Autodesk® Moldflow Insight 2024

Validation of Coupled Analyses of Fiber Orientation and Polymer Flow

Executive Summary

The Autodesk Moldflow Insight 2024 software release includes new features that consider the effect of fiber orientation on the anisotropic thermal conductivity and rheology of polymer composites in 3D analyses. This report describes the mathematical models for fiber-flow coupled analyses, introduces the new solver options and result, and demonstrates the impacts of coupling on simulation results in various verification and validation cases.

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Introduction

When using the standard flow equations in previous releases of Autodesk Moldflow software, the Flow solver calculates the fiber orientation in polymer composites based on the flow solution during the molding process, but it does not consider the effect of the fibers on the polymer flow. This approach is known as a *decoupled* flow analysis, where the thermal conductivity and viscosity of the polymer flow are assumed to be isotropic and independent of the fiber orientation.

However, in reality, the thermal conductivity in polymer composites is typically anisotropic due to the difference between the thermal conductivities of the fiber and the polymer matrix. The degree of anisotropy varies with the fiber orientation. Additionally, the polymer flow experiences resistance around the fibers, resulting in fully anisotropic polymer rheology that varies in different directions depending on the fiber orientation and velocity gradient in the flow.

In the Autodesk Moldflow Insight 2024 release, two new options are available in 3D analyses to consider the fiber orientation's impact on thermal conductivity and polymer rheology, respectively. With these options enabled, the fiber solution and flow solution are fully *coupled* in the Flow solver. This means that the fiber solution is not only calculated based on the flow solution but also subsequently impacts the flow solution.

Mathematical Modeling

Fiber orientation effect on thermal conductivity

In a polymer composite with cylindrical fibers fully aligned in the first direction, the three diagonal components of the anisotropic thermal conductivity tensor are described as follows [1][2]:

$$k_i^{\mathrm{UD}} = k_i^m \frac{[(V_f - 1)S_{ii} - V_f]\left(k_i^f / k_i^m - 1\right) - 1}{(V_f - 1)S_{ii}\left(k_i^f / k_i^m - 1\right) - 1}$$

with

$$S_{11} = 1 - g$$

$$S_{22} = S_{33} = g/2$$

$$g = \begin{cases} \dfrac{r}{(r^2-1)^{3/2}}\left[r\left(r^2-1\right)^{1/2} - \cosh^{-1} r\right] & (r > 1) \\ \dfrac{r}{(1-r^2)^{3/2}}\left[\cos^{-1} r - r\left(1-r^2\right)^{1/2}\right] & (r < 1) \end{cases}$$

where k_i^f and k_i^m are the thermal conductivities of the fiber and the polymer matrix, respectively, in the i-th direction (i = 1, 2, 3), V_f is the fiber volumetric fraction, and r is the fiber aspect ratio of the length to the diameter. For any given fiber orientation distribution, orientation averaging is applied to calculate the thermal conductivity tensor of the polymer composite.

Typically, the fiber in a polymer composite has a higher thermal conductivity than the polymer matrix. As a result, the composite's thermal conductivity is highest in the direction along which the most fibers are aligned. In thin molded parts, where most fibers ($r > 1$) are typically aligned in the plane parallel to the mold cavity surface, the composite's thermal conductivity in the thickness direction is lower than in other directions.

As the thermal conductivity data in the material database represent bulk values of a composite with a certain fiber orientation in a measurement sample, the isotropic thermal conductivity of the polymer matrix is first separated from the database values by assuming a specific fiber orientation.

During each time step in the simulation of the molding process, once the fiber orientation solution is obtained based on the flow solution, an updated thermal conductivity tensor is calculated for each tetrahedral element. The finite element form of the energy equation for the next time step is then modified to incorporate the updated anisotropic thermal conductivity.

Fiber orientation effect on polymer rheology

The constitutive equation of the polymer melt, which accounts for the anisotropic contribution from fibers, is expressed as follows [3]:

$$\tau_{ij} = \eta_I \left(\dot{\gamma}_{ij} + N_p A_{ijkl} \dot{\gamma}_{kl} \right)$$

where τ_{ij} is the extra stress tensor, $\dot{\gamma}_{ij}/2$ is the deformation rate tensor, η_I is the isotropic viscosity, A_{ijkl} is the fourth-order fiber orientation tensor, and N_p is a scalar called the *Particle Number*.

On the right-hand side of the constitutive equation, $\eta_I \dot{\gamma}_{ij}$ represents the typical isotropic term, while $\eta_I N_p A_{ijkl} \dot{\gamma}_{kl}$ describes the anisotropic effect from fibers. The strength of this effect depends on the value of the Particle Number (N_p) and the degree of stretching or compression along the fiber alignment direction. The Particle Number (N_p) is automatically calculated based on the fiber aspect ratio, fiber volumetric fraction, and the strength of fiber alignment. N_p increases with higher fiber aspect ratios or volumetric fractions, or with decreased strength of fiber alignment.

