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Predicting Warpage and Residual Stresses in Isotactic Polypropylene using Microstructure-Based Multiscale Simulations

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Abstract

In injection-molded of semi-crystalline polymers, warpage cannot be predicted reliably by macroscopic pvT-based shrinkage modelling alone. The reason is that the local thermal and pressure histories during processing generate pronounced gradients in crystallization degree, microstructure, effective properties, and residual stresses, which collectively determine the final part distortion. This study presents an integrated multiscale framework for isotactic polypropylene that couples non-isothermal filling, packing, and cooling simulation with DSC/Flash-DSC-based crystallization modelling, hierarchical lamella-spherulite homogenization, and thermo-mechanical warpage analysis of a stepped-plate benchmark. The simulations a more thermally expansive skin layers and a stiffer core, in agreement with the measured through-thickness property. Incorporating local crystallization-dependent properties improves the warpage prediction from 50.94 to 32.82 µm, compared with an experimental value of 35.4 µm, reducing the prediction error from 15.54 to 2.58 µm, corresponding to an improvement factor of approximately six. Residual packing pressure has little effect on global shrinkage, but substantially alters local residual stress distributions.

Keywords

Injection molding; isotactic polypropylene; multiscale simulation; warpage; residual stresses

1 Introduction

The increasing geometrical complexity of injection molded thermoplastic parts, together with ever tighter dimensional tolerances, has intensified the need to predict and control shrinkage and warpage. For semi-crystalline thermoplastics in particular, these distortion phenomena arise from strongly inhomogeneous thermal and solidification history within the material [HT01]. A principal cause is the development of non-uniform shrinkage across the part thickness, which originates from

cooling-rate gradients. This is especially pronounced in thick-walled geometries [SKR21]. The resulting non-uniform contraction generates residual stresses that ultimately drive part distortion. In addition, the overall magnitude of shrinkage is affected by process parameters such as packing pressure and packing time, while the local volumetric evolution during solidification is commonly described by pressure-volume-temperature (pvT) behavior [AKL+24, LAH+26].

In thick-walled polypropylene (PP) components, the local cooling rate may differ by several orders of magnitude between the rapidly solidifying skin layers adjacent at the mold wall and the more slowly cooling core region [ACH23]. These local thermal histories govern not only the attainable crystallization degree, but also the formation of the underlying spherulitic microstructure. Since the thermo-mechanical behavior of the material is determined by locally evolving microstructure, the deformation of the final part cannot be described adequately by homogeneous material data or by simplified pvT-based shrinkage modelling alone (Figure 1A). This limitation becomes even more relevant when the pressure state is idealized as dropping instantaneously to ambient after packing, although residual cavity pressure can persist well into the cooling phase and influence the development of residual stresses [LAH+25]. Figure 1B illustrates this idealized representation.

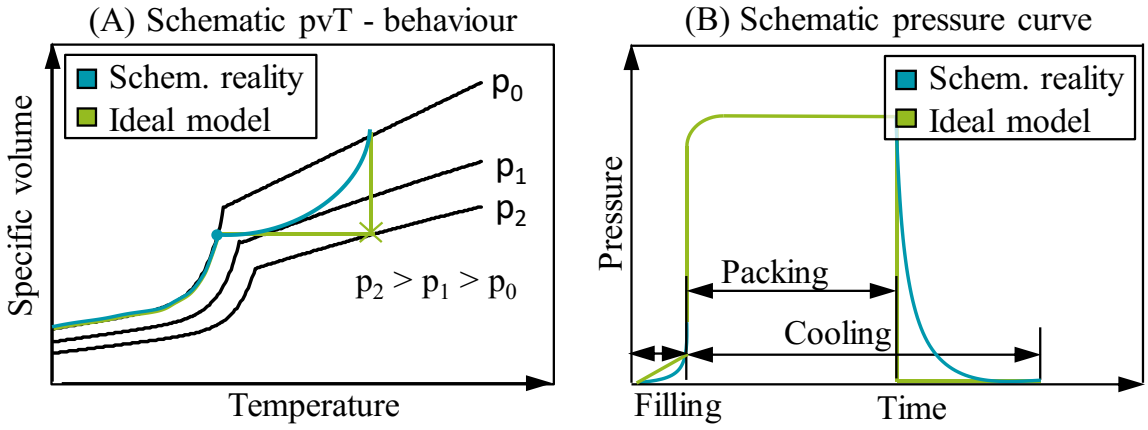


Figure 1: Schematic comparison of simplified and real pvT behavior (A) and cavity pressure (B)

