COMPARISON OF MESH PARTITIONING TECHNIQUE WITH LEVEL-SET METHOD FOR COEXTRUSION SIMULATION

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Abstract

Multilayer flow is simulated in five different coextrusion dies using the mesh partitioning technique as well as by the level-set method. These simulations show that depending upon the layer structure in the die, one of the two techniques may be more suitable for the coextrusion simulation. In general, the layer structure predicted by the mesh partitioning technique is found to be more accurate than the corresponding predictions from the level-set method. Level-set method requires that the layers should be arranged in a sequential manner, which is not necessary if the mesh partitioning technique is used. The mesh partitioning technique cannot simulate a multilayer flow if an interface between the polymer layers splits into two interfaces, or if two interfaces, which start separately, merge into a single interface in the die.

Introduction

During coextrusion, different polymers are extruded simultaneously through a die. By combining the functionalities of several different polymers, the coextruded products have unique properties which cannot be obtained by any single component polymer [1]. However, design of coextrusion dies is difficult if the coextruded polymers have widely different viscosities because in such a system the layer structure can change dramatically as the polymers flow side-by-side in the die [2, 3]. Therefore, a software package which can accurately predict the development of layer structure in a coextrusion die is an extremely valuable design tool for a die designer.

To simulate a multi-layer flow during polymer coextrusion, many different numerical techniques have been used in the literature. Each of these techniques has advantages (and disadvantages) relative to other techniques, and therefore, may be more suitable depending upon the layer structure employed in the die. A brief review of various coextrusion simulation techniques is presented in the next section. To demonstrate the suitability of each technique, simulations of multilayer flow in five different coextrusion dies are presented later in this paper.

Numerical Techniques for Coextrusion Simulation

The main difficulty in simulation of a multilayer flow is enforcement of the different material properties of the two polymers, when an element in the finite element mesh is occupied by more than one polymer. Each of the three techniques discussed below employ different approach for enforcing different material properties in such elements.

Moving Mesh Technique

In earlier attempts to simulate coextrusion, the node locations in the finite element mesh were moved after each flow simulation iteration (while keeping the mesh topology/connectivity the same), such that the interface between the adjacent polymer layers coincided with the inter-element boundaries in the mesh [2]. With the inter-element boundaries coinciding with interface between adjacent layers, each element is occupied by only one polymer. Therefore, different material properties on two sides of the interface can be easily enforced in the modified mesh. Computer implementation of a moving mesh technique for coextrusion simulation is relatively simple. However, for real life coextrusion systems, with complex three-dimensional die channel geometry, repeated modification of the finite element mesh to obtain interface-matched elements is impractical. Therefore, a moving mesh technique is typically employed for a two-dimensional simulation of coextrusion, or for simple three-dimensional dies such as those for extruding rectangular cross sections.

Mesh Partitioning Technique

The mesh partitioning technique has been employed in all of our coextrusion simulations so far [3 – 6]. In the mesh partitioning technique, the interface between adjacent polymer layers is represented by a mesh of triangular finite elements. This mesh of triangular elements is then used to partition the tetrahedral elements in the die which are intersected by an interface into two different finite elements. The two new elements generated by partitioning an original tetrahedral element in the die can be tetrahedral, pyramidal or prismatic in shape. Further details of the mesh partitioning technique are available in an earlier paper [4].

Once the elements, which are intersected by an interface, are partitioned into two different elements, different material properties on two sides of the interface can be easily enforced in the simulation. Since the finite element mesh remains unaltered during the entire simulation, the mesh partitioning technique can easily simulate a multi-layer flow irrespective of the complexity of the die geometry or that of the layer structure in the coextrusion die. However, the current implementation of the mesh partitioning technique in our software assumes that each interface between adjacent polymer layers is maintained as an individual interface throughout the die. If an interface is split into multiple interfaces inside the die, or multiple interfaces, which start separately, are merged into a single interface in the die, our current implement of the mesh partitioning technique cannot simulate such cases. These cases, with the splitting or joining of interfaces, can be simulated by the level-set method, which is discussed in the next section.

However, splitting and joining of interfaces is rare in coextrusion dies. Therefore, mesh partitioning technique can be efficiently employed to simulate the flow in almost all coextrusion systems. The main disadvantage of the mesh partitioning technique is the complexity of implementing the technique in a software package.

Level-Set Method

In the level-set method, a scalar variable (*f*) is initialized to different values at the various die entrances. The layer structure (or polymer level, *f*) inