Three Dimensional Simulation of Coextrusion in a Complex Profile Die

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Abstract

Mesh partitioning technique is used to simulate bilayer coextrusion in a complex profile extrusion die. Mesh partitioning technique allows coextrusion simulation without changing the finite element mesh as the interface between the adjacent polymer layers is changed during a coextrusion simulation. Since the finite element mesh in the die remains fixed during the simulation, the mesh partitioning technique allows coextrusion simulation even in highly complicated profile dies. Effect of polymer viscosity on interface shape, velocity, pressure, shear rate, and residence time distribution in a profile coextrusion die is analyzed. It is found that polymer viscosity has significant effect on the interface shape, velocity, pressure, and shear rate, but only a minor effect on the residence time distribution in the die.

Introduction

Coextrusion, which involves simultaneous extrusion of several different polymers through a die to form a single multilayered product, combines the functionalities and benefits of several polymers into a single product [1]. Despite this inherent advantage of coextrusion, growth of coextrusion market has been slowed down by the complexity of coextrusion die design. Depending upon the rheology of polymers used for coextrusion, the polymers in various layers may get redistributed as they flow through the die such that the distribution of various polymers at the inlet and at the exit of the die may be quite different. Because of this redistribution of polymer layers, finding a die geometry which will give the required layer distribution in the final product can be extremely difficult.

Coextrusion dies are currently designed using a “trial and error” approach. This repetitive approach is not only highly time-consuming and costly, but also requires highly experienced engineers and rarely provides an optimum die design. Therefore, a coextrusion simulation software, which can accurately predict the shape of the interface between different polymer layers, is an excellent design-aide for a coextrusion die designer. A coextrusion software not only tremendously simplifies the coextrusion die design process, the software can also be exploited for a proper selection of the material in different layers and for optimization of the processing conditions.

Coextrusion Simulation Equations

For simulation of a multilayer flow of polymers during coextrusion, the velocity and stresses are required to be continuous across the interface between the adjacent polymer layers [2]. That is,

$$\vec{v}_i^{(1)} = \vec{v}_i^{(2)} \qquad \forall i \in I \qquad (1)$$

$$\tilde{\tau}_i^{(1)} = \tilde{\tau}_i^{(2)} \qquad \forall i \in I \qquad (2)$$

where I contains all finite elements nodes on the interface, v(vector)$_i^{(1)}$ and τ~$_i^{(1)}$ are the velocities and stresses on one side of the interface, with v(vector)$_i^{(2)}$ and τ~$_i^{(2)}$ being the velocities and stresses on the other side of the interface. Besides the continuity of velocity and stress, coextrusion simulation requires enforcement of the no-cross-flow condition at the interface. That is, the velocity component normal to the interface must be zero at all interface nodes:

$$\vec{v}_i \cdot \vec{n}_i = 0 \qquad \forall i \in I \qquad (3)$$

where v(vector)$_i$ is the velocity, and n(vector)$_i$ is the unit vector perpendicular to the interface.

Mesh Partitioning Technique

In most three-dimensional simulations of coextrusion reported in the literature, finite element mesh is modified after each flow simulation iteration, such that the interelement boundaries coincide with the interface between adjacent layers of different polymers [2]. 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 [3] 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 domain 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 three-dimensional finite elements. When a two-dimensional plane intersects a tetrahedral finite element, it leads to one of the following combinations of two finite elements.
o One tetrahedral and one prismatic element (Fig. 1 a),
o Two tetrahedral elements (Fig. 1 b),
o One pyramidal and one tetrahedral element (Fig. 1 c)
o Two prismatic elements (Fig. 1 d).
In the coextrusion software used, each of the tetrahedral elements which are intersected by the interface between adjacent polymer layers is replaced by one of these four combinations of the two finite elements.

Prediction of Interface Shape

The shape of the interface between adjacent polymer layers is defined by the no-cross-flow boundary condition (Eqn. 3). In the coextrusion software used in this work, a weighted residual form of Eqn. 3 is solved to predict the interface shape [4].

$$\int_{\Gamma} (\vec{v} \cdot \vec{n}) N_i \, ds = 0 \qquad \forall N_i \in I_s \qquad (4)$$

where I_s is the space of weighting functions (same as the shape functions) on the interface and Γ denotes the interface surface.