Consequently, warpage prediction requires more than a purely macroscopic pvT-based description of shrinkage. Rather, it requires a physically consistent process-structure-property framework that relates local thermal and pressure histories to crystallization kinetics, microstructure formation, effective material behavior, and the resulting residual stress and distortion state [ACH23, AKL+24, LAH+26, AWH26].

This study presents an integrated multiscale simulation framework for predicting shrinkage and warpage in injection-molded semi-crystalline isotactic polypropylene (iPP). The approach combines injection molding process simulation of filling, packing, and cooling with microstructure evolution modeling and a hierarchical homogenization strategy to derive local crystallization- and microstructure-dependent thermoelastic and thermal properties across the part thickness. On this basis, the macroscopic shrinkage related deformation of a staggered iPP plate is analyzed and validated against warpage measurements. Particular emphasis is placed on demonstrating that local crystallization-dependent property gradients are essential for recovering the correct warpage

behavior, while the inclusion of residual packing pressure is a necessary refinement for representing evolving residual stresses with greater physical fidelity.

2 Integrative Multiscale Simulation Framework

To capture the coupling between process conditions, microstructure formation, local material behavior, and final part distortion, an integrative multiscale simulation framework is developed (Figure 2). Its central objective is to resolve the local inhomogeneous mechanical properties formed during solidification in the filling simulation and to transfer their effects consistently to the warpage prediction of the final part. The framework, therefore, links processing conditions to microstructure development and microstructure related mechanical properties to macroscopic part behavior to predict part warpage.

