Effect of Polymer Viscosity on Post-Die Extrudate Shape Change in Coextruded Profiles

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Abstract

Bi-layer flow in a profile coextrusion die was simulated. Prediction of post-die changes in extrudate profile was included in the simulation. Mesh partitioning technique was used to allow the coextrusion simulation without modifying the finite element mesh in the profile die. Effect of polymer viscosities on the change in profile shape after the polymers leave the die is analyzed. It is found that a difference in the viscosities of the coextruded polymers can lead to a highly non-uniform velocity distribution at die exit. Accordingly, post-die changes in extrudate shape were found to be widely different when the polymers in the two coextruded layers were changed.

Introduction

The main goal in design of a die for extrusion of a complex profile is to get a uniform velocity distribution at the die exit (die balancing) [1]. If the velocity at die exit is different in different portions of the profile, the polymer gets redistributed after it comes out of the die till a uniform velocity is obtained away from the die. In general after the polymer leaves the die the thickness of the profile will increase at the locations with larger velocity, and will decrease at low velocity locations. Besides this change in thickness, redistribution of the polymer after it leaves the die can also lead to a significant distortion in the profile shape beyond die exit.

The degree of difficulty in balancing a complex profile die is increased multifold, if instead of extruding a single polymer, multiple polymers with different viscosities are to be coextruded through the die. Because of the difference in viscosities, the exit velocity can be quite different in the portions with different polymers. As expected, velocity is higher in the low viscosity polymer and lower in the high viscosity polymer. Due to this non-uniform exit velocity distribution, a coextruded profile can distort to a large extent beyond the die exit.

As discussed in our earlier papers [2, 3], if the viscosity of the two polymers are very different, polymer layer also get redistributed as they flow within the die. Redistribution of polymer layers in coextrusion dies is well documented in the literature [4], and is not discussed here. Instead, this paper is focused on the effect of polymer viscosities on post-die changes in the shape of the coextruded profiles.

Governing Equations

In the present work, the mass and momentum conservation equations [4] for inertia-less, incompressible flow with shear-thinning viscosity were solved for coextrusion simulation. Besides the flow equations, energy equation [4] was also solved to include non-isothermal effects. As discussed in our earlier publication [3], continuity of velocity and stress was enforced across the interface between adjacent polymer layers. The interface between the polymer layers was determined by using the no-cross-flow condition on the interface [3].

To determine the shape of the extrudate beyond die exit, the no-traction condition (Eqn. 1), and no-cross-flow condition (Eqn. 2) were applied on the free surface.

$$\vec{T} = \tilde{\tau} \cdot \vec{n} = 0 \tag{1}$$

$$\vec{v} \cdot \vec{n} = 0 \tag{2}$$

where $\vec{T}$ is the traction force, $\tilde{\tau}$ is stress, $\vec{v}$ is velocity, and $\vec{n}$ is the unit vector perpendicular to the free surface. At the end of the extrudate length used for post-die analysis, the draw-down velocity equal to the average velocity at die exit was enforced for the coextrusion simulations presented in this paper.

Mesh Partitioning Technique

In the three-dimensional simulations of coextrusion reported in the literature, finite element mesh is modified after each flow simulation iteration, such that the inter-element boundaries coincide with the interface between adjacent layers of different polymers [5]. Such an approach using an interface-matched finite element mesh can only be employed for simulating a two-dimensional system or a simple three-dimensional system such as a rectangular die. For real-life coextrusion systems, with complex three-dimensional die channel geometry, repeated generation and modification of interface-matched finite element meshes is impractical.

In the present work, polyXtrue software [6] was used to simulate the flow in a bi-layer profile coextrusion die. In this software a three-dimensional mesh of tetrahedral finite elements is generated over the complete flow channel in the die. This finite element mesh is not modified or regenerated at any stage during coextrusion simulation. Thereby, allowing simulation of even highly complex coextrusion systems.

