above T_s. The tensor C_{ijkl} is the viscoelastic relaxation modulus of the material, and β_{ij} is the tensor of thermal coefficient of expansion. The material is assumed to be thermo-rheologically simple and therefore the time-temperature superposition (TTS) principle is used to account for the temperature dependence of the material response. In the above equation, ξ is the pseudo-time defined as

$$\xi(t) = \int_{0}^{t} \frac{1}{a_T} dt'$$

where a_T is the time-temperature shift factor characterized by either the WLF equation or the Arrhenius equation depending on the material and the temperature range.

The residual stress is modelled by solving the force balance at each time step[22,23,24]. There are many complications inside the formulation. Above all, the solidification temperature is a complex concept. For amorphous polymer, the solidification temperature should be a function of pressure and cooling rate. For semi-crystalline, solidification temperature should be determined by crystallinity which requires the crystallization kinetics predicted in the simulation. The strain and temperature variables in the equation largely depend on the local temperature and pressure histories of the filling, packing and cooling phases of the molding process. On the other hand, C_{ijkl} and β_{ij} are strongly dependent on the temperature and processing-related internal structures which themselves are in turn affected by processing conditions, particularly for those systems involving semi-crystalline materials and phase change.

Multi-layered skin-core structures have often been observed in injection molded parts. The number of layers depends on the material, molding conditions and the location in the part. For semi-crystalline polymer, the deformation of polymers during the flow has dramatic effects on the crystallization and subsequent solidification of polymers in two aspects: enhancement of crystallization rate and formation of thread-like nuclei that grow into shish-kebab structures. These phenomena are known as flow-induced crystallization (FIC), and significantly influence the resulting morphology which includes the degree of crystallinity, the shape, the sizes, and the orientation of the crystalline structures[1,2,25]. The crystallization and material property prediction has been a hot research topic for many years. The relationship between polymer processing, morphology evolution and final mechanical properties of semi-crystalline polymer is shown in Figure 2[25].

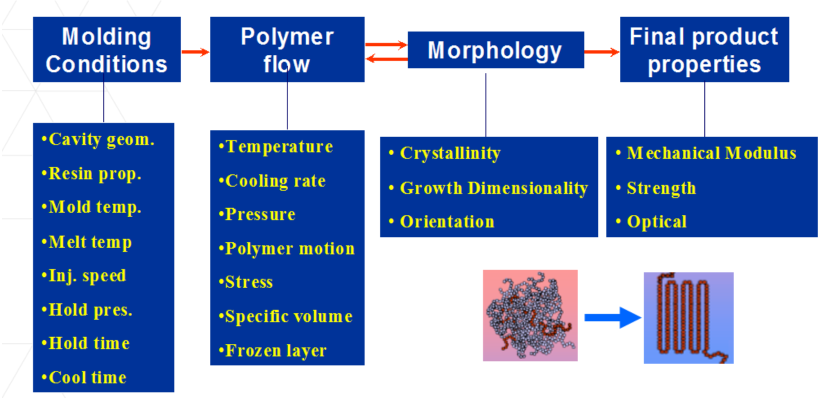


Figure 2. Prediction of semi-crystalline polymer properties [25]

For discontinuous fiber filled polymers, the geometry, concentration, thermo-mechanical properties, and orientation distribution of the fibers, as well as the thermo-mechanical properties of the polymer matrix, significantly affect the mechanical and thermal performances of the composite material. It should be noted that the velocity gradients of the melt during filling and packing determines the orientation of fibers. That means that all the assumptions used in filling and packing simulation will have an effect on the fiber orientation prediction. The procedure for predicting the mechanical properties of fiber-filled polymer can be summarized in Figure 3.