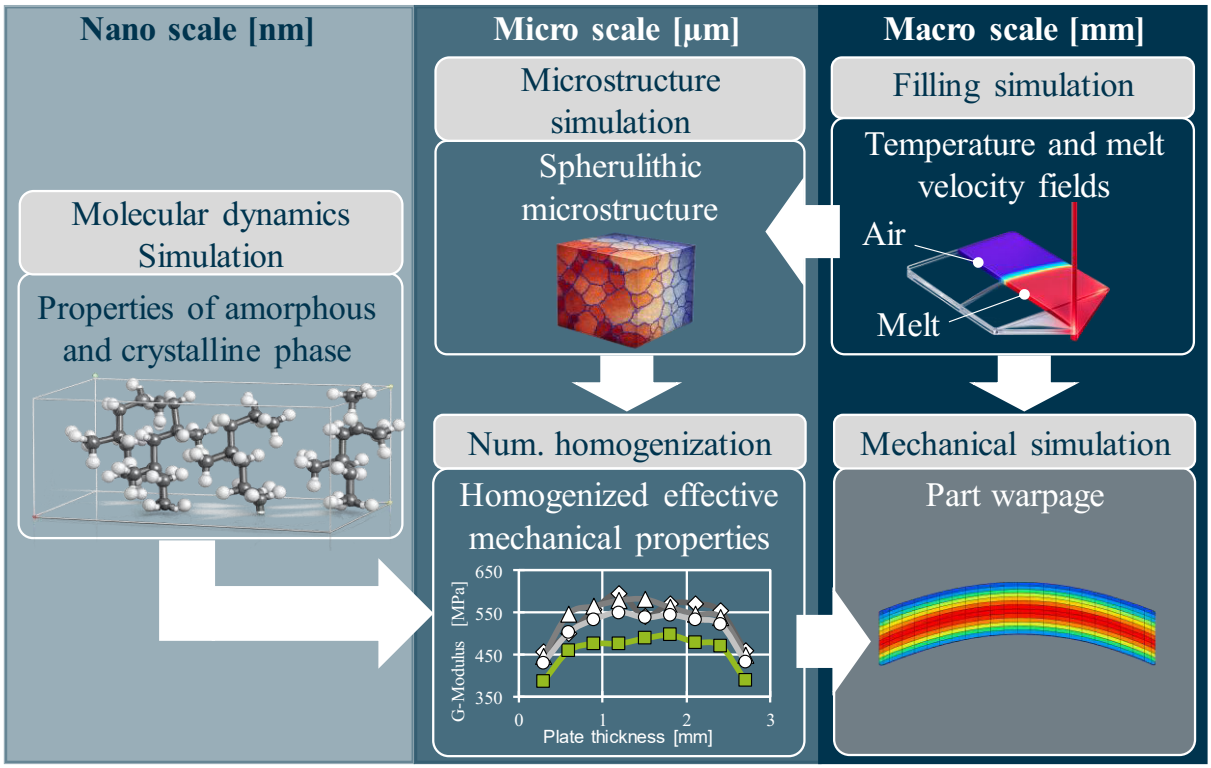


Figure 2: Integrative multiscale simulation framework for predicting of shrinkage and warpage in injection-molded parts

First, the injection-molding process is simulated in COMSOL Multiphysics in order to obtain the local temperature, melt-velocity, and pressure histories during filling, packing, and cooling [AKL+24, AWH26]. The filling stage assumes non-isothermal melt flow. In the post-packing state, residual packing pressure is allowed to relax during cooling, capturing a more realistic temperature and pressure evolution in the cavity. The local temperature and pressure histories control crystallization and volumetric shrinkage and thus define the boundary conditions for all lower-scale analyses.

The second stage describes the evolution of the semi-crystalline microstructure. For this purpose, the time-dependent temperature and velocity fields obtained from the injection-molding simulation are transferred to a microscale crystallization model. Based on these local process histories,

spherulitic microstructures are predicted in representative volume elements (RVEs) distributed across the component thickness. A cellular automaton model combining Ziabicki athermal nucleation with Hoffman-Lauritzen-Davis growth is implemented in the SphaeroSim software [AKL+24, LAH+26]. In parallel, the local crystallization degree assigned to these RVEs is derived from differential scanning calorimetry (DSC) and Flash-DSC measurements as a function of cooling rate [LAM+25]. Because these spherulitic microstructures are composed of crystalline-amorphous lamellar substructures, they define the microstructural basis for the subsequent hierarchical homogenization.

In the third stage, the predicted crystallization degree and spherulitic morphology are converted into local effective material properties by hierarchical homogenization. First, the lamella RVE is homogenized at the nanoscale to determine the effective lamella properties. These properties are then transferred to the predicted spherulitic RVEs and homogenized at the microscale using a radial spherulite model. The resulting local thermo-elastic and thermal properties across the thickness provide the material input for the macroscale warpage simulation [LAM+25, LAH+26]. These local effective properties are then mapped, together with the temperature and pressure fields from the injection-molding simulation, to a 2D thermomechanical plane-strain model [LAH+26, AWH26]. The analysis includes both in-mold and post-demolding cooling. By accounting for residual packing pressure during cooling, the model represents the delayed onset of shrinkage more consistently than a purely thermal approach. This enables direct analysis of the interaction among local shrinkage, stiffness gradients, and residual stresses in the final warpage of the component [LAH+26, AWH26].

A staggered plate serves as benchmark geometry for this investigation (Figure 3). Its defined thickness variation from 4 mm to 1 mm generates strong local differences in cooling rate, solidification, and pressure loss.