In the coextrusion software used in this work, the interface between adjacent layers of different polymers is represented by a surface mesh of linear triangular finite elements. However, the surface mesh of triangular elements on the interface and the three-dimensional mesh of tetrahedral elements in the coextrusion die are completely independent of each other. This decoupling between the two finite-element meshes is possible because in the mesh partitioning technique for coextrusion simulation, the interface between adjacent polymer layers is not required to match with the inter-element boundaries in the three-dimensional mesh of tetrahedral finite elements. Instead, in the software used in this work, the interface is allowed to pass through the interior of the tetrahedral finite elements in the three-dimensional mesh.

In the mesh partitioning technique for coextrusion simulation the tetrahedral elements which are intersected by the mesh of triangular elements on the interface are partitioned into two tetrahedral, pyramidal, or prismatic finite elements. Further details of the mesh partitioning technique are available in our earlier publications [2, 3].

Resins

To simulate the flow in a bi-layer coextrusion die, an acrylonitrile butadiene styrene (ABS) resin manufactured by The Dow Chemical Company with a melt flow rate (MFR) of 2.5 dg/min (230°C, 3.8 kg) [7], and a polystyrene from BASF with MFR of 0.3 cm^3/min (200 ^{o}C, 5 kg) were used. The viscosities (η) of the ABS and polystyrene, shown in Fig. 1, were modeled by the Cross-WLF equation given below [8].

$$\eta = \frac{\eta_0}{1+\left(\eta_0 \dot{\gamma}/\tau^*\right)^{1-n}} \qquad (3)$$

$$\eta_0 = D_1 \exp\left[-\frac{A_1 (T - T_a)}{A_2 + (T - T_a)}\right] \qquad (4)$$

where A_1, A_2, D_1, T_a, τ^* and n are material parameters, and $\dot{\gamma}$ is the shear rate. For the ABS and polystyrene used in the work, the values of the material parameters are given in Table 1.

In Fig. 1, it should be noted that at 500K, the temperature specified for die walls and at die entrance for all the simulations in this paper, the viscosity of ABS is higher than the viscosity of polystyrene. For instance at 500K and shear rate of 100 s^{-1}, the viscosity of ABS is 1581.4 Pa·s, whereas that of polystyrene is 542.1 Pa·s.

Results and Discussion

To analyze the effect of the viscosities of the coextruded polymers on the post-die changes in extrudate shape, a bi-layer flow in a profile die was analyzed in this work. The geometry of the die analyzed is shown in Fig. 2. The cross-section at the exit of the profile die in Fig. 2 consists of a J-shaped portion to the right connected to a C-shaped portion in the upper left. The thickness of the C-shaped portion of the profile (2.96 mm) is slightly larger than the thickness of the J-shaped portion (2.27 mm). The J-shaped portion of the profile is completely made up of the substrate polymer which enters the die from a 6.34 cm diameter circular entrance at the back of the die. Besides the substrate polymer, the C-shaped portion of the profile also has a thin cap layer which enters through an 8.73 mm diameter circular channel on the left side in Fig. 2. This circular channel for the cap layer entrance is followed by the thicker C-shaped distribution channel which is connected to the main die channel by a thin C-shaped land region with only 0.5 mm opening. Because of this thin land region, before meeting the substrate polymer with a uniform velocity, the cap polymer flows around in the C-shaped distribution channel. At the entrance of the cap layer the velocity is 1 cm/s, whereas the entrance velocity for the substrate polymer is 1 mm/s. Both polymers enter the die at 500K, and the die wall temperature is also 500K.

Flow in the profile die was simulated for three different material combinations (*i*) ABS in the substrate as well as the cap layer, (*ii*) ABS in the substrate and polystyrene in the cap layer, and (*iii*) polystyrene in the substrate and ABS in the cap layer. The predicted extrudate profile for ABS in both layers was very similar to the profile predicted for polystyrene in both layers. Therefore, the results for the case with polystyrene in both layers are not presented in this paper.

<u>*ABS in Substrate as well as Cap layer*</u>

The velocity distribution in various cross-sections of the profile die for the case with ABS in substrate as well as cap layer is shown in Fig. 3, and the velocity distribution at the die exit is shown in Fig. 4 (a). As expected, velocity in Fig. 3 is the largest in the cross-section passing through the thin land region of the feeder channel for the cap layer. After the two polymers meet, till die exit, in Figs. 3 and 4 (a) the velocity in the thicker C-shaped portion is larger than the velocity in the thinner J-shaped portion of the profile.

