MESH PARTITIONING TECHNIQUE FOR THREE-DIMENSIONAL SIMULATION OF COEXTRUSION

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Abstract

A new algorithm for simulation of polymer coextrusion is introduced. In the new algorithm, the finite element mesh of tetrahedral elements remains unaltered as the interface shape between adjacent polymer layers is developed during the simulation. The use of a fixed finite element mesh for coextrusion simulation is possible because in the new algorithm the interface between the two polymers is not required to match with an inter-element boundary of the tetrahedral elements in the mesh. Instead, by partitioning the tetrahedral elements intersected by the interface into two tetrahedral, pyramidal or prismatic finite elements, in the new algorithm, the interface is allowed to pass through the interior of the tetrahedral elements in the original finite element mesh.

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]. Three different types of die designs, namely, multi-lip design, multi-manifold design and feed-block design are commonly used for coextrusion [1]. Multi-lip design is difficult to use for more than two layers, whereas multi-manifold can be used for up to four layers. In contrast, in a feed block design, a single conventional die is used along with an adapter (or feed block). The feed block feeds the various polymer streams into the die inlet. Feed block design is simple, relatively inexpensive, and allows the use of existing dies with minor or no modifications. Any number of individual layers can be combined in the feed block design. Therefore, most coextrusion systems these days use the feed block design. However, depending upon the rheology of the polymers used for coextrusion, the polymers in different layers may be redistributed as they flow through the die such that the distribution of various polymers at the exit and at the inlet of the die may be quite different. Therefore, even though the feed block design for polymer coextrusion is inexpensive and versatile, design of a feed-block is difficult.

Coextrusion Simulation Equations

For simulation of a multilayer flow 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, $\vec{v}_i^{(1)}$ and $\tilde{\tau}_i^{(1)}$ are the velocities and stresses on one side of the interface, with $\vec{v}_i^{(2)}$ and $\tilde{\tau}_i^{(2)}$ 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 $\vec{v}_i$ is the velocity, and $\vec{n}_i$ is the unit vector perpendicular to the interface.

New Algorithm for Coextrusion Simulation

In all 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 [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 contrast, in the new algorithm developed in this work, 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 new algorithm, 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 in the new algorithm developed in this research because the interface between different polymer layers is not required to match with the inter-element boundaries in the three-dimensional mesh of tetrahedral finite elements. Instead, in the new coextrusion simulation algorithm, the interface is allowed to pass through the interior of the tetrahedral finite elements in the three-dimensional mesh.

Mesh Partitioning Technique

In the multilayer flow simulation algorithm developed in this research, 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.

- One tetrahedral and one prismatic element (Fig. 1 a),
- Two tetrahedral elements (Fig. 1 b),
- One pyramidal and one tetrahedral element (Fig. 1 c)
- Two prismatic elements (Fig. 1 d).

In our new coextrusion software, 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 present work, a weighted residual form of the no-cross-flow condition was solved to predict the interface shape [3].

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

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

If the standard Galerkin method is used to discretize Eqn. (4) it leads to oscillations in the predicted interface shape. In the present work, oscillations in the interface were eliminated by modifying the weighting functions (N_i) such that a higher weight is given to the points on upstream side of the node i (streamline-upwind-Petrov-Galerkin (SUPG) method [4]). In each coextrusion simulation iteration, after solving Eqn. 4, the interface shape was updated by moving the nodes in the mesh of triangular finite elements on the interface without affecting the topology of the mesh.

Resins

The generalized Newtonian formulation 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 200 ^oC for the two grades of LDPE is shown in Fig. 2. Experimental data from reference [5] (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. These two grades of LDPE were selected for the flow simulation, because of the large difference in their viscosities.