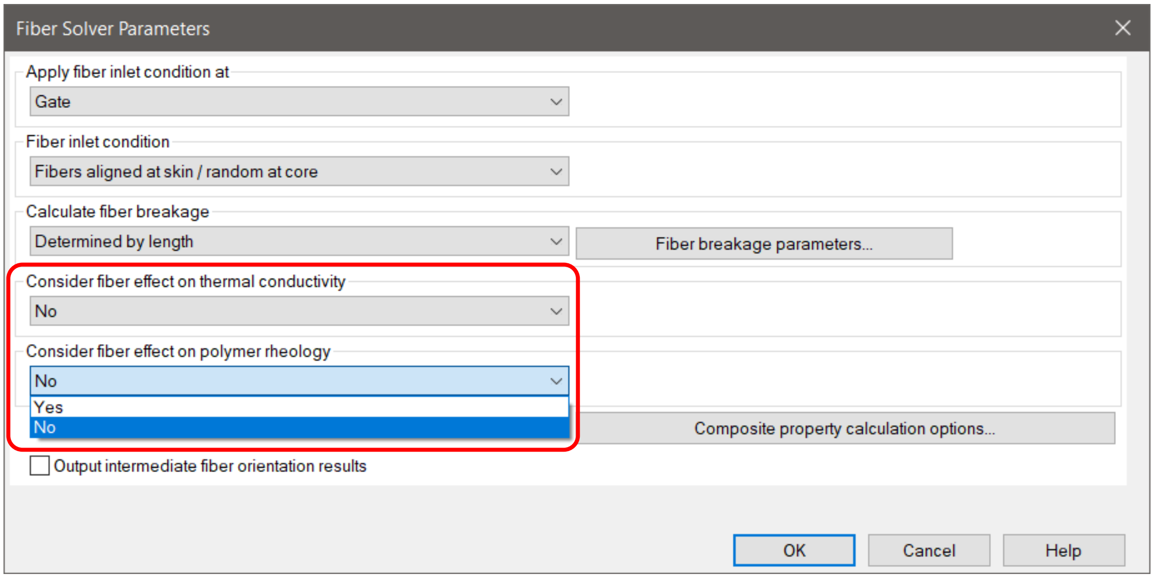
As for the viscosity data, the scalar values supplied in the material database or specified via the Solver API represent the bulk values of the polymer composite with a certain fiber orientation. To account for this, the isotropic viscosity (η_I) is first separated from the given viscosity value using an empirical fiber orientation.

During each time step in the simulation of the molding process, once the fiber orientation solution is obtained based on the flow solution, the finite element forms of the momentum and energy equations for the next time step are then modified to incorporate the anisotropic contribution of fibers.

Solver Options and Results

In the Autodesk Moldflow Insight 2024 software, there are new options available in the **Fiber Solver Parameters** dialog box: “**Consider fiber effect on thermal conductivity**” and “**Consider fiber effect on polymer rheology**,” as shown in Figure 1. These options allow users to take into account the impact of fibers on thermal conductivity or polymer rheology during the simulation. By default, both options are set to “No,” meaning that the fiber effect is not considered. Users can modify these settings according to their specific analysis requirements.

The thermal conductivity data in the material database can be either a bulk value or an anisotropic through-thickness value. The measurement type is specified in the **Test information (Thermal Conductivity Data)** dialog box as shown in Figure 2. When decomposing the matrix thermal conductivity, the bulk value of a polymer composite from the material database is required. If the option “Consider fiber effect on thermal conductivity” is set to “Yes” and the thermal conductivity data from the material database is anisotropic through-thickness value, the Flow solver will display a warning message and will not consider the fiber effect on thermal conductivity.



Fiber Solver Parameters

Apply fiber inlet condition at: Gate

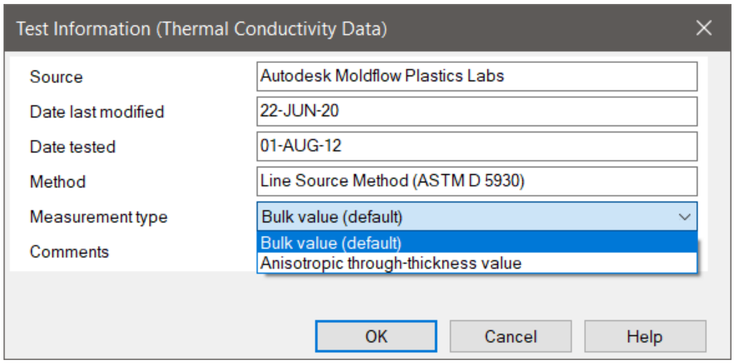
Fiber inlet condition: Fibers aligned at skin / random at core

Calculate fiber breakage: Determined by length

Consider fiber effect on thermal conductivity: No

Consider fiber effect on polymer rheology: No

Figure 1. Solver options of “Consider fiber effect on thermal conductivity” and “Consider fiber effect on polymer rheology”.



Test Information (Thermal Conductivity Data)

Source	Autodesk Moldflow Plastics Labs
Date last modified	22-JUN-20
Date tested	01-AUG-12
Method	Line Source Method (ASTM D 5930)
Measurement type	Bulk value (default)
Comments	

Figure 2. “Measurement type” specified in the “Test information (Thermal Conductivity Data)” dialog box.

When the option “Consider fiber effect on thermal conductivity” is set to “Yes,” the Flow solver will generate a new result called the **Thermal conductivity tensor** for a composite material filled with fibers or disk-like fillers. This result allows examination of the thermal conductivity in different directions and at various locations within the final molded part. It can also be exported in an interface file for subsequent structural and thermal analyses.

When the option “Consider fiber effect on polymer rheology” is set to “Yes,” the Flow solver will not generate the viscosity result for a composite material filled with fibers or disk-like fillers. This is because the scalar value result cannot accurately represent the anisotropic rheology in the polymer flow.