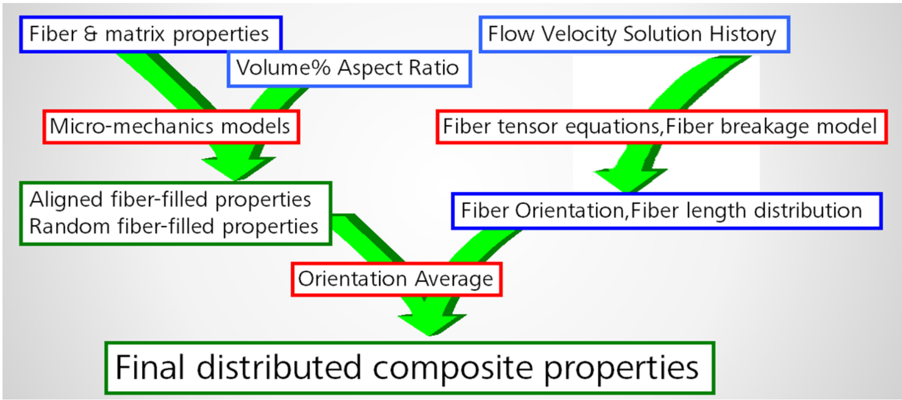


Figure 3. Prediction of discontinuous fiber reinforced composite properties

In order to achieve a reliable description of morphology evolution during polymer processing, one needs: a thermo-mechanical model which accounts for the main phenomena that take place, a good description of geometry and thermal boundary conditions, an accurate and comprehensive material characterization of rheological behaviour, viscosity and viscoelasticity and effect of crystallinity, crystallization kinetics, including the effect of flow on the morphology development, but it is nearly impossible to get a full set of characterization data for a given material in the range of process variables of interest for injection molding.

Reliable data collected from the real system in actual operation is desirable in any simulations. In fact, most material properties for injection molding simulation are obtained using laboratory tests under well controlled conditions. For example, specific heat, thermal conductivity and PVT data are generally measured at much lower cooling rate than rates in injection molding. The material properties are strongly dependent on the details of the thermo-mechanical history experienced by the material during processing. The mechanical properties and the coefficient of thermal expansion in material database are measured with a 3mm thickness specimen molded with a certain processing condition, and there are some approximations when they are used as a general material data for all other cases.

The heat transfer coefficient (HTC) value between the mold and the polymer surface is another difficult parameter, which is related to non-perfect contact between polymer and mold surfaces and gases allocated between them. As the contact condition keeps changing in the injection molding process, the time-dependent heat transfer coefficient has to be used. The heat transfer coefficient is critical to the temperature evolution in the layers of polymer very close to part surface, and therefore could have a significant impact on the morphology and properties of the skin layer of an injection molded part [26].

It is clear that the characterization of material properties cannot be carried out without an effort in the collection of experimental data in the range of process variables of interest for injection molding. The good-quality material data for anisotropic thermo-viscoelastic residual stress calculation and crystallization simulation are normally unavailable. Though standard material characterization is expected to be unsuitable for the development of process modeling, some material data used as the critical input for the mathematical modelling in commercial simulation programs are normally the readily available material data in the material database, and some approximations are unavoidably involved. In fact, the thermo-viscous-elastic residual stress model with a constant solidification temperature are commonly used in industrial applications [27].

4 VALIDATION AND CALIBRATION

Validation and calibration are important steps for ensuring the credibility of injection molding simulation results. Some uncertainties and approximations exist in the assumptions of either the conceptual or mathematical model, the initial conditions or boundary conditions, input of material properties and the parameters in the mathematical model. These sources of uncertainty are propagated to uncertainties in the simulation results. Validation is the process of assessing the physical accuracy of a mathematical model based on comparisons between computational results and experimental data. Calibration is the process of adjusting the parameters used in the model to ensure that the output matches observed data.

As discussed in the previous section, the lack of good material data in anisotropic thermo-viscoelastic residual stress calculation and crystallization simulation necessitates use of simplified thermo-viscous-elastic residual stress model with a constant solidification temperature and various readily available material data obtained under laboratory condition. It can generally provide acceptable results which help users to optimize the processing condition and mold and part design. The model calibration and correction can generally improve the prediction accuracy further [28,29].