Results and Discussion

Flow in a Square Die with a Circular Core

The finite element mesh of tetrahedral elements used to simulate a core-and-shell type of multilayer flow in a square die is shown in Fig. 3 (a). The cross-section of the square die in Fig. 3 is 1 × 1 cm, and the total length of the die in the axial direction is 6 cm. For the first 1 cm length of the die, the two polymers flow in separate channels. As shown in Fig. 3 (b), in the plane of first contact between the two polymers the interface is a circle with 0.4 cm diameter. The center of the circle is located along one of the two primary diagonals of square cross-section. The distance between the axis of the square die and the center of the circular interface is 0.21 cm. It should be noted that the flow in this coextrusion die is symmetric about the lower-left to upper-right (LLUR) diagonal. Therefore, as the two polymers flow along the die and the interface shape is developed, the symmetry about the LLUR diagonal is expected to be maintained throughout the die. For all the coextrusion simulation reported here for the die in Fig. 3 (a), the interface shape was initialized to the circular cylinder shown in Fig. 3 (b).

To analyze the effect of polymer viscosity on the shape of the interface, the flow in the core-and-shell square die was simulated for three different material combinations: (*i*) LDPE-A in core as well as shell, (*ii*) LDPE-D and LDPE-A, respectively, in core and shell layers, and (*iii*) for LDPE-A in shell and LDPE-D in core layer. For all three material combinations, in order to obtain similar velocities in the two layers when they come in contact, the flow rate specified at the entrance was proportional to the cross-sectional area of the core and shell layers in the plane of contact, which, as mentioned in the last paragraph, is at distance of 1 cm from the die entrance. In the plane of contact, the cross-sectional areas of the core and shell layers for the square die are 0.126 and 0.874 cm^2, respectively. Therefore, flow rates of 0.126 and 0.874 cm^3/s, respectively, were enforced at the entrance of the core and shell layers. To analyze the effect of flow rate on the interface shape, the flow with LDPE-A in both layers was also simulated for the flow rate of 0.378 and 0.622 cm^3/s in the core and shell layers respectively. The total flow rate in this non-synchronized flow rate (NSFR) case is the same as that for the three synchronized flow rate cases, but now the flow rate through the core layer is increased whereas the flow rate through the shell layer is decreased.

Fig. 4 shows the interface shape and velocity distribution for the four coextrusion simulations in the core and shell square die. For all four simulations, the shape of the interface at the die exit is shown in Fig. 5, which also shows the interface shape in the plane of first contact between the two polymers (entrance profile). For LDPE-A in core as well as shell layer, and the flow rates in the two layers synchronized according to the ratio of their cross-sectional areas in the plane of contact, the interface shape and velocity distribution are shown in Fig. 4 (a). It is noted that for the initial interface shape shown in Fig. 3 (b), for a fully developed velocity profile at the die exit, the flow rate through the core will be higher than the flow rate in the core at the plane of contact. Therefore, for the synchronized flow rate at the entrance, for mass conservation, the area of cross-section of the core at the die exit is expected to be smaller than that in the plane of contact. Also, for the same cross-sectional area, the flow rate in the core will decrease if the core moves away from the die axis. The decrease in the cross-sectional area as well as the movement of the core away from the die axis is confirmed by the predicted interface shape in Fig. 4 (a) and Fig. 5. Fig. 4 (b) shows the results for LDPE-D in the core layer and LDPE-A in the shell layer. With the higher viscosity polymer (LDPE-D) in the core layer, the velocity in the core layer is now smaller than that in Fig. 4 (a). Therefore, with LDPE-D in the core layer, in Fig. 4 (b) and in Fig. 5, in comparison to the interface shape for LDPE-A in both layers, the area of cross-section of the core is larger at the exit and the core moves further away from the die axis. The opposite trends are observed for LDPE-A in the core and LDPE-D in the shell layer (Fig. 4 c). With the lower viscosity polymer in the core layer, the flow in the core is faster; the area of cross-section of the core at the exit is smaller; and in comparison to the case with LDPE-A in both layers, movement of the core away from the axis is smaller.