Predicted shape of the profile and that of the interface at the end of the extrudate, along with the profile shape at the die exit, is shown in Fig. 4 (b). Because of the larger velocity in the C-shaped portion, thickness of C-shaped portion of the profile increases after the polymer leaves the die, whereas the extrudate thickness is the smallest near the ends of the J-shaped portions where the exit velocity is the smallest. Beyond die exit, as some of the high velocity polymer in the C-shaped portion moves towards the low velocity polymer in J-shaped profile, the C-shaped portion is bent towards the J-shaped portion, and a large distortion is obtained in the vertical link connecting the C-shaped and the J-shaped portions.

Development of the interface starting from the contact line, where the two polymers meet for the first time, till the die exit, and in the extrudate beyond the exit is shown in Fig. 5. The interface shape at the end of the extrudate was also shown in Fig. 4 (b). With ABS in both layers the thickness of the cap layer is quite uniform over the complete C-shaped portion of the die. Similar interface and extrudate shapes were obtained when polystyrene was used in the substrate as well as the cap layer.

Pressure variation along the die in Fig. 6 follows the expected trends. At die exit and in the extrudate beyond the die exit, the pressure is zero. The pressure increases towards the two entrances. Due to the large pressure drop in the thin land region of the feeder channel for the cap layer, the pressure is the maximum at the entrance of the cap layer.

Temperature distribution in the profile die is shown in Fig. 7. In the thin land region of the feeder channel for the cap layer because of the high shear rate, and hence large heat generations due to viscosity dissipations, the polymer temperature increases by about 4°. This high temperature polymer is then convected all the way to die exit. Beyond die exit, temperature of the polymer extrudate decreases as the heat is lost to the atmosphere by natural convection.

ABS in Substrate and Polystyrene in Cap layer

For the case with the lower viscosity polymer (polystyrene) in the cap layer, and the higher viscosity polymer (ABS) in the substrate, the predicted velocity distribution in the profile die is shown in Figs. 8 and 9 (a). Because of the lower viscosity of polystyrene in the cap layer, which acts as a lubricating layer, coupled with the fact that profile thickness in the C-shaped portion of the profile is larger, the exit velocity is the C-shaped portion is now much larger than the velocity in the remaining profile. Because of this large imbalance in velocity distribution at the die exit, in the post-die extrudate in Figs. 8 and 9 (b), there is a large increase in the thickness of the C-shaped portion and the thickness of the J-shaped portion decreases significantly. Also, transfer of some of the high velocity polymer from the C-shaped portion to the J-shaped portion results in a large distortion of the vertical link between the two sections of the profile. The bending of C-shaped portion towards the J-shaped portion is now quite excessive to the extent that by the end of the extrudate the lower arm of the C-shaped portion is touching the J-shaped portion.

Development of the interface in the die channel and in the post-die extrudate is shown in Fig. 10. The interface shape at the end of the extrudate was also shown in Fig. 9 (b). Because of the large velocity in the C-shaped portion, for mass balance the thickness of the polystyrene cap layer is now very small. Also, it is noted that a small portion of the upper arm of the C-shaped portion in Figs. 9 (b) and 10 has no cap layer.

For polystyrene cap and ABS substrate the pressure distribution is shown in Fig. 11. With low viscosity polystyrene in the cap layer, the total pressure drop in the die is much smaller than the pressure drop in Fig. 6. However, the highest pressure in Fig. 11 is still at the entrance of the cap layer.

Variation in the temperature along the profile die with polystyrene in the cap layer, shown in Fig. 12, is very similar to the temperature variation in Fig. 7 for the case with ABS in the substrate as well as in the cap layer.

Polystyrene in Substrate and ABS in Cap layer

For the case with ABS in the cap layer and polystyrene in the substrate, the velocity distribution shown in Fig. 13 is very different than the velocity distributions in Fig. 3 and 8 for the previous two cases. As expected, the maximum velocity in the die is still in the thin land region of the feeder channel for the cap layer. However, after the cap layer meets with substrate, the velocity in the C-shaped portion of the profile is now smaller than the velocity in the J-shaped portion, with the maximum velocity in the profile being at the T-junction of the J-shaped portion.