In our earlier publication [5] on coextrusion simulation for simpler extrudate shapes, an initial estimate of the interface shape had to be specified as an input to the coextrusion software. Starting with the initial estimate of the interface shape, the earlier version of the software then accurately predicted the interface shape between the adjacent polymer layers. For complicated profile coextrusion dies, such as the die analyzed in this work, it is difficult to determine the initial estimate of the interface between the adjacent polymer layers. Therefore, in the current version of the polyXtrue software, using the streamlines for the flow simulation in the previous iteration, an initial estimate of the interface between the adjacent polymer layers is automatically determined by the software. This initial estimate of the interface shape obtained from the streamlines for the previous flow iteration is then updated according to the predictions from the weighted residual form of the no-cross-flow condition (Eqn. 4).

Resins

The generalized Newtonian formulation for an inertialess, incompressible flow with shear-thinning viscosity was used for the coextrusion simulations. To simulate a multilayer flow in coextrusion dies, two different grades of low-density polyethylene (LDPE) were used in this work. The shear viscosity data at 200oC for the two grades of LDPE is shown in Fig. 2. Experimental data from reference [6] (Fig. 2) was used to obtain the parameters for the Cross model (Table 1).

$$\eta_s = \frac{\eta_0}{1 + (\eta_0 \dot{\gamma} / \tau^*)^{(1-n)}} \qquad (6)$$

Fig. 2 also shows the viscosity curves based upon the Cross model parameters given in Table 1.

Results and Discussion

The geometry of the complex profile die analyzed, and the mesh of tetrahedral elements used for coextrusion simulation is shown in Fig. 3. Most of the extruded profile (substrate) is made of one polymer, but it has a thin cap layer on the top wall. As shown in Fig. 4, the cap layer also wraps around the vertical tab on the left side of the part. For substrate of the profile the polymer enters along the axial direction into a circular channel which is gradually transformed into the profile shape. The cap layer enters through a circular channel on top, which is perpendicular to the die axis. In order to distribute the polymer from the circular channel to the thin cap layer, the circular channel is followed by two distribution channels. Both distribution channels have circular crosssections, and are connected by a channel with uniform narrow opening. Because of the narrow channel between the two distribution channels, the polymer first flows along the transverse direction and is distributed in the first distribution channel before it enters into the second distribution channel. The second distribution channel is connected to the entrance of the cap layer in the die, again by a narrow channel which further distributes the polymer in the second distribution channel before the polymer uniformly reaches the contact line where the cap layer meets the substrate for the first time.

The flow in the bi-layer profile die was simulated for the following three different combinations of LDPE-A and LDPE-D in the substrate and the cap layer.

Substrate	Cap layer
LDPE-A	LDPE-A
LDPE-A	LDPE-D
LDPE-D	LDPE-A

For these three combinations of LDPE-A and LDPE-D, the velocities at the circular entrances of the substrate and cap layer were 0.1 cm/s and 1.5 cm/s, respectively. These values of entrance velocities were used so that the velocities of the two polymers are similar when the two polymers come in contact inside the die. The bi-layer flow in the die was also simulated for entrance velocity of 3.0 cm/s for the cap layer, while keeping the entrance velocity for substrate to 0.1 cm/s