For the non-synchronized flow rate (NSFR), the predicted interface shape and velocity distribution are shown in Fig. 4 (d). With the larger flow rate in the core, immediately after the plane of contact the polymer in the core fountains out, resulting in the outward movement of the interface. Even though, for the NSFR case, the shape of the interface at the entrance and at the exit in Fig. 4 (d) and Fig. 5 are very different, it is noted that the symmetry of the interface about the LLUR diagonal is still maintained. With the different flow rates of LDPE-A in the core and shell layers, even though the velocity distributions in the feed block portion of the die in Fig. 4 (a) and (d) are very different, after the plane of contact the velocity distributions in these two simulations with LDPE-A in both layers are almost the same.

<u>*Flow in a Square Die with Flat Interface*</u>

The finite element mesh used to simulate a bi-layer flow in a square coextrusion die is shown in Fig. 6. The geometry of the die in Fig. 6 is similar to the die geometry used by Dooley and Rudolph [5] for their experimental work. The dimensions of square die cross-section are 0.95×0.95 cm. For the first 2.54 cm of the die in the coextrusion simulation, separate flow channels were used for the two polymers. After flowing separately in this feed block, the two polymers come in contact 2.54 cm inside the die. In the plane of contact, the top polymer layer consists of the 20% of the square cross-section and the bottom polymer layer is the lower 80% of the square.

The bi-layer flow in the square die was also simulated for three-combinations of LDPE-A and LDPE-D with the flow rate synchronized according to the ratio of the cross-sectional area of the two layers in the plane of contact. For the total flow rate of 7.2 Kg/hr (2.05 cm^3/s) used by Dooley and Rudolph [5], flow rates of 0.41 and 1.64 cm^3/s were enforced at the entrance of the top and bottom layers, respectively. Also, to analyze the effect of flow rate on the interface shape, the bi-layer coextrusion in the square die was also simulated for equal flow rates (1.025 cm^3/s) of LDPE-A through the top and bottom layers.

For all four coextrusion simulations in the square die, the interface shape was initialized to a flat surface shown in Fig. 6 (b). It should be noted that the interface surface in Fig. 6 (b) is extended beyond the die boundary. In the present work, we started with interface only between the die walls. However, with interface only between the die walls, as the interface nodes on the die boundary are moved during interface development, some of the interface nodes move outside the die boundary, whereas some move inside the die. At the locations, where the interface boundary nodes move inside the die, the separation between the two polymer layers is lost, and the coextrusion simulation is no more valid and is aborted. With the interface mesh in Fig. 6 (b) extended beyond the die boundaries, during interface development, the partition between the two polymer layers is maintained. However, to solve the no-cross-flow condition over the complete interface mesh, the velocity somehow needs to be fictitiously specified for the nodes outside the die walls. In the present work, the velocity at the interface nodes just inside the die walls was extrapolated outward to specify the velocity at the nodes outside the die walls.

Fig. 7 shows the interface shape and velocity distribution for the four bi-layer coextrusion simulations in the square die. For all four simulations, the shape of the interface at the die exit is shown in Fig. 8, which also shows the interface shape in the plane of first contact between the two polymers. For the flow rate in the two layers at the entrance synchronized according the cross-sectional areas of the two layers at the plane of contact, the interface shape for LDPE-A in both layers is shown in Fig. 7 (a). For a fully developed velocity profile in the square die, the flow rate in the top 20% of the square cross-section is less than 20% of the total flow rate. Therefore, for the synchronized flow rate at the entrance, as expected for mass balance, beyond the plane of contact the interface moves downward to satisfy the no-cross-flow condition. With LDPE in both layers, further downstream from the plane of contact, the velocity is the maximum along the die axis and decreases towards the die walls.

With the higher viscosity polymer (LDPE-D) in the top layer the flow in the top layers is slowed down, whereas the flow in the bottom layer is accelerated. Therefore, with LDPE-D in the top layer, to satisfy the no-cross-flow condition, the interface between the two layers in Fig. 7 (b) and Fig. 8 moves further lower than the interface for LDPE-A in both layer. Again, these trends are reversed when LDPE-A is used in the top layer and LDPE-D in the bottom layer (Fig. 7 c). With the higher viscosity now in the bottom layer, the flow in the bottom layer is slowed down, whereas the flow in the top layer is accelerated, resulting in the higher interface for this case in Fig. 7 (c) and Fig. 8.