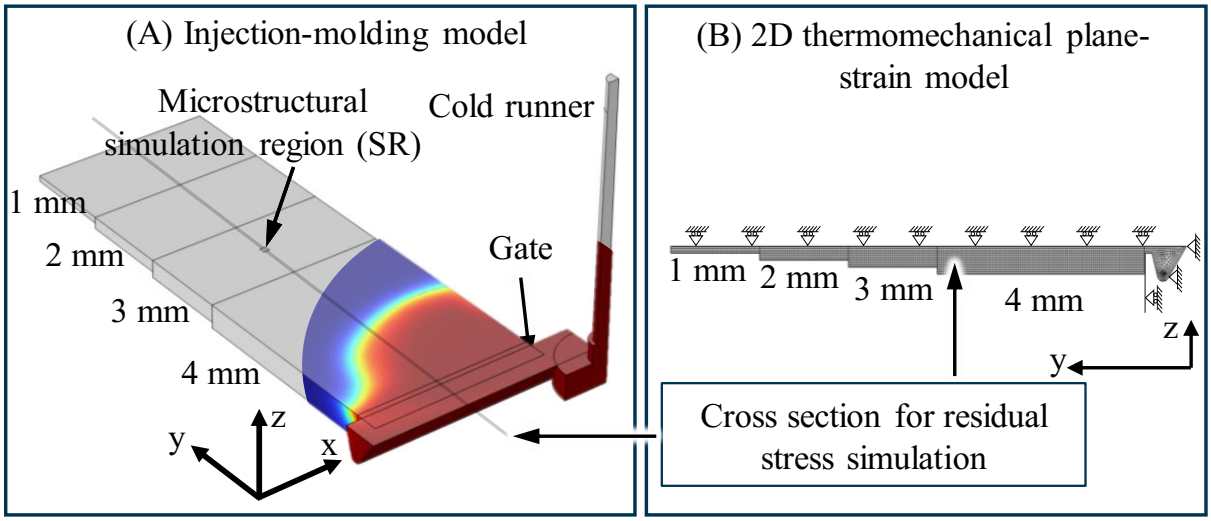


Figure 3: Staggered plate model for injection-molding process simulation (A) and thermomechanical plane-strain analysis (B)

These differences promote pronounced gradients in crystallization degree, spherulitic morphology, local effective properties, and residual stresses, while the geometry remains simple enough for

systematic analysis and experimental validation. The present investigation uses the middle region of the 3 mm thick segment as the simulation region (SR) to analyze the full multiscale chain (Figure 3A), and the cross-section of the staggered plate for the thermomechanical analysis (Figure 3B). The benchmark material is isotactic polypropylene PP505P from Sabic, selected for its industrial relevance, low cost, and well-defined spherulitic α-iPP morphology. Because iPP responds strongly to locally non-uniform cooling, it is particularly suitable for studying the process-induced microstructural inhomogeneities and resulting warpage addressed here. Together, the selected geometry, material, and processing conditions define the basis of the present investigation.

3 Prediction of Effective Thermo-Elastic and Thermal Properties

The injection-molding process of the stepped plate is simulated using the pvT-model parameters, process parameters, and boundary conditions reported in [WHS+19, LAH+26, AWH26]. In SR, the simulation predicts cooling rates from about 2.6 °C/s in the core to about 700 °C/s at the mold wall, while the temperature difference between the upper and lower surfaces remains below 2.0 °C during packing and cooling [LAH+26]. Although the applied packing pressure is reduced from 600 bar to 1 bar after 15 s, residual cavity pressures of up to 46 MPa are still present. Ambient pressure is reached only after about 24 s. After demolding, the plate cools further by natural convection and reaches nearly room temperature after about 135 s [LAH+26, AWH26].

The resulting temperature and melt-velocity fields are transferred to the microstructure analysis in SR. Across the 3 mm thickness, 30 cubic spherulitic RVEs with an edge length of 100 µm are defined. For each spherulitic RVE, the local cooling rate at solidification is evaluated and converted into a local crystallization degree by means of the empirical DSC/Flash-DSC cooling-rate relation [LAM+25]. This local crystallization degree defines the corresponding crystalline-amorphous lamella RVE and, after nanoscale homogenization, the associated effective lamella properties. These local lamella properties are subsequently assigned to the predicted spherulitic RVEs, whose solidified microstructures are transferred to HOMAT for thermoelastic and thermal homogenization [NN20]. The resulting predictions provide the local effective Poisson's ratios, elastic moduli, coefficients of thermal expansion, and thermal conductivities.