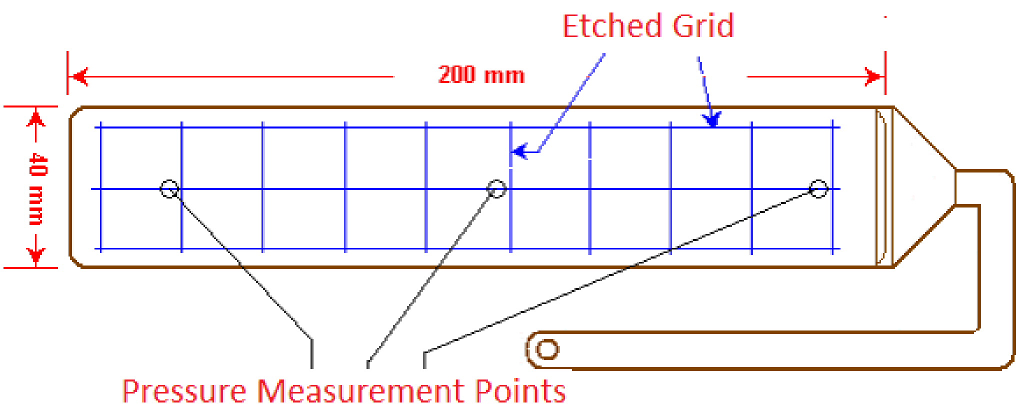


Figure 4. Molded shrinkage sample- tagdie model

For the purpose of model calibration for a given material, up to 28 samples are molded, each with different processing conditions or thickness. The processing condition variables include melt temperature, mold temperature, injection time and profile, packing time and profile, and cooling time.

A grid is etched on the mold to facilitate shrinkage measurements. A sample model is shown in Figure 4. After molding at each of the 28 conditions, the shrinkage is measured both in the flow direction and transverse to flow. The measured shrinkage data is collected from the real processing system in actual injection molding.

A hybrid model, the CRIMS (Corrected Residual In-Mold Stress) model, has been developed for 2.5 D shell solution to utilize shrinkage measurement data [28]. The approach uses the theoretical model as one of the independent variables in a hybrid model that is correlated with measured shrinkage data in order to reduce the discrepancy between measured and predicted shrinkage. Figure 5 shows the excellent match between the experimental and calculated parallel shrinkages using the CRIMS model for an unfilled polypropylene material.

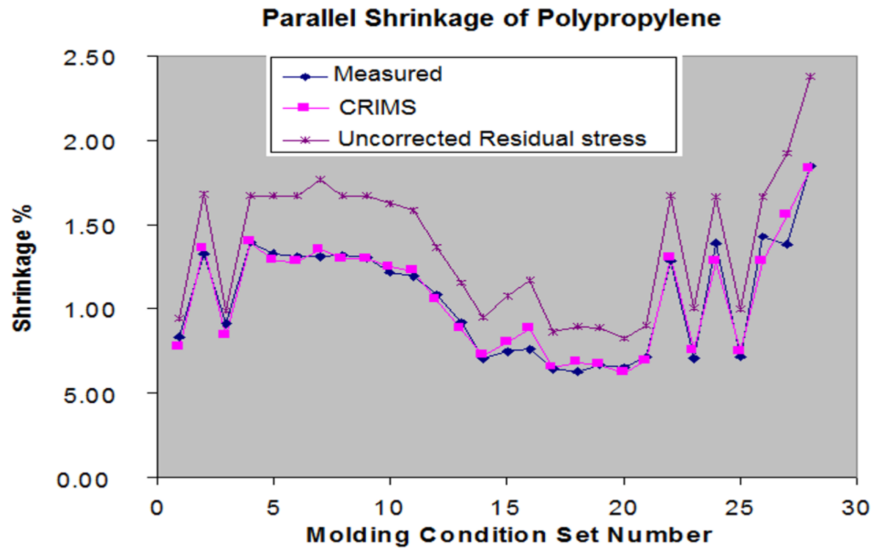


Figure 5. Shrinkage prediction comparison for 28 experimental sets in 2.5D shell solution

A different calibration approach has been developed for three-dimensional shrinkage and warpage simulation for unfilled materials. The shrinkage measurement is used to calibrate the special thermal expansion coefficients of material. The 3D anisotropic thermo-viscous-elastic residual stress model with the shrinkage-calibrated thermal expansion coefficients can generate a more realistic shrinkage and warpage prediction. Figure 6 shows a significant improvement on shrinkage prediction after the special