To further validate the accuracy of the coextrusion simulation, the bi-layer flow in the square die was simulated with equal flow rate of LDPE-A through the top and bottom layers. With 50% of the polymer coming through the top 20% area, immediately after the plane of contact the polymer in the top layer fountains out, and the interface in Fig. 7 (d) and Fig. 8 moves downward accordingly. If the interface profile at the exit was a straight line, the interface for the NSFR case in Fig. 8 would have been exactly at the middle of die. However, since the interface at the exit is slightly higher in the middle (where the velocity is larger) and lower at the two ends (where the velocity is smaller), for mass conservation, the area of cross-section of the top layer at the exit is expected to be slightly smaller than that of the bottom layer. With the equal flow rate through the two layers, for the predicted interface shape at the exit in Fig. 8, the cross-sectional area of the top and bottom layers are 0.4533 and 0.4539 cm^2, respectively. Again, as observed for the core and shell flow in the last section, for the bi-layer flow also, for flow of LDPE-A in both layers, the velocity distributions further downstream of the plane of contact, are almost identical in Fig. 7 (a) and (d).

In contrast to the interface shape predicted for LDPE-A in the top layer and LDPE-D in the bottom layer in Fig. 7 (c), in the experiments with these two materials, Dooley and Rudolph [5] observed encapsulation of higher viscosity polymer (LDPE-D) by less viscous polymer (LDPE-A) (Fig. 9). Dooley and Rudolph [5] postulated that the encapsulation is caused by the difference between the viscosities of the two polymers. However, our simulation, as well as previous publications by other research groups [2], could not capture the encapsulation with a purely viscous generalized Newtonian formulation. We believe that the encapsulation is caused by the difference in the viscoelastic properties, in particular, second normal stress difference, of the two polymers.

Conclusions

A new algorithm for simulation of a multilayer flow in polymer coextrusion is introduced in this work. The new algorithm does not require the interface between different polymer layers to match with the inter-element boundaries. Instead, the interface is allowed to cut through the tetrahedral finite elements. A weighted residual form of the no-cross-flow condition was used to predict the interface shape. The simulation results presented here clearly demonstrate that our new algorithm can simulate any complex coextrusion system.

Acknowledgement

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References

1. C. Rauwendaal, “Polymer Extrusion”, Hanser Publishers, New York (1994).
2. A. Karagiannis, A. N. Hyrmak, and J. Vlachopoulos, Rheologica Acta, Vol. 29, 71 – 87 (1990).
3. J. Dheur and M. J.Crochet, Rheologica Acta, Vol. 26, 401 – 413 (1987).
4. A. N. Brooks and T. J. R. Hughes, Computer Methods in Applied Mechanics and Engineering, Vol. 32, 199 – 259 (1982).
5. J. Dooley and L. Rudolph, Journal of Plastic Film and Sheeting, Vol. 19, 111 – 123 (2003).