To assess the effect of the local crystallization gradient on the predicted effective properties, the properties predicted with the local crystallization model are compared with those obtained under the assumption of constant crystallization degree properties [LAM+25, LAH+26]. Figure 4 shows the effective Poisson's ratios and elastic moduli across the plate thickness in SR. The comparison shows that the use of local crystallization properties mainly affects the skin regions, whereas the constant-crytallization-degree model remains almost uniform across the thickness. For the effective Poisson's ratios, both approaches predict similar values in the central part of the plate, but the local model yields a pronounced increase near both surfaces. The effect on the elastic modulus is even more pronounced. While the constant model predicts an almost uniform stiffness across the thickness, the local-crystallization-degree model shows an increase from the surface toward the

core. This trend is confirmed by experiments, which show similar behavior across the thickness. Further details on the experimental validation are provided in [LAH+26].

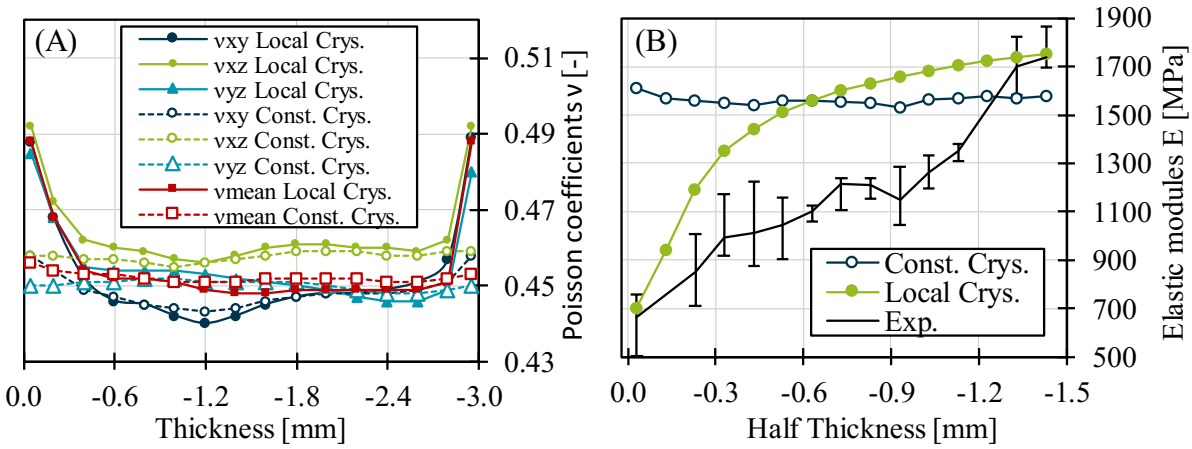


Figure 4: Variation over the plate thickness of the effective Poisson coefficients (A) and elastic modules (B) predicted with constant and variable effective properties and comparison to experiments.

Figure 5 shows the results of the predicted thermal response across the plate thickness in SR. Both models predict a pronounced orthotropy of the effective thermal expansion coefficients, with the general tendency $\alpha_z > \alpha_x > \alpha_y$ throughout the plate thickness. The differences between the two approaches appear near the plate surfaces, close to the mold walls. While the constant crystallization model predicts nearly uniform properties, the local model predicts an increase in all thermal expansion coefficients in the layers near the plate surfaces. A similar observation is obtained for the effective thermal conductivity. Whereas the constant model predicts an almost uniform conductivity across the thickness, the local model yields a clear reduction near the surfaces.