For the three different combinations of LDPE-A and LDPE-D, as well as for the case with larger flow rate (LFR) through the cap layer, Fig. 5 shows the predicted interface shape between the two layers. In Fig. 5, all four interface profiles look very similar, except for the interface shape in Fig. 5 (b). In Fig. 5 (b), the interface shape near the contact line in the vertical tab on the left where the cap layer wraps around the substrate is quite different than the interface shape for the other three cases. This difference in the interface shape for the case with higher viscosity polymer (LDPE-D) in the cap layer and lower viscosity polymer (LDPE-A) in the substrate is further clarified in Fig. 6. When the viscosity of the polymer in the cap layer is the same (Fig. 6 a, d) or lower (Fig. 6 c) than the viscosity for the polymer in the substrate, after the two polymers come in contact at the contact line, the interface between the two layers goes towards the exit along the axial direction. However, for the case with higher viscosity polymer in the cap layer (Fig. 6 b), in the vertical tab on the left where the cap layer wrap around the substrate, the interface first goes toward the entrance before reversing back and starting to move toward the exit. It was confirmed that for this case with the higher viscosity polymer in the cap layer, the polymer velocity in this region near the vertical tab is in fact towards the entrance. Because of this initial movement of the interface towards the entrance, for the case with the higher viscosity polymer (LDPE-D) in the cap layer, the vertical tab on the left is almost completely occupied by the higher viscosity polymer (green line in Fig. 7). That is, for this case there is almost no substrate polymer in the vertical tab. For the horizontal wall on top of the extrudate profile, effect of the polymer viscosity on the interface location at the die exit is shown in Fig. 7 (b). Effect of viscosity on the interface location in the horizontal wall can be explained by examining the velocity distributions shown in Fig. 8. In comparison to the case with low viscosity polymer (LDPE-A) in the substrate as well as the cap layer (Fig. 8 a), for the case with higher viscosity polymer (LDPE-D) in the cap layer (Fig. 8 b), the velocity of the polymer in the cap layer is lower at the die exit. Therefore, in Fig. 7 (b) in order to satisfy the mass balance, the interface in the horizontal wall at the die exit is lower for this case (green line). In contrast, for the case with higher viscosity polymer (LDPE-D) in the substrate and the lower viscosity polymer (LDPE-A) in the cap layer, as expected, the velocity in Fig. 8 (c) is higher in the cap layer. Therefore, in order to satisfy the mass balance, the interface for this case is located at the highest position in Fig. 7 (b) (blue line). That is, the cap layer is the thinnest for this case. It is evident from Fig 7 (a) that the cap layer for this case may be too thin in the region where the vertical tab on the left connects with the horizontal wall. In this region where the vertical tab is joined with the horizontal wall, for the case with higher viscosity polymer (LDPE-D) in the substrate, the interface is almost touching the die wall. That is, for this case there may not be any cap layer in this region where the vertical tab connects with the horizontal wall. For the last case with LDPE-A in the substrate as well as the cap layer, but larger (double) flow rate in the cap layer, (Fig. 8 d, and black line in Fig 7), as expected, the interface is lower in comparison to the case with smaller velocity in the cap layer and with LDPE-A in both layers (red line in Fig. 7).

For the three cases with different polymer combinations and the case with larger flow rate (LFR) through the cap layer, the velocity distribution at the die exit and the velocity distribution in the plane where the cap layer first comes in contact with the substrate are shown in Fig. 9. It should be noted that the range of scale bars in Fig. 8 and Fig. 9 are different. For all four cases, the flow in the substrate is not very well balanced. In particular, the velocity is significantly higher in the vertical wall connecting the circle in the middle with the bottom horizontal wall. This higher velocity in the vertical wall can be easily reduced, that is, the floor at the die exit can be easily balanced, by reducing the opening in this region in the die plates between the circular entrance and the final die plate at the exit.

Fig. 10 shows the pressure distributions for the four coextrusion simulations in the profile die. As expected, the pressure is zero at the exit, and because of its smaller cross-section and higher velocity, the pressure is the highest in the circular channel at the entrance of the cap layer. In comparison to the pressure for the case with LDPE-A in both layers, the pressure in the die increases when the higher viscosity polymer (LDPE-D) is used in the substrate (Fig. 10 c) or in the cap layer (Fig. 10 b). Also, the pressure in the two distribution channels and the circular entrance channel increases for the case with larger flow rate in the cap layer (Fig. 10 d).

The shear rate on the die walls for the four coextrusion simulations is shown in Fig. 11. For all four cases the shear rate is the highest in the cap layer in the plane where it meets the substrate for the first time. Also, it is noted that after the two polymers meet, the shear rate in the cap layer is higher for the case with the higher viscosity polymer (LDPE-D) in the substrate (Fig. 11 c) because after the two polymers meet the velocity in the cap layer is higher for this case (see Fig. 8 c). For the case with higher velocity through the cap layer (Fig. 11 d), as expected, the shear rate is higher in the narrow channel connecting the two distribution channels for the cap layer and in the narrow channel connecting the second distribution channel with the contact line where the two polymers meet.