Since the velocity distribution for this case with polystyrene in the substrate is very different than the velocity for the previous two cases, as expected, the predicted post-die change in the extrudate shape in Fig. 14 (b) is also very different than that in Figs. 4 (b) and 9 (b). After the two polymers leave the die, the thickness of the J-shaped portion now increases, whereas the thickness of the C-shaped portion of the profile decreases. Furthermore, in contrast to the previous two cases, in Fig. 14 (b) instead of bending towards the J-shaped portion, the C-shaped portion now bends away from the J-shaped portion of the profile.

Development of interface between the two layers is shown in Fig. 15. For this case with polystyrene in the substrate, the shape of the interface at the end of the extrudate was shown in Fig. 14 (b). It is evident from Fig. 14 (b) that the C-shaped portion of the profile is now made almost completely by the cap material (ABS) with only a very thin layer of the substrate material (polystyrene). Furthermore, it is noted that cap layer of ABS has now wrapped around and penetrated in the vertical link between the C- and the J-shaped portions of the profile.

The pressure and temperature variations in Fig. 16 and 17 for this third case with polystyrene in the substrate are very similar to those for the previous two cases in Figs. 6, 7, 11, and 12. Again, the maximum pressure is at the entrance of the feeder channel for the cap layer; the high temperature polymer due to heat generated in the land region of the feeder channel for the cap layer is convected all the way to the die exit; and beyond the die exit the temperature of the extrudate decreases due to the heat convected to the atmosphere.

Conclusions

For extrusion of a multi-layer profile, balancing of the velocity distribution at the die exit can be difficult if viscosities of coextruded polymers are very different. The non-uniformities in exit velocity distribution can lead to a large distortion in extrudate profile after the polymers leave the die. Therefore, as the polymers in the two layers of a coextruded profile were changed, the post-die distortion in the extrudate shape was found to be very different for different polymer combinations.

References

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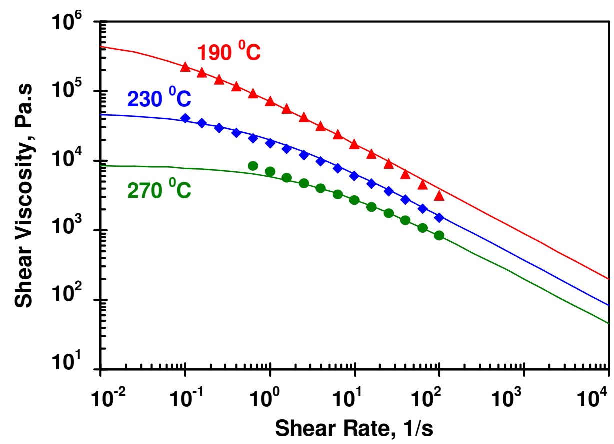
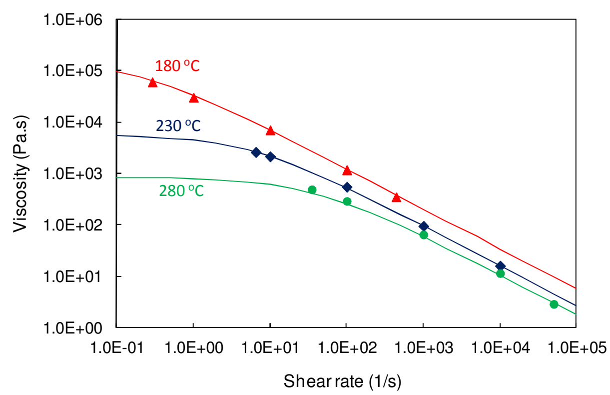
Table 1: Properties of the ABS and polystyrene

	ABS	Polystyrene
Viscosity parameters		
D_1 *(Pa.s)*	3.631×10^{11}	2.02×10^{12}
A_1	27.21	28.69
A_2 (K)	92.85	58.2
T_a (K)	373.0	375.4
τ^* (Pa)	2.9×10^4	2.95×10^4
n	0.33	0.225
Other material properties		
Density (kg/m^3)	940.0	936.0
Heat Capacity (J/kg K)	2345.0	2300.0
Thermal conductivity (W/m K)	0.18	0.155



(a)



(b)

Fig. 1 Shear viscosity data (symbols) and Cross-WLF model fit (curves) to the viscosity data for the ABS (a), and polystyrene (b) resins.