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

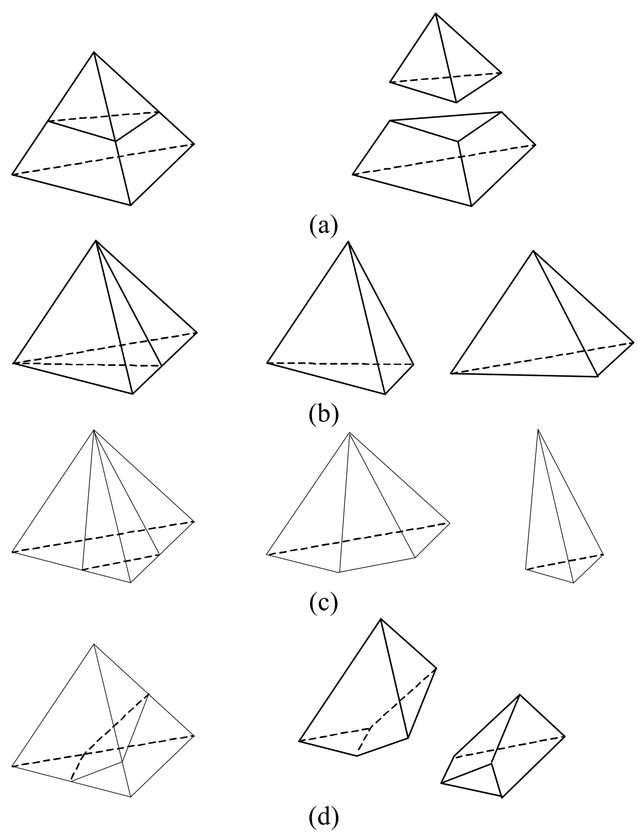


Fig. 1 Four possible combinations of the two finite elements obtained by partitioning a tetrahedral finite element. Each of the figures on the left shows a tetrahedral element with an intersecting plane. Figures on the right show the two finite elements generated by the intersection.

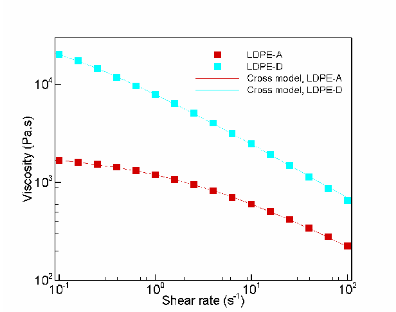
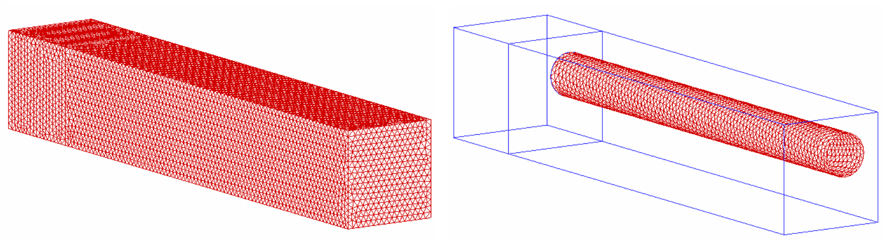


Fig. 2 Viscosity of two different grades of LDPEs [5].



(a) (b)

Fig. 3 Finite element mesh of (a) tetrahedral elements in the square die, (b) triangular elements on the initial interface.