Verification and Validation

Fiber orientation effect on thermal conductivity

To validate the fiber orientation effect on the thermal conductivity, a series of plaques were injection molded in the Autodesk Moldflow Plastics Lab using a polypropylene material filled with 20wt% short carbon fibers. The thicknesses of the plaques were 2, 3, and 5 mm. The pressure history during the molding process was recorded at the middle of the part. Samples were cut from the middle of the molded parts to measure the thermal conductivity using two different methods. One method measured the bulk thermal conductivity, while the other measured the thermal conductivities in the thickness and radial directions [4]. The part geometry is illustrated in Figure 3, and the measurement location is marked accordingly. The measured bulk thermal conductivity of the composite ranged from 0.32 to 0.45 W/m·C, depending on the temperature, while the thermal conductivity of the carbon fibers was 8.36 W/m·C.

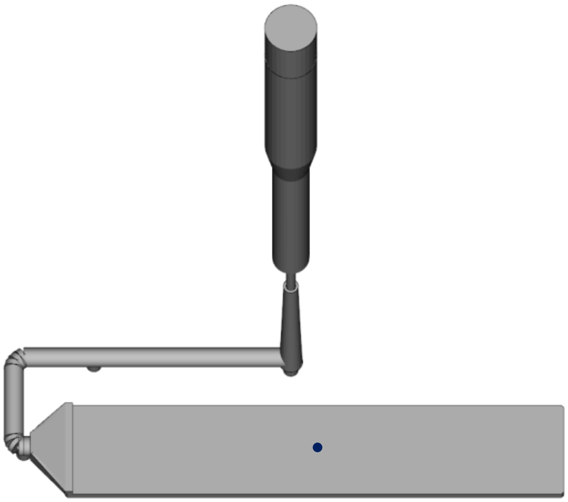
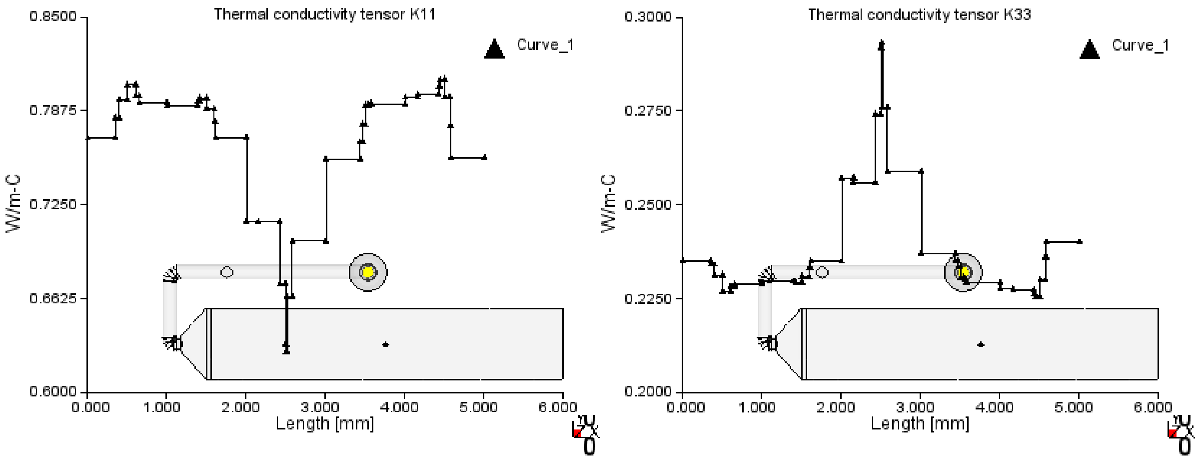
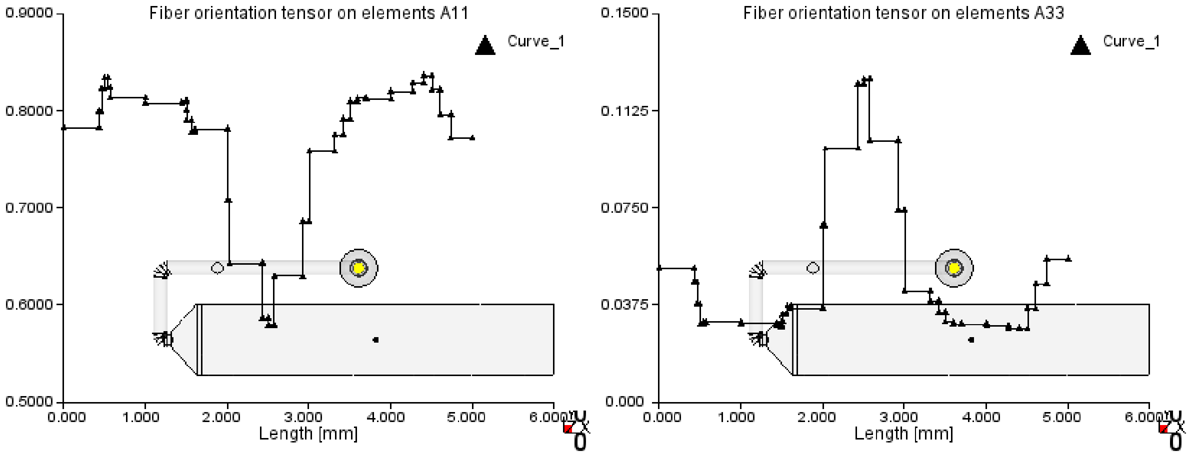


Figure 3. Geometry and measurement location of the plaque.