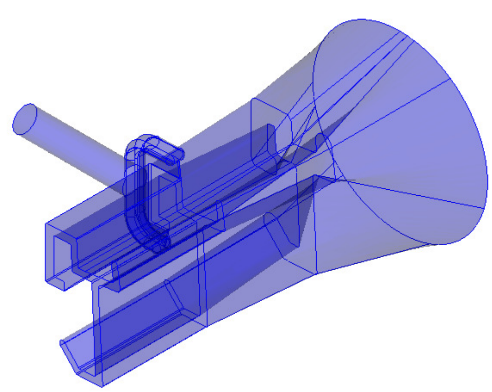


Fig. 2 Geometry of a bi-layer profile die.

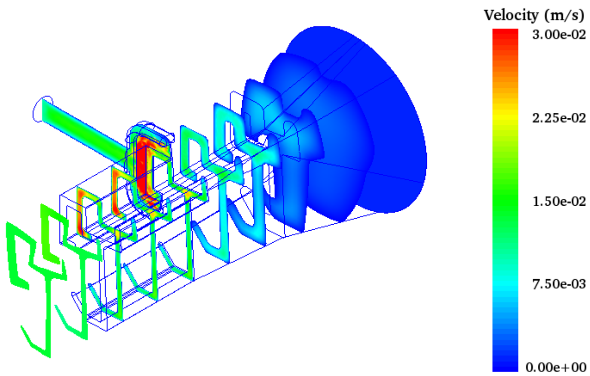
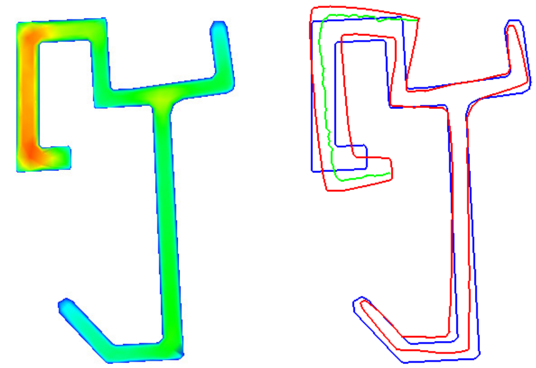


Fig. 3 Velocity distribution in the profile die with ABS in the substrate as well as the cap layer.



(a) (b)

Fig. 4 (a) Velocity distribution at die exit, (b) extrudate profile (red), and interface (green) at the end of the extrudate with ABS in the substrate as well as the cap layer. Blue line shows the shape of the profile at die exit.

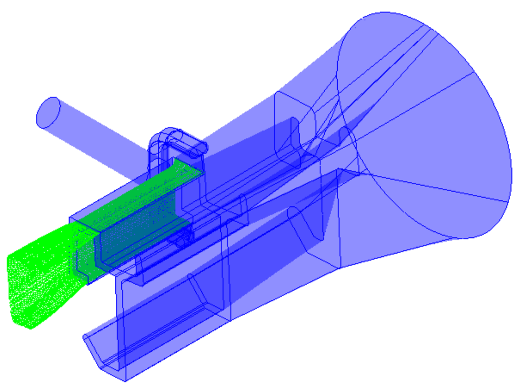


Fig. 5 Interface between the cap layer and substrate with ABS in the substrate as well as the cap layer.