Fig. 12 shows the residence time distributions for the polymers in the substrate and the cap layer. In Fig. 12, for the four coextrusion simulations, the residence time for the substrate is much larger than the residence time for the cap layer. The larger residence time for the substrate is expected because the circular entrance channel for the substrate has a larger cross-sectional area. Accordingly, a smaller velocity (1 mm/s) was specified at the entrance of the circular entrance channel for substrate, whereas a much higher velocity (1.5 cm/s or 3.0 cm/s) was specified at the entrance of the circular entrance channel for cap layer. Also, as expected, the residence time for the cap layer is smaller for the case with larger flow rate through the cap layer (black line with square symbol in Fig. 12). For the three cases with different polymer combinations in the substrate and the cap layer, even though the residence time distribution for the cap layer (and also for substrate) are different for different polymer combinations, the difference in the residence time for the cap layer (and also for substrate) for the three cases is small, and is probably within the accuracy of the predictions. That is, for the three different polymer combinations, viscosities of the polymers seem to have only a minor effect on the residence time distribution.

Conclusions

Mesh partitioning technique was used for simulation of a bi-layer coextrusion in a complex profile die. Since the mesh partitioning technique does not require the interface between different polymer layers to match with the inter-element boundaries (instead, allowing the interface to cut through the tetrahedral finite elements), this technique could be used to simulate the flow in a highly complex bi-layer coextrusion die. Effect of polymer viscosity on interface shape, velocity, pressure, shear rate, and residence time distribution was analyzed. Viscosities of the two polymers were found to have significant effect on the interface shape, velocity, pressure, and shear rate in the die, but only a minor effect on the residence time distributions of the two polymers.

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Table 1 Cross-model parameters for two LDPEs.

	η_0 (Pa·s)	τ^* (Pa)	n
LDPE-A	2.01×10^3	4.14×10^3	0.462
LDPE-D	5.11×10^4	2.49×10^3	0.439

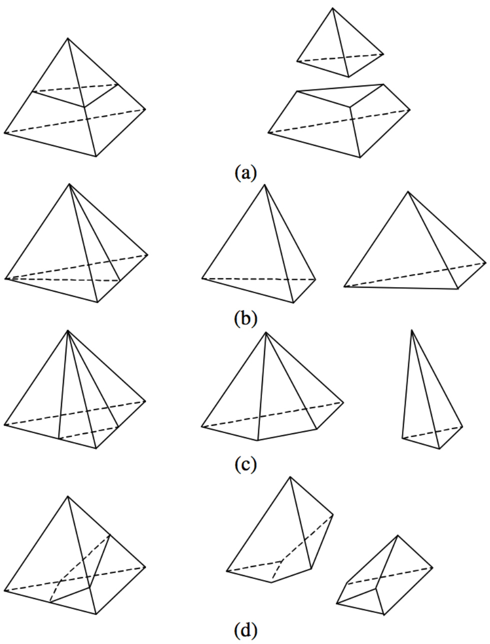


Fig. 1 Four possible combinations of the two finite elements obtained by partitioning a tetrahedral finite element. Each of the figures on the left shows a tetrahedral element with an intersecting plane. Figures on the right show the two finite elements generated by the intersection.

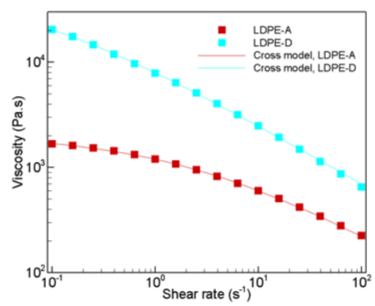


Fig. 2 Viscosity of two different grades of LDPEs [6].