Figure 4(a) shows the thermal conductivity tensor result, which is generated by the Flow solver when the option “Consider fiber effect on thermal conductivity” is set to “Yes”. In this figure, the number 1 denotes the flow direction, and the number 3 denotes the thickness direction. It is evident that the thermal conductivity in the thickness direction is much lower than that in the flow direction. This is because most fibers are aligned in the flow direction in this part and the carbon fiber’s thermal conductivity is much higher than the matrix polymer’s thermal conductivity. The thermal conductivity in the thickness direction is also lower than the bulk thermal conductivity. The through-thickness profile of the thermal conductivity tensor also exhibits a shell-core-shell structure, which is correlated with the profile of the fiber orientation tensor shown in Figure 4(b). The thermal conductivity in the thickness direction was then averaged through the thickness and compared with the measured data in Figure 5. The predictions show very good agreement with the measurements.



(a) Thermal conductivity tensor



(b) Fiber orientation tensor

Figure 4. Predictions of the thermal conductivity and fiber orientation tensors through thickness at the middle of the molded 5 mm plaque.

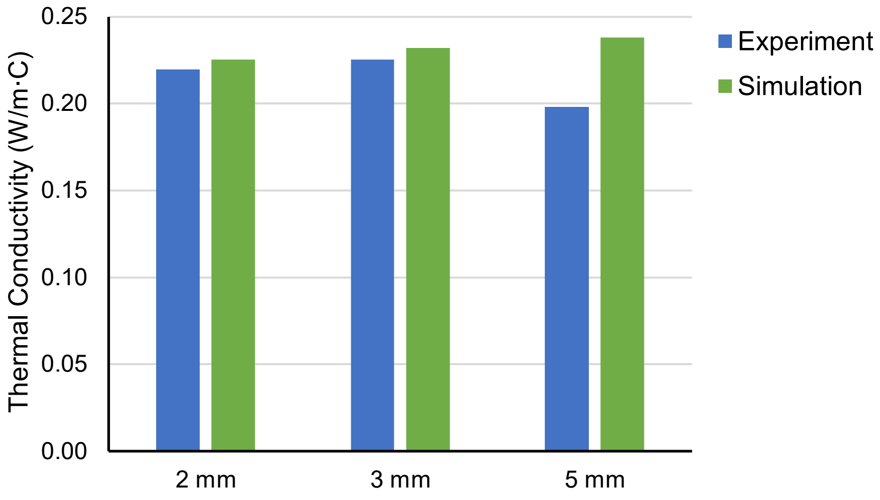


Figure 5. Comparison of the measured and predicted thermal conductivity in the thickness direction.

The predictions of the pressure history, when the option “Consider fiber effect on thermal conductivity” is set to both “No” (decoupled) and “Yes” (coupled), are compared with the experimental measurements in Figure 6. When the fiber effect is considered, the thermal conductivity is lower in the thickness direction, resulting in weaker heat transfer in that direction. As a result, the pressure decay during the packing stage is slower in the coupled analysis compared to the decoupled analysis. The coupled analysis produces better agreement with the measured data than the decoupled analysis.