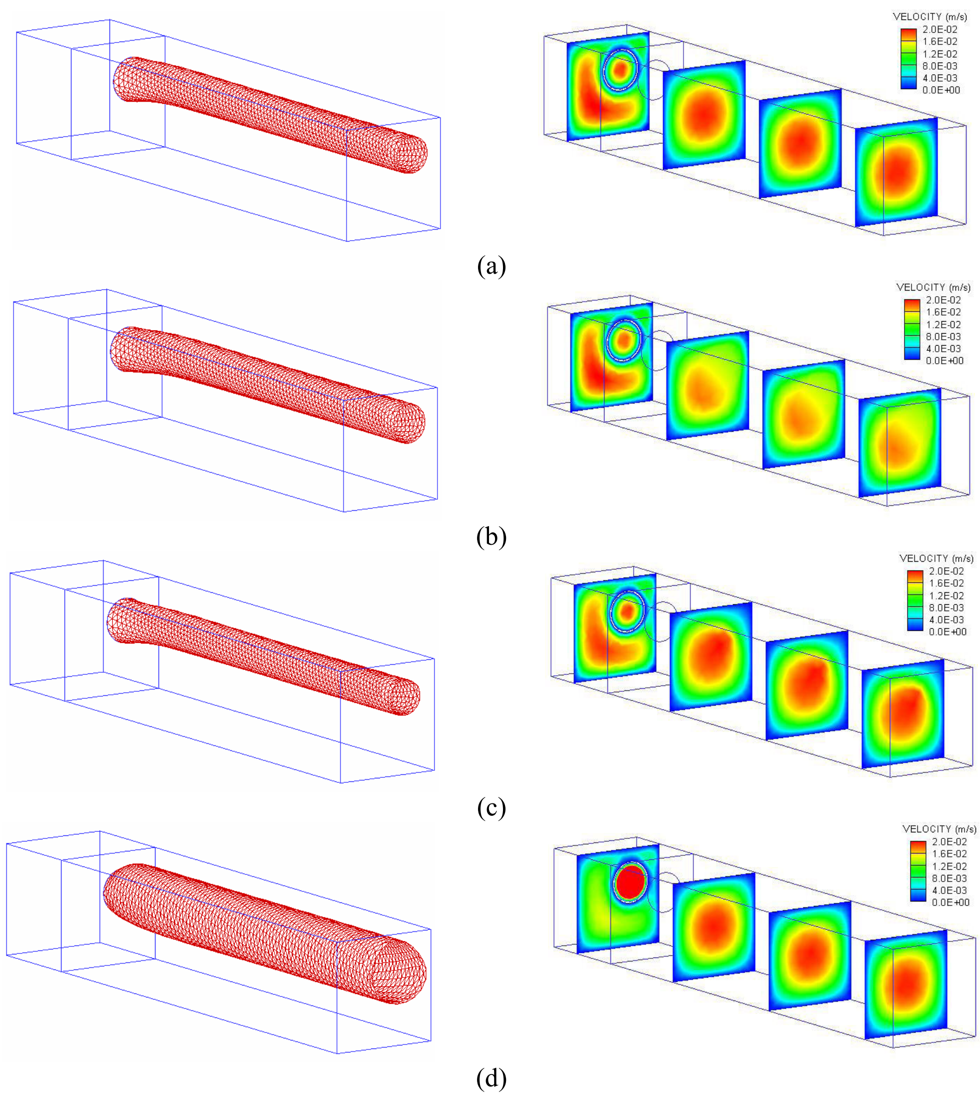


Fig. 4 Interface shape (left) and velocity distribution (right) for the core and shell coextrusion in a square die. (a) Core: LDPE-A, Shell: LDPE-A, (b) Core: LDPE-D, Shell: LDPE-A, (c) Core: LDPE-A, Shell: LDPE-D, (d) Core: LDPE-A, Shell: LDPE-A with higher flow rate through the core.