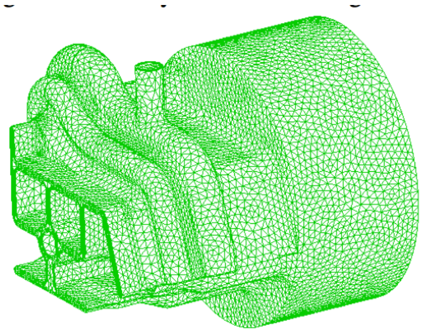


Fig. 3 Finite element mesh of tetrahedral elements in the profile die.

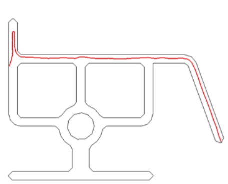


Fig. 4 Shape of the cap layer in the profile die. Interface between the cap layer and substrate is shown by red line.

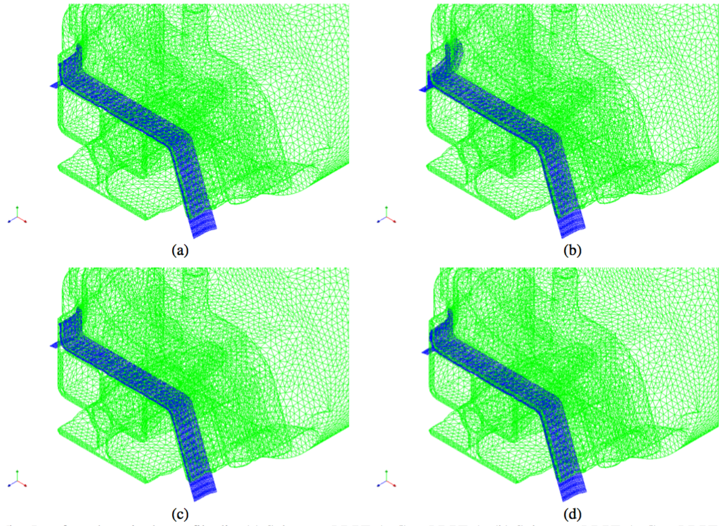


Fig. 5 Interface shape in the profile die. (a) Substrate: LDPE-A, Cap: LDPE-A, (b) Substrate: LDPE-A, Cap: LDPE-D, (c) Substrate: LDPE-D, Cap: LDPE-A, (d) Substrate: LDPE-A, Cap: LDPE-A with larger flow rate (LFR) through the cap layer.

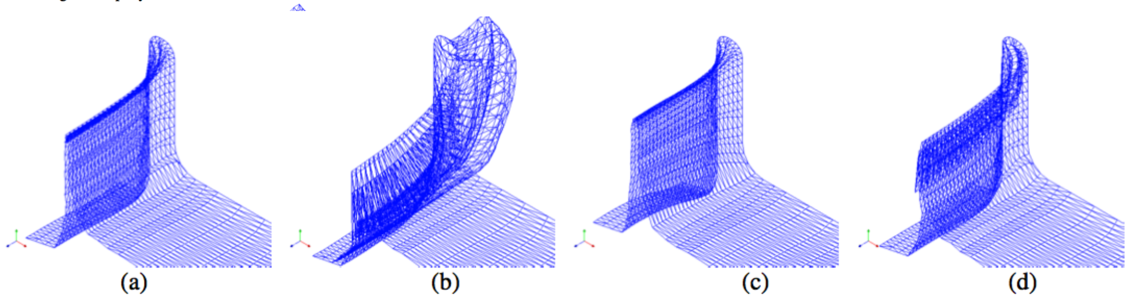


Fig. 6 Interface shape near the vertical tab in the profile die. (a) Substrate: LDPE-A, Cap: LDPE-A, (b) Substrate: LDPE-A, Cap: LDPE-D, (c) Substrate: LDPE-D, Cap: LDPE-A, (d) Substrate: LDPE-A, Cap: LDPE-A with larger flow rate (LFR) through the cap layer.