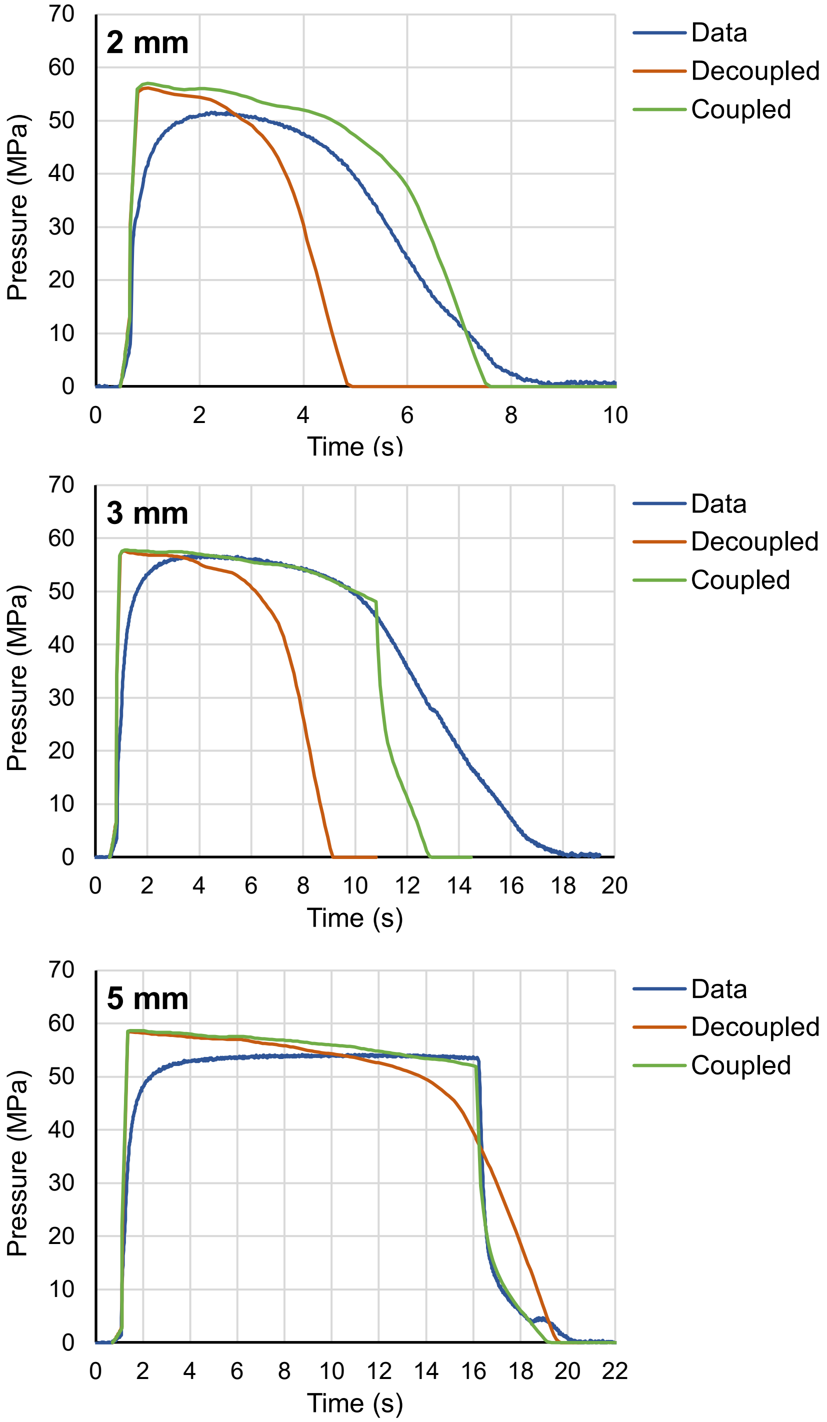


Figure 6. Comparison of the measured and predicted pressure history during the molding process.

Fiber orientation effect on polymer rheology

The results from simulations are compared in this section when the option “Consider fiber effect on polymer rheology” is set to both “No” (decoupled) and “Yes” (coupled) for several compression molding and injection molding cases. The coupling of fiber orientation and polymer rheology has a significant impact on the filling pattern, particularly in compression molding. The coupling affects the prediction of fiber orientation, primarily through its influence on the filling pattern or velocity profiles. However, its effect is relatively small for some short fiber materials. Additionally, the coupling also affects the pressure prediction.

A useful verification case for the coupled analysis is a compression molding of a simple disk, as illustrated in Figure 7. The initial charge is compressed to mold a 2.5 mm thick disk using a polypropylene material filled with 25wt% short glass fibers. In the decoupled analysis, the flow pattern is not influenced by fibers and exhibits a perfect circular shape, as shown in Figure 8(a). In the coupled analysis, the initial charge is first given a planar random orientation, represented by the red axes in Figure 8(b). The orientation effect is isotropic in the plane of the part, and the filling pattern remains circular. However, in Figure 8(c), where all fibers in the initial charge are aligned in one direction, the polymer melt experiences strong resistance from the fibers in that direction. Therefore, the polymer flows more slowly in the direction of fiber alignment compared to perpendicular to the fiber alignment, resulting in an oval-shaped filling pattern that stretches in the perpendicular direction. These filling patterns are accurately captured by the coupled analysis in Autodesk Moldflow Insight software.

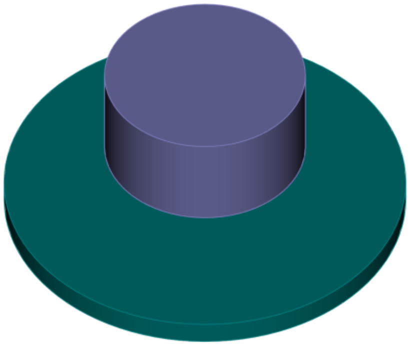
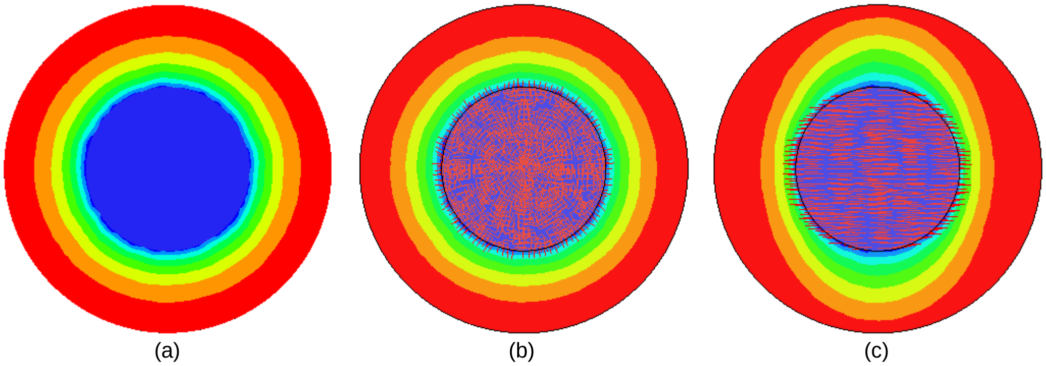