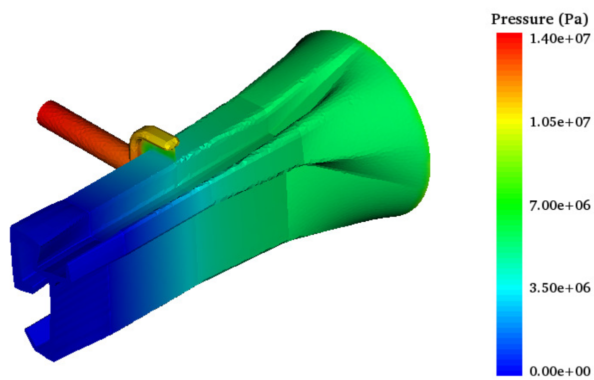
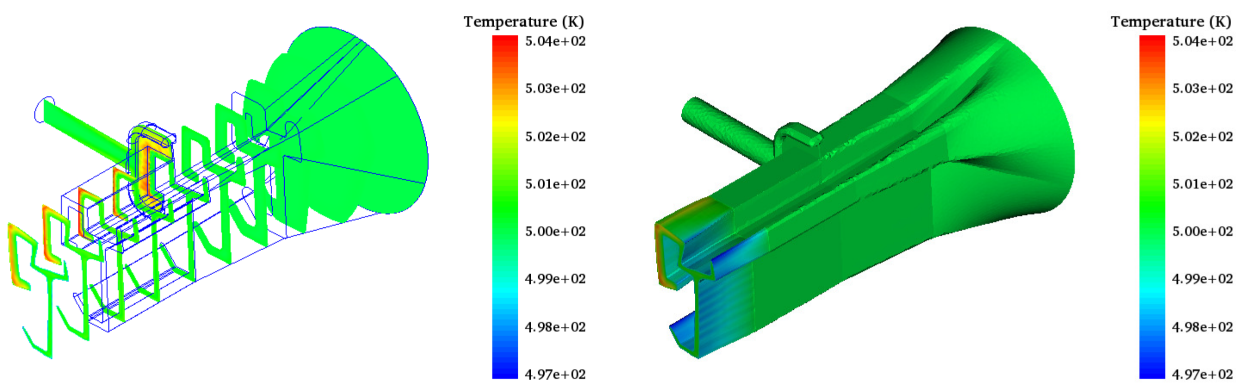


Fig. 6 Pressure distribution in the profile die with ABS in the substrate as well as the cap layer.



(a) (b)

Fig. 7 Temperature distribution inside the die (a), and on the extrudate surface (b) of the profile die with ABS in the substrate as well as the cap layer.

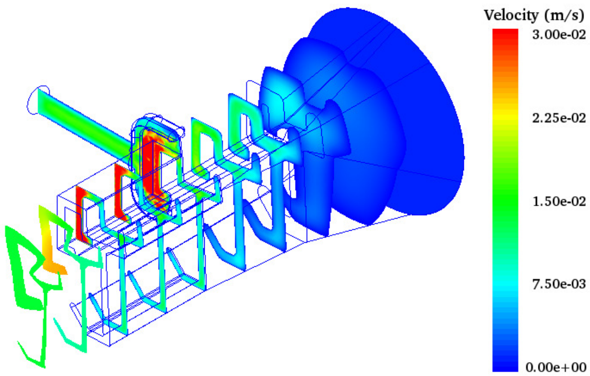
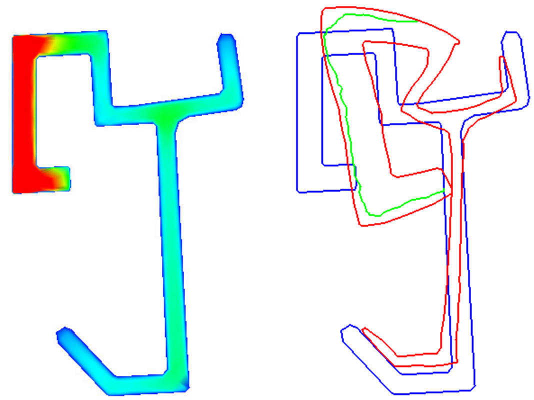


Fig. 8 Velocity distribution in the profile die with ABS in substrate and polystyrene in cap layer.



(a) (b)

Fig. 9 (a) Velocity distribution at die exit, (b) extrudate profile (red), and interface (green) at the end of the extrudate with ABS in substrate and polystyrene in cap layer. Blue line shows the shape of the profile at die exit.