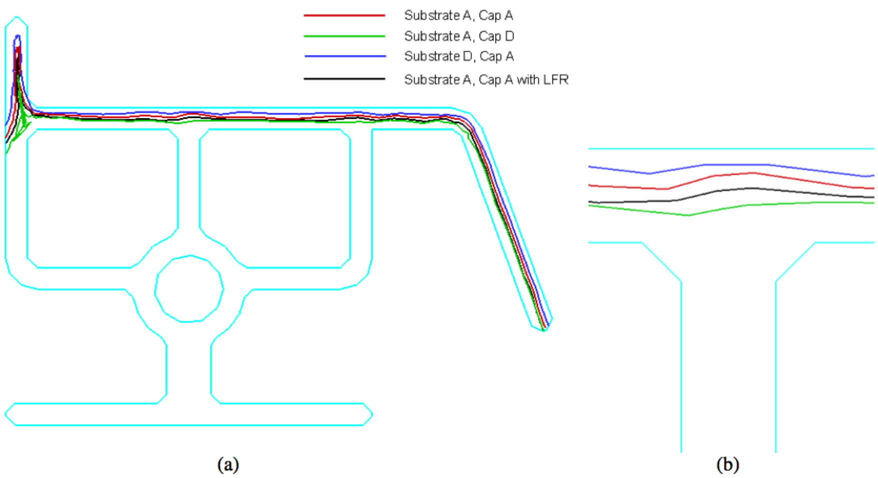


Fig. 7 Interface profiles at the exit of the profile die, (a) complete profile, (b) near the middle of the upper horizontal wall. (LFR: Larger Flow Rate in the cap layer)

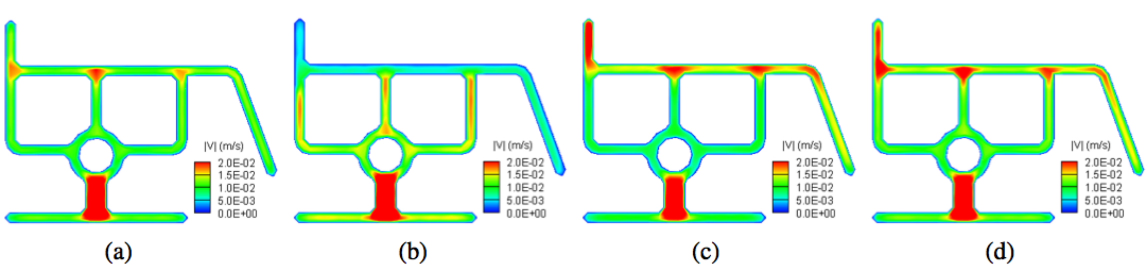
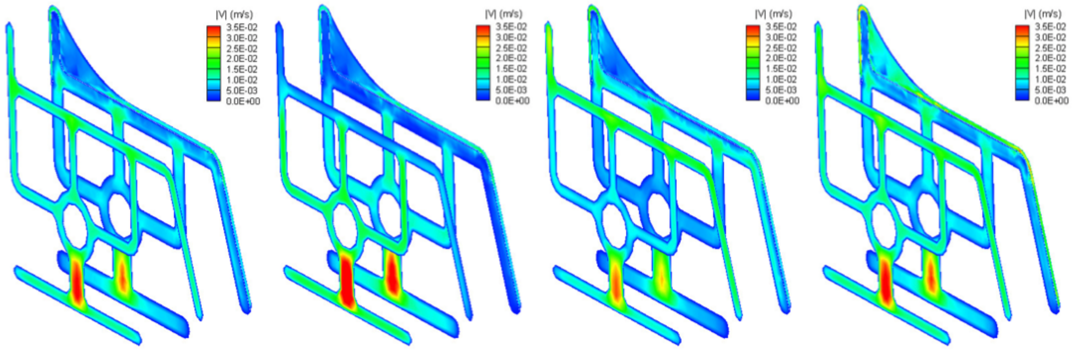
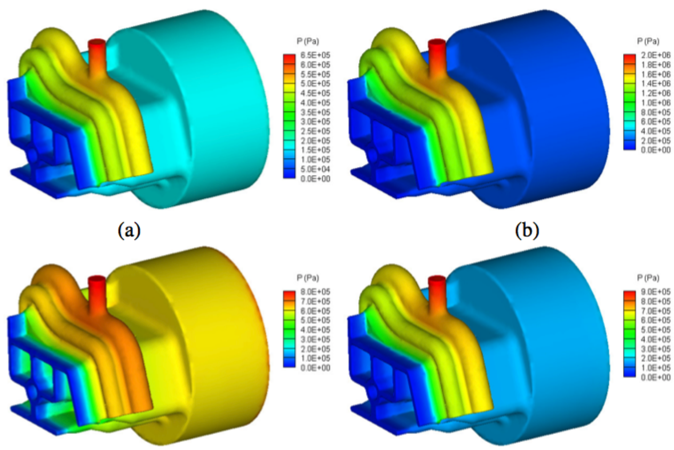