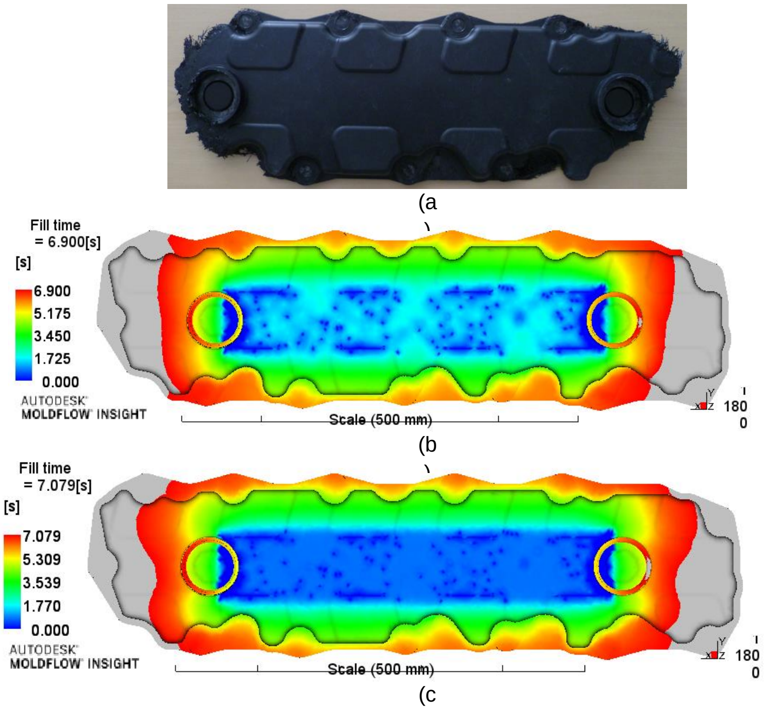
Figure 7. Compression molding geometries: the initial charge (top) and the compression molded disk (bottom).



(a) (b) (c)

Figure 8. Comparison of the filling predictions: (a) from the decoupled analysis, (b) from the coupled analysis with a planar random orientation in the initial charge, and (c) from the coupled analysis with a fully aligned orientation in the initial charge.

In a compression molding validation case-study, a larger panel was compression molded using a thermoset sheet molding compound filled with 34wt% long fibers. In the initial charge, the fibers are assumed to be randomly aligned in the plane. Figure 9 compares the filling patterns from the decoupled and coupled analysis with the actual short shot molding, specifically when two bosses on the part are almost filled. In the decoupled analysis, the flow front appears almost flat after the bosses. However, in the coupled analysis, the flow goes around the bosses and moves faster near the edges compared to the middle. Although there are still some discrepancies between the predictions and the actual short shot molding, the coupled analysis shows better agreement with the actual molding compared to the decoupled analysis.



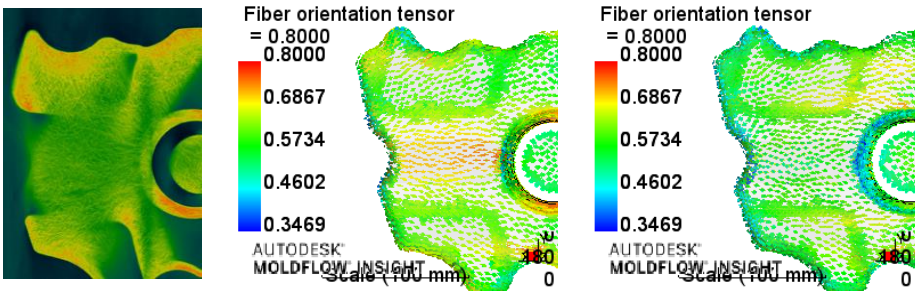
(a)

(b)

(c)

Figure 9. Comparison of the filling patterns (a) from the short-shot molding, (b) from the decoupled analysis, and (c) from the coupled analysis.

The fiber orientation inside the part is visualized using a CT scan and compared with the simulation results in Figure 10. In the decoupled analysis, stronger fiber alignment along the flow direction is predicted after the boss. In contrast, the coupled analysis predicts a more random orientation. The significant difference in the orientation predictions is primarily attributed to the different filling patterns observed in the coupled and decoupled analyses.



(a) (b) (c)

Figure 10. Comparison of the fiber orientation: (a) from the CT scan of the molded part, (b) from the decoupled analysis, and (c) from the coupled analysis.

In an injection molding case-study, a 3 mm thick plaque was injection molded using a polyamide 66 filled with 35wt% short glass fibers. The fiber orientation through the part thickness was measured at several locations within the part. The part geometry is illustrated in Figure 11, and the measurement locations are marked accordingly.

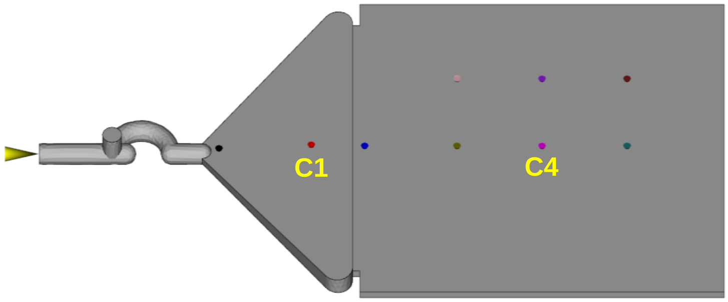


Figure 11. Geometry and measurement locations of the 3 mm thick plaque.