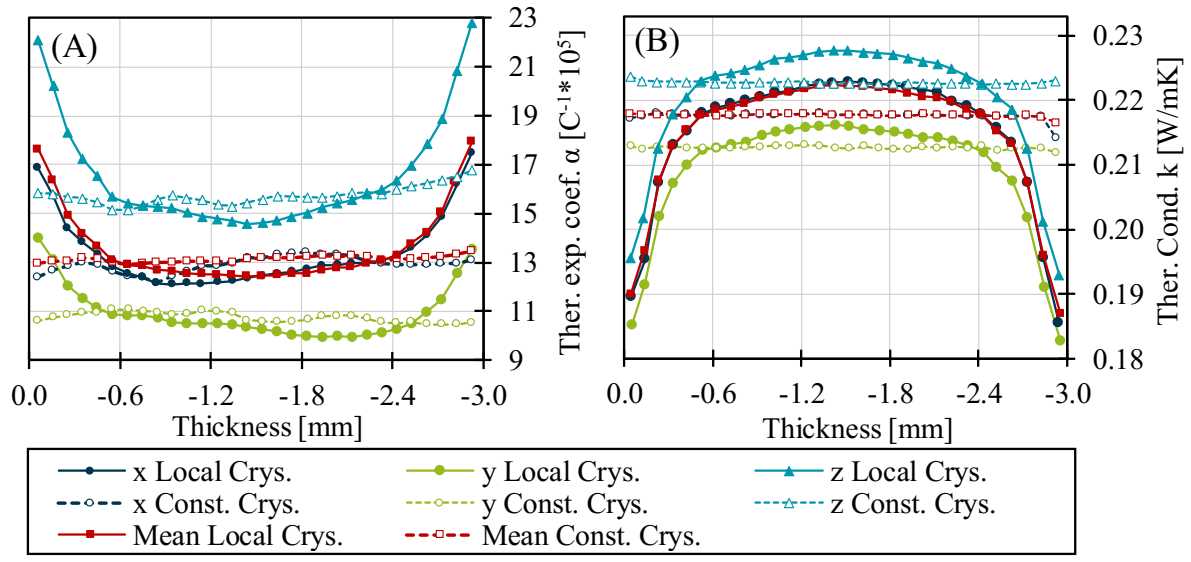


Figure 5: Variation over the plate thickness of the effective thermal expansion coefficients (A) and thermal conductivity (B) predicted with constant and variable effective properties.

These results show that the local crystallization history mainly changes the effective properties in the near-surface regions. Near the plate surfaces, where the crystallization degree is lowest, higher Poisson's ratios, higher thermal expansion coefficients, and lower thermal conductivities are

predicted, while the elastic moduli decrease. Towards the highly crystallized core, the material becomes stiffer and thermally less expansive. Further details regarding the degree of crystallization can be found in [AKL+24]. This demonstrates that local crystallization must be considered to predict realistic effective-property distributions. Its effect on the prediction of shrinkage and warpage in the molded part is analyzed in the next section.

4 Distortion and Warpage Prediction

The local effective thermoelastic and thermal properties derived in the previous section are subsequently transferred to the thermomechanical plane-strain model to evaluate their effect on the macroscopic distortion behavior of the 3 mm plate section. Further details on the plane-strain model are provided in [LAH+26]. To quantify the influence of the local crystallization gradient, the predictions obtained with crystallization-dependent local properties are compared with those based on constant effective properties across the plate thickness [LAH+26, AWH26]. Figure 6 shows the evolution of the predicted shrinkage after mold opening. In both the width and thickness directions, the model with local properties predicts greater shrinkage than the constant-property model. This difference is caused by the weakly crystallized skin layers, which contract more during cooling.