Fig. 8 Velocity distribution at the exit of the profile die. (a) Substrate: LDPE-A, Cap: LDPE-A, (b) Substrate: LDPE-A, Cap: LDPE-D, (c) Substrate: LDPE-D, Cap: LDPE-A, (d) Substrate: LDPE-A, Cap: LDPE-A with larger flow rate (LFR) through the cap layer.



(a) (b) (c) (d)

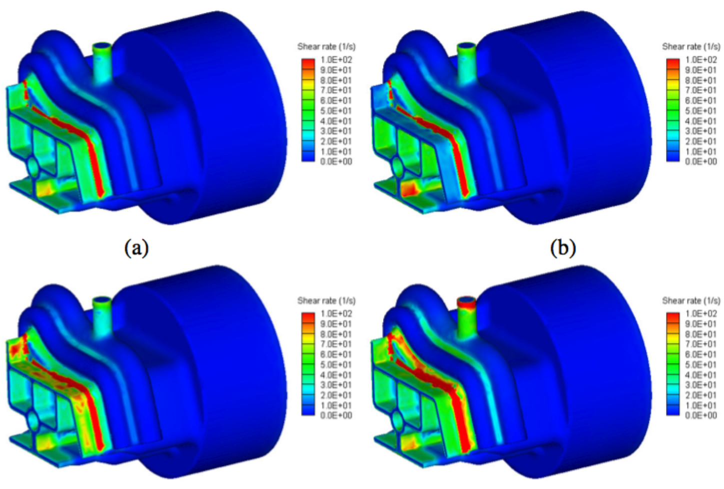
Fig. 9 Velocity distribution at the exit, and in the plane of the contact line of the profile die. (a) Substrate: LDPE-A, Cap: LDPE-A, (b) Substrate: LDPE-A, Cap: LDPE-D, (c) Substrate: LDPE-D, Cap: LDPE-A, (d) Substrate: LDPE-A, Cap: LDPE-A with larger flow rate (LFR) through the cap layer.



(a) (b)

(c) (d)

Fig. 10 Pressure distribution in the profile die. (a) Substrate: LDPE-A, Cap: LDPE-A, (b) Substrate: LDPE-A, Cap: LDPE-D, (c) Substrate: LDPE-D, Cap: LDPE-A, (d) Substrate: LDPE-A, Cap: LDPE-A with larger flow rate (LFR) through the cap layer.



(a) (b)

(c) (d)

Fig. 11 Shear rate distribution in the profile die. (a) Substrate: LDPE-A, Cap: LDPE-A, (b) Substrate: LDPE-A, Cap: LDPE-D, (c) Substrate: LDPE-D, Cap: LDPE-A, (d) Substrate: LDPE-A, Cap: LDPE-A with larger flow rate (LFR) through the cap layer.

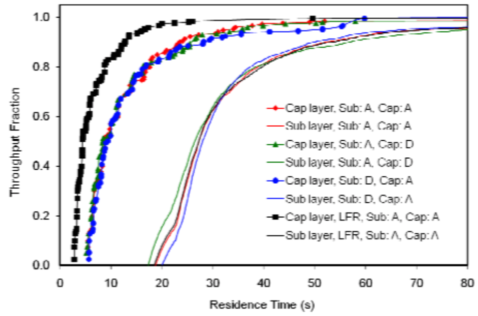


Fig. 12 Residence time distribution for the substrate and the cap layer of the profile die. (LFR: Larger Flow Rate in the cap layer)

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