The fiber orientation predictions from the decoupled and coupled analyses are compared with the measured data in Figure 12. In this figure, the number 1 denotes the flow direction, and the number 2 denotes the crossflow direction. Both the measurements and predictions exhibit the typical shell-core-shell orientation structure observed in thin injection-molded parts. This structure includes transverse alignment in the middle of the thickness and strong flow direction alignment near the surfaces. The fiber orientation predictions from the decoupled and coupled analyses are almost identical. This suggests that coupling the fiber orientation with the polymer rheology has a very small influence in this case.

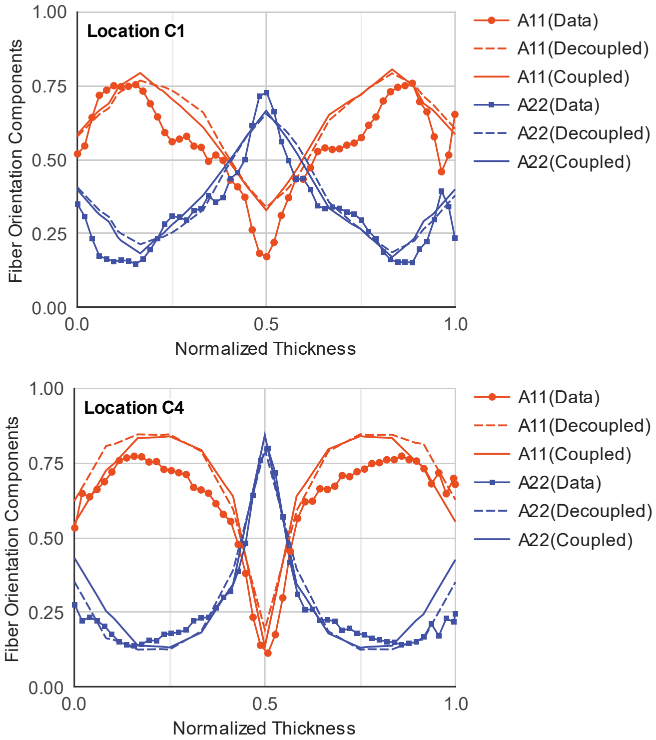


Figure 12. Comparison of the predicted fiber orientation from the decoupled and coupled analyses with measured fiber orientation data for the 3mm thick plaque.

In a second injection molding validation case-study, a 3.18 mm thick plaque was molded using a polyamide 66 material filled with 50wt% long carbon fibers. The fiber orientation through the part thickness was measured at several locations within the part. The part geometry is illustrated in Figure 13, and the measurement locations are marked accordingly.

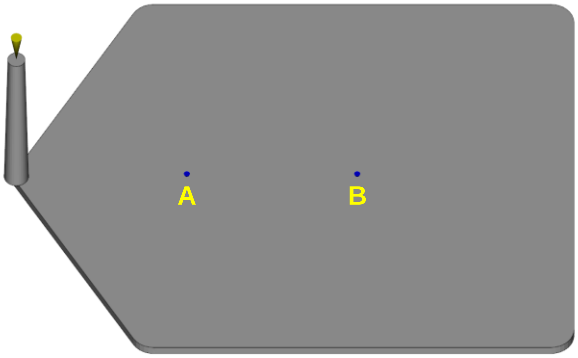


Figure 13. Geometry and measurement locations of the 3.18 mm thick plaque.

The predictions and measurements are compared in Figure 14, demonstrating that the coupled analysis predicts a wider core and shows better agreement with the measured data compared to the decoupled analysis at both locations. Additionally, at location A, which is close to the end of the fan gate, the prediction from the coupled analysis is less symmetric through the thickness compared to the prediction from the decoupled analysis. This observation is reasonable because the polymer was injected from the top surface, indicating that the fiber orientation effect on the rheology is more pronounced around the gate where the flow is more complex than a simple shear flow. Furthermore, the Particle Number (N_p) increases with the fiber aspect ratio. Therefore, the fiber orientation effect on the polymer rheology for the long fiber material in this case is stronger than the effect observed for the short fiber material in the previous case.

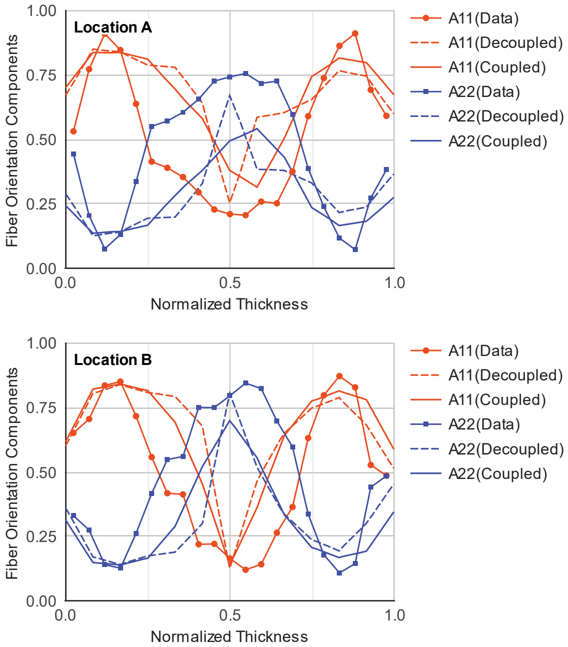


Figure 14. Comparison of the predicted fiber orientation from the decoupled and coupled analyses with measured fiber orientation data for the 3.18mm thick plaque.