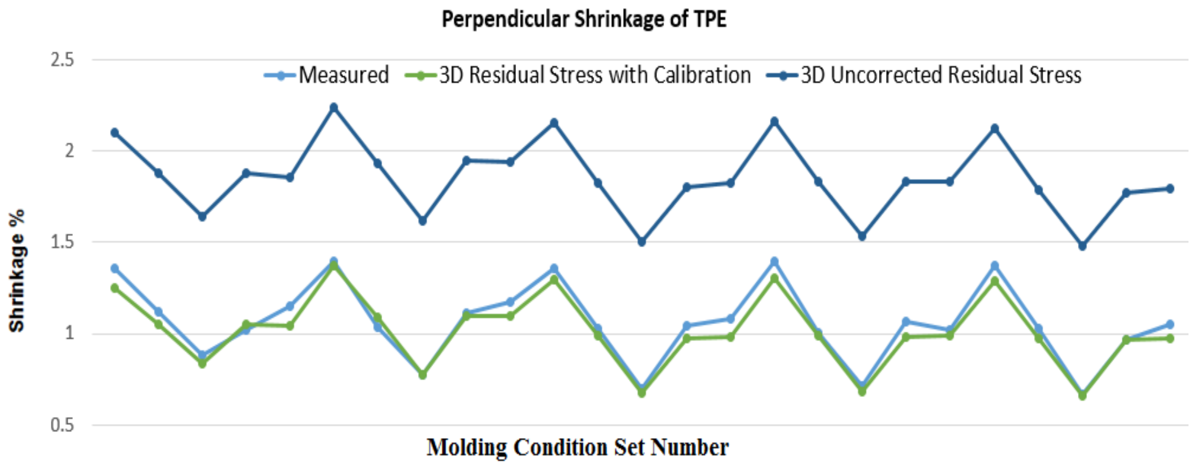


Figure 6. Shrinkage prediction comparison for 25 experimental sets in 3D solution

shrinkage-calibrated thermal expansion coefficient is employed for an unfilled TPE material. Though the uncorrected residual stress model predicts excellent shrinkage variation trend with the different molding sets, it significantly over-predicts shrinkage magnitude for all 25 molding conditions in this special case, and it is probably due to some unreliable material properties in the material database. In the real-world industrial application of injection simulation, to use supplemental values is not uncommon when some specific material properties are not available. By calibration using the measured shrinkage, a theoretical model can be tuned to represent a system over a realistic range of operating conditions.

Although there exist some limitations in the state-of-the-art simulation technology of injection molding, simulation can provide meaningful insight into performance sensitivities to process, geometry and material, even without calibration. These sensitivities may be used by engineers to improve product design and process settings for actual production. A validation case is presented here to illustrate the effectiveness of injection molding simulation.

The conformal cooling box has been 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 7,8). The parts were produced with four combinations of the moving and fixed mold halves [30].