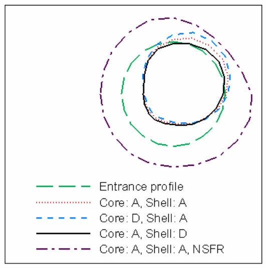
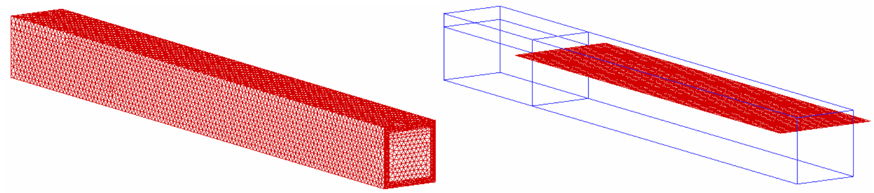
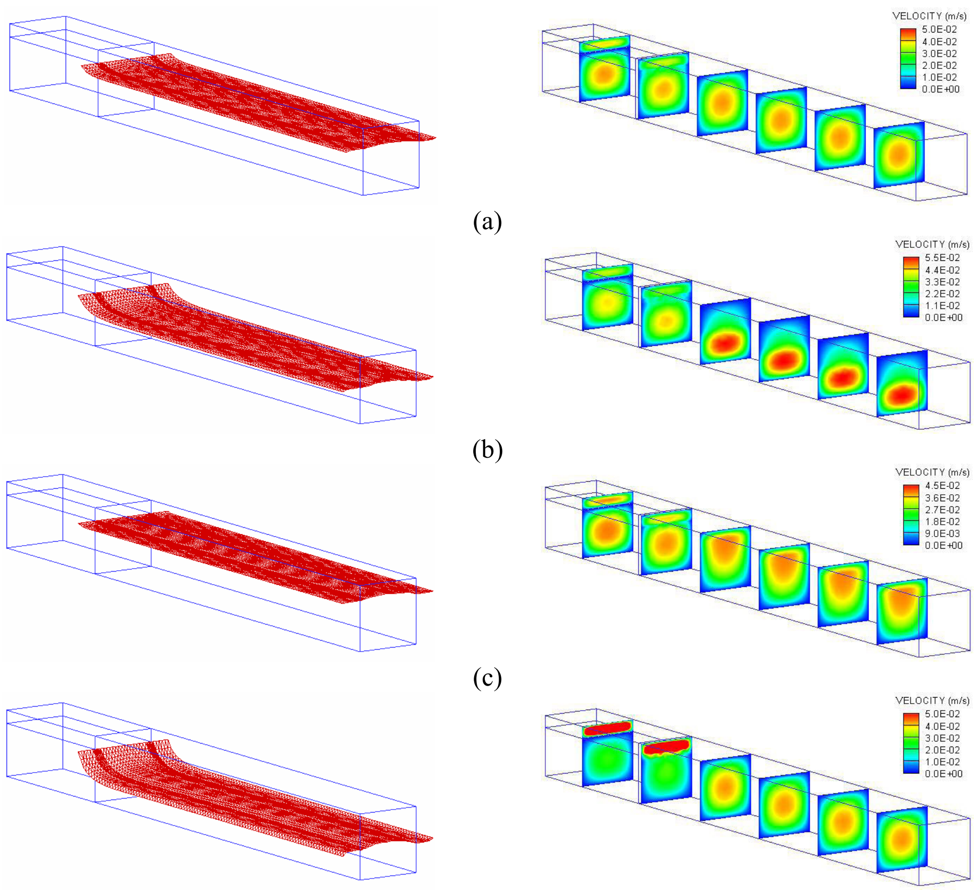


Fig. 5 Interface profiles at the exit of core and shell square die.



(a) (b)

Fig. 6 Finite element mesh of (a) tetrahedral elements in the square die, (b) triangular elements on the initial interface.



(a)

(b)

(c)

(d)

Fig. 7 Interface shape (left) and velocity distributions (right) for the bi-layer coextrusion in a square die. (a) Top: LDPE-A, Bottom: LDPE-A, (b) Top: LDPE-D, Bottom: LDPE-A, (c) Top: LDPE-A, Bottom: LDPE-D, (d) Top: LDPE-A, Bottom: LDPE-A with higher flow rate through the top layer.

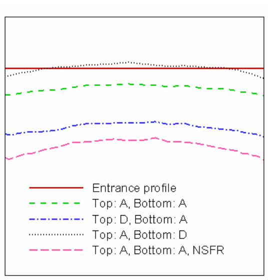
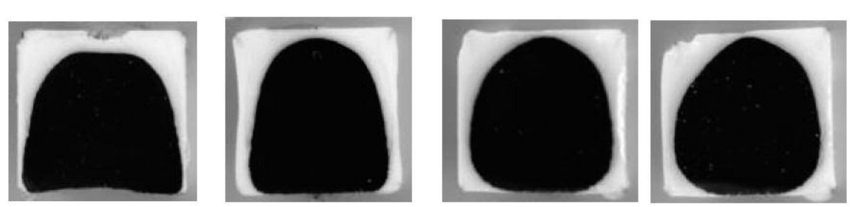


Fig. 8 Interface profiles at the exit of the bi-layer square die.



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

Fig. 9 Interface shape in coextrusion experiments with LDPE-A in the top layer and LDPE-D in the bottom layer [5]. (a) Near the entrance, (b and c) intermediate, (d) near the exit.