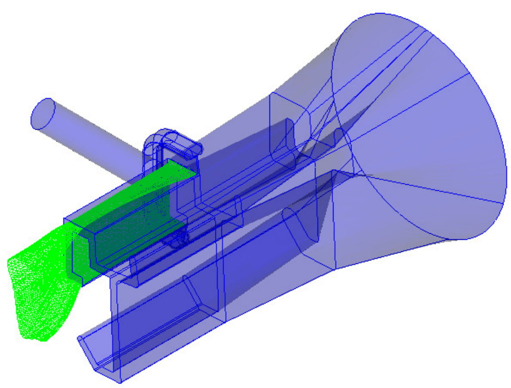


Fig. 10 Interface between the cap layer and substrate with ABS in substrate and polystyrene in cap layer.

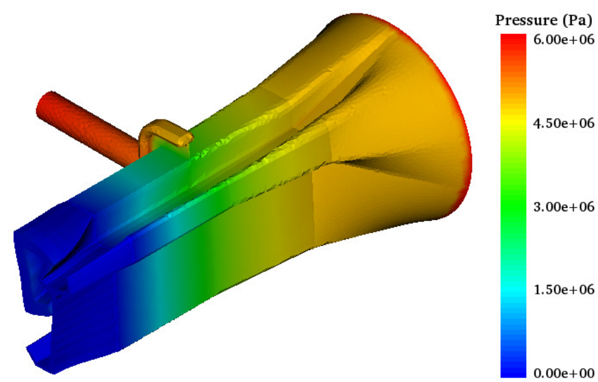
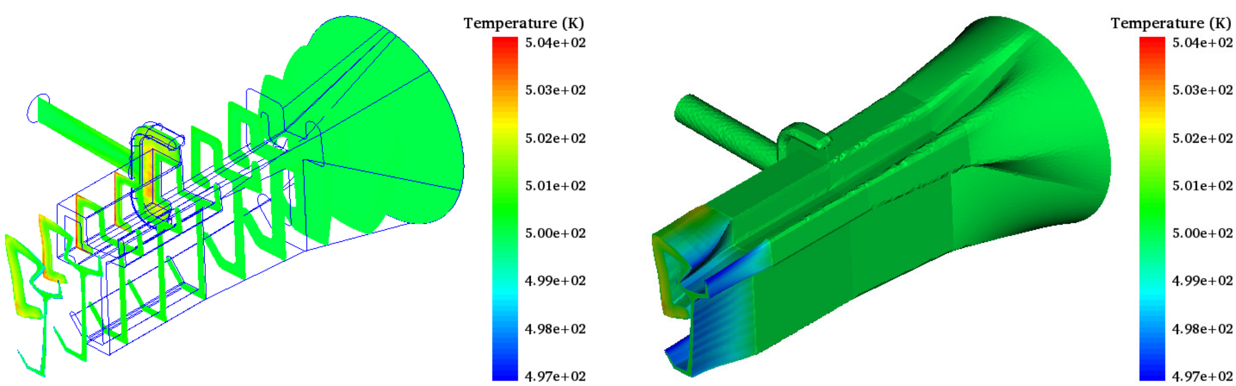


Fig. 11 Pressure distribution in the profile die with ABS in substrate and polystyrene in the cap layer.



(a) (b)

Fig. 12 Temperature distribution inside the die (a), and on the extrudate surface (b) of the profile die with ABS in substrate and polystyrene in cap layer.

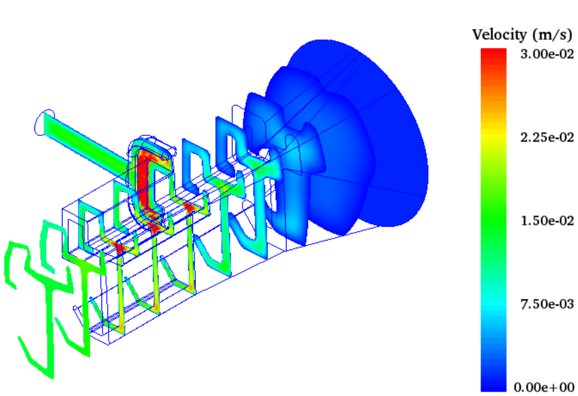
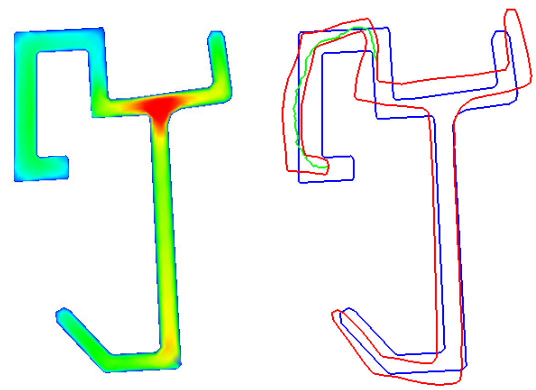


Fig. 13 Velocity distribution in the profile die with polystyrene in substrate and ABS in cap layer.