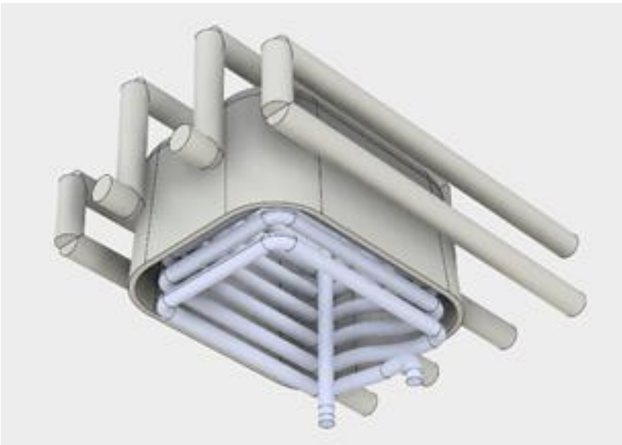


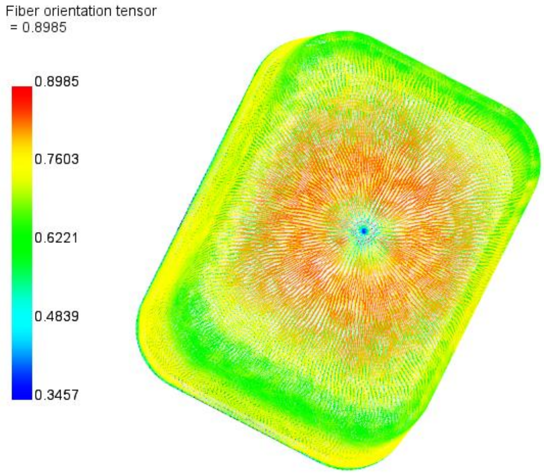
Figure 7. Part and combined cooling circuit

Figure 8. Experimental setup

The part model is meshed into 2,285,777 tetrahedral elements, and the mold model into 3,303,544 tetrahedral elements. 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. A sequence of “Cool(FEM) + Fill + Pack + Warp” analyses were run to predict the final box shape. No model calibration procedure is used in this example.

The figures 9 and 10 show the simulated fiber orientation and Young’s modulus results for the case with 80°C/80°C temperature combination on both mold halves.

The simulation and measured warpage results are compared. The larger inward deflection at the longer wall section is plotted for each condition in Figure 11. 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



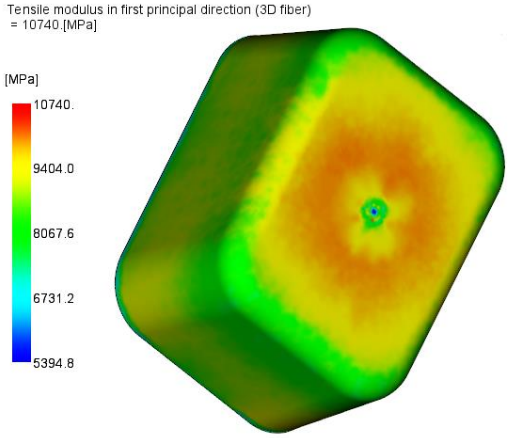


Figure 9. Fiber orientation (1st principal direction)   Figure 10. Tensile modulus (1st principal direction)

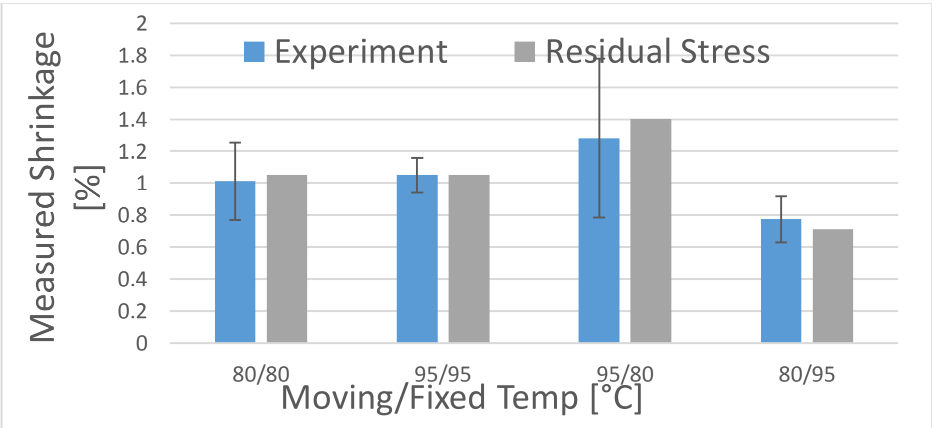


Figure 11. Experimental and simulated deflections between box's edges along the longest length

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. the 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.

5 CONCLUDING REMARKS

Computer Aided Engineering (CAE) for plastic injection molding is arguably the most sophisticated and successful example in the field of process simulation. Further research efforts are required on the reliable and robust morphology and property prediction. On the other hand, the model calibration based on shrinkage measurement is an effective approach for improving the accuracy of shrinkage and warpage simulation.

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