In a third injection molding example, a 2 mm plaque was molded using a polyamide 6 material filled with 40wt% short glass fibers, and the fiber orientation was measured at several locations within the part. The part geometry is illustrated in Figure 15, and the measurement locations are marked accordingly.

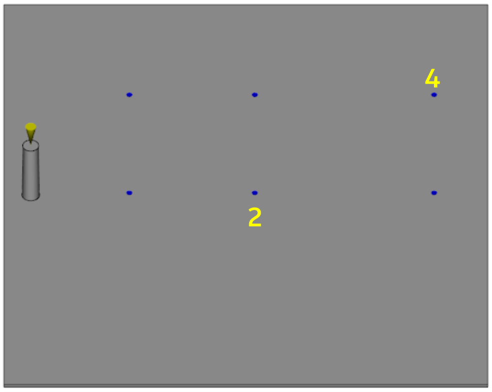


Figure 15. Geometry and measurement locations of the 2 mm thick plaque.

The predicted and measured fiber orientation data are compared in Figure 16. At location 2, the predictions from the decoupled and coupled analyses are very similar and both match the measured data very well. Coupling does not have a significant impact on the fiber orientation result at the middle of the part. However, at location 4, the predictions from the decoupled and coupled analyses differ considerably. The decoupled analysis still predicts the typical shell-core-shell orientation structure, while the coupled analysis predicts very similar A_{11} and A_{22} orientation components in the shell layers. The coupled analysis provides better agreement with the measurements compared to the decoupled analysis.

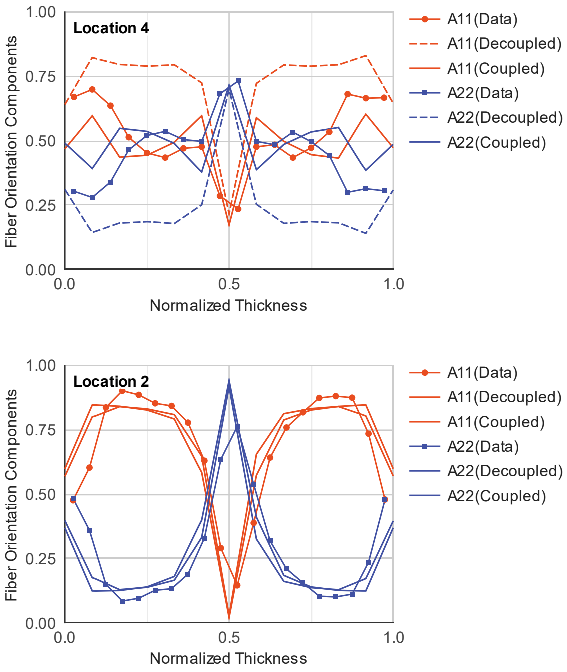


Figure 16. Comparison of the predicted fiber orientation from the decoupled and coupled analyses with the measured fiber orientation data for the 2mm thick plaque.

This improvement is mainly attributed to the change in the filling pattern, as demonstrated in Figure 17. Initially, the polymer melt exhibits a strong radial flow from the gate. In the decoupled analysis, the polymer at the edge gradually catches up, resulting in a more uniform flow front where shear is still dominant in the 1-3 direction. In contrast, the coupled analysis shows that the polymer still exhibits a radial flow towards the corner, with shear being dominant in the flow direction towards the corner. The measured data and the predictions from the coupled analysis still exhibit the shell-core-shell orientation structure in a coordinate system along the radial direction, but no longer in the global coordinate system.

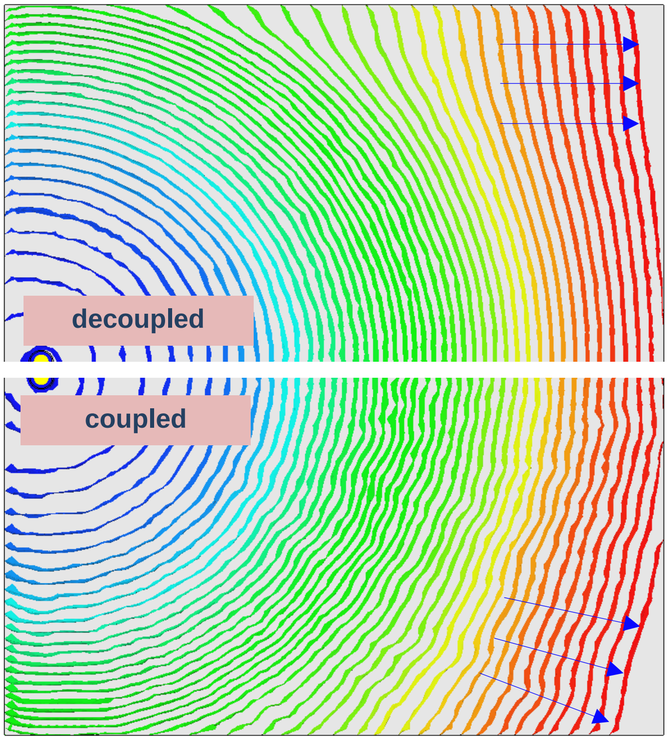


Figure 17. Comparison of the filling predictions from the decoupled and coupled analyses of the 2mm thick plaque. Figure 18. Geometry and measurement locations of the 2 mm thick plaque.

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