(a) (b)

Fig. 14 (a) Velocity distribution at die exit, (b) extrudate profile (red), and interface (green) at the end of the extrudate with polystyrene in substrate and ABS in cap layer. Blue line shows the shape of the profile at die exit.

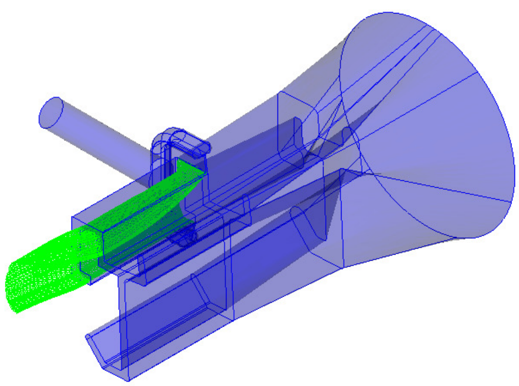


Fig. 15 Interface between the cap layer and substrate with polystyrene in substrate and ABS in cap layer.

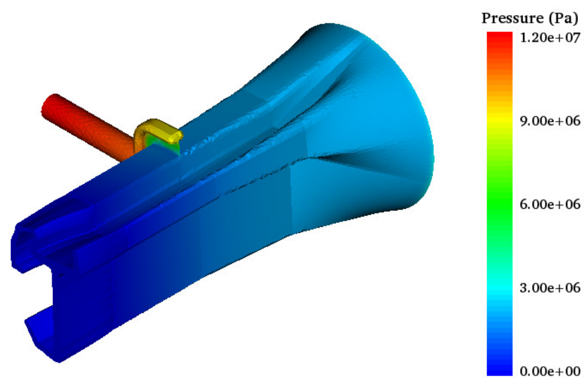
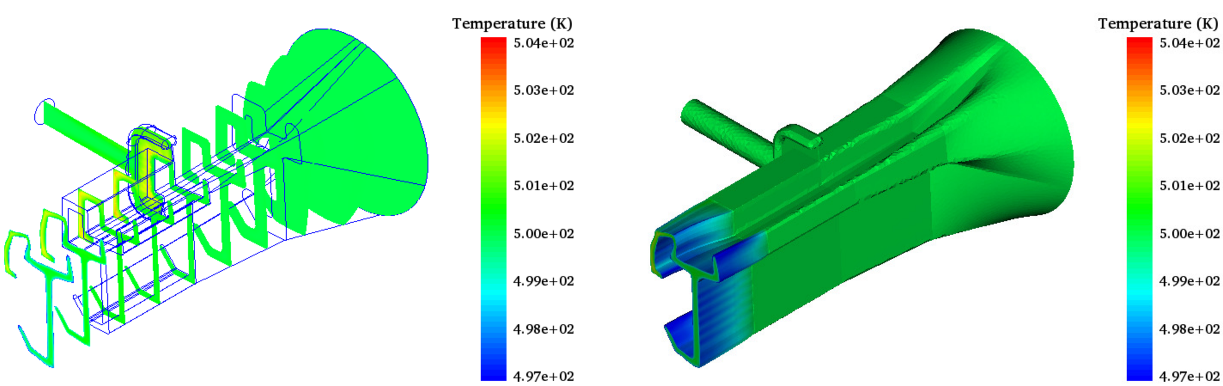


Fig. 16 Pressure distribution in the profile die with polystyrene in substrate and ABS in the cap layer.



(a) (b)

Fig. 17 Temperature distribution inside the die (a), and on the extrudate surface (b) of the profile die with polystyrene in substrate and ABS in cap layer.