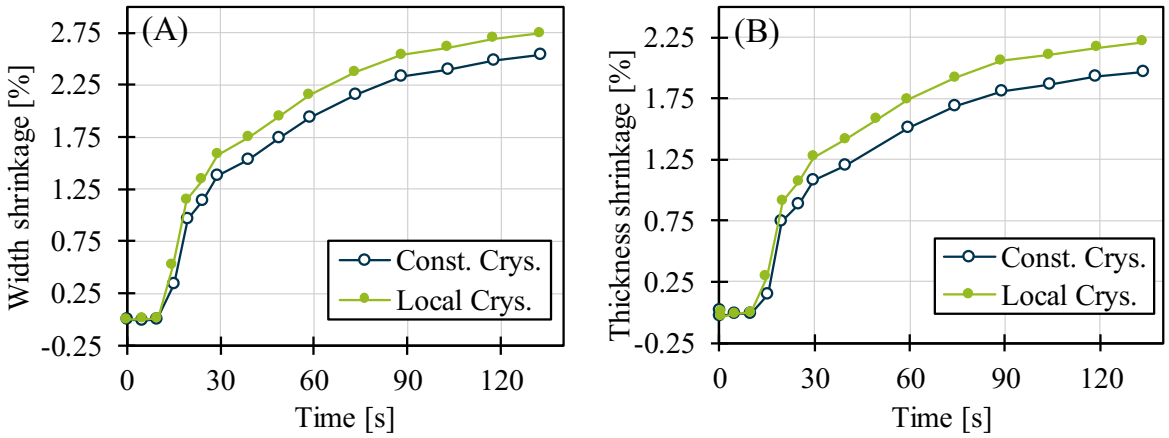


Figure 6: Evolution of the width shrinkage (A) and thickness shrinkage (B) predicted by the two model variants.

The effect on warpage after mold opening is shown in Figure 7. In the present analysis, warpage is defined as the vertical displacement Uy of the bottom node at the right-hand side of the 3 mm plate section. For validation, the final warpage was measured on five iPP plates by optical 3D scanning using a GOM ATOS system. The measured mean value was used for comparison with the simulation. Further details on the experimental warpage measurement are provided in [LAH+26]. Although the local-property model predicts greater shrinkage, it leads to smaller final warpage. The simulation with constant properties yields a predicted warpage of 50.94 µm, whereas accounting for local crystallization-dependent properties reduces the predicted warpage to 32.82 µm. The experimental reference value is 35.4 µm. As a result, the prediction error decreases from 15.54 µm to 2.58 µm, corresponding to an improvement factor of 6 in predictive accuracy.

Overall, the distortion analysis confirms the central role of local crystallization in predicting the final part geometry. A constant-property description is not sufficient to represent the actual

shrinkage and warpage behavior. Instead, local crystallization-dependent effective properties must be considered to predict realistic distortion in injection-molded semi-crystalline iPP components.

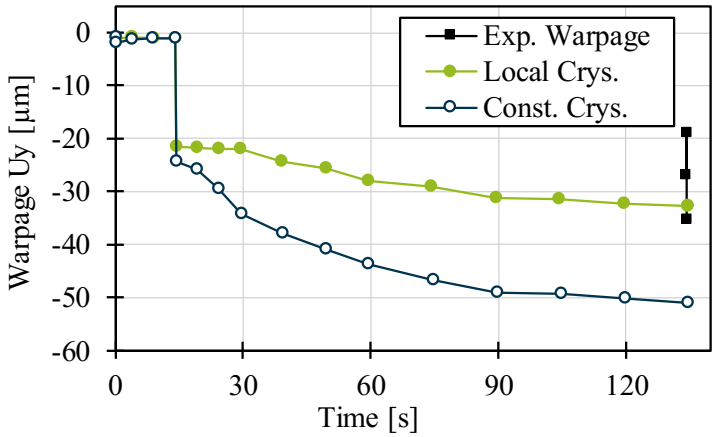


Figure 7: Warpage evolution after mold opening predicted with constant and variable effective properties

5 Process Refinement Through Residual Packing Pressure and Residual Stresses

A further refinement concerns the transfer of the pressure state from packing to cooling. In conventional shrinkage analyses, the cavity pressure is often assumed to drop instantaneously to ambient pressure once the applied packing pressure is released. For the present iPP stepped plate, however, the process simulation shows that this assumption is not valid. Although the applied packing pressure is reduced from 600 bar to 1 bar after 15 s, residual cavity pressures of up to 46 MPa are still present at 15.05 s, and ambient pressure is reached in section SR only after about 24 s. The cooling phase can therefore not be treated as purely thermal from the end of packing onward. Instead, volumetric shrinkage can fully develop only after the local residual pressure has relaxed sufficiently.

This process refinement has only a minor effect on the overall shrinkage prediction. When residual in-mold pressure is taken into account, the effective time at ambient pressure during cooling is reduced to about 6 s instead of about 15 s. Nevertheless, the difference in shrinkage along the longest part axis remains small, with a maximum deviation of only 3.5 µm, which is within the measurement uncertainty of the optical 3D scanning system. From the viewpoint of global shrinkage, the residual packing pressure may, therefore, be neglected.

In terms of the development of process-induced residual stresses (Figure 8), the simulations show that the local stress distribution at the end of cooling changes when residual packing pressure is considered. The strongest differences occur in the early-solidifying 1 mm and 2 mm sections and in the gate region, where local stresses are frozen in before the pressure can relax completely. This should not be interpreted as a sustained pressure effect. The absolute stress levels must therefore be assessed with caution, since viscoelastic relaxation is not yet fully represented in the present framework. This result is of direct relevance for warpage prediction, since the final distortion results not only from the shrinkage magnitude, but also from the interaction between shrinkage and the residual stress state present at demolding. The refinement introduced here, therefore, shows that

accurate future warpage predictions must combine local crystallization-dependent material properties with a realistic process-induced initial stress state [AWH26].

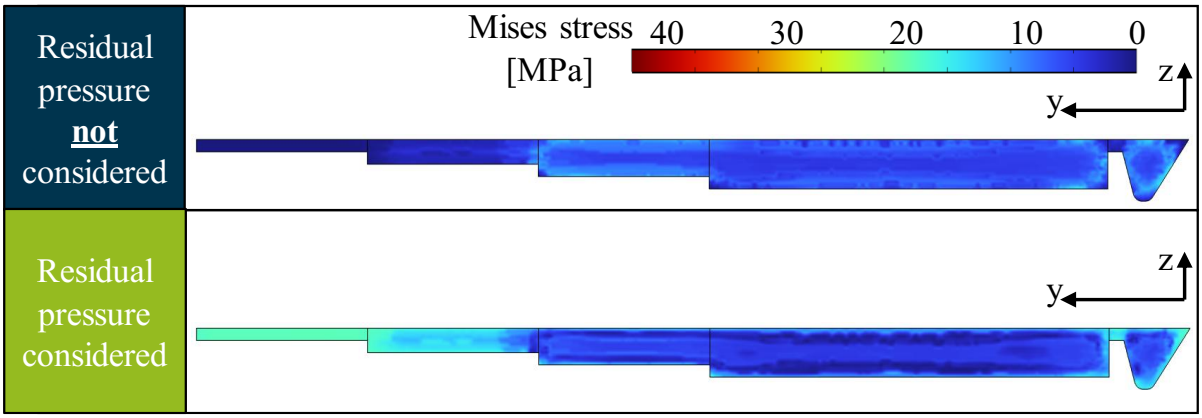


Figure 8: Comparison of the residual stresses with and without consideration of residual packing pressure

6 Summary and Conclusions

This study shows that accurate warpage prediction for injection-molded semi-crystalline isotactic polypropylene requires an integrated process-structure-property framework. At the component level, the developed multiscale simulation chain captures how local cooling conditions determine crystallization degree, microstructure, effective thermos-elastic properties, and ultimately part distortion.

The comparison between the two modeling approaches demonstrates the importance of local crystallization-dependent properties. The simulation with constant material properties predicts a warpage of 50.94 µm, whereas the model with local crystallization-dependent properties predicts 32.82 µm, compared with an experimental value of 35.4 µm. Accordingly, the prediction error decreases from 15.54 µm to 2.58 µm, corresponding to an approximate **improvement factor of 6** in predictive accuracy. These results confirm that a constant-property description is not sufficient to reproduce the actual shrinkage and warpage behavior of the molded part.

The results further show that residual packing pressure has only a minor effect on global shrinkage, but a pronounced effect on the local residual stresses. This is especially relevant in the early-solidifying 1 mm and 2 mm sections and in the gate region, where stresses can be frozen in before pressure relaxation is complete. Future refinement of the framework should, therefore, focus on expanding it to include other polymers, polymers with polycrystalline microstructures, or filled/anisotropic materials.

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Conflict of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data supporting the findings of this study are available at:
http://hdl.handle.net/21.11102/7ab0387c-f490-4863-baaf-4668a867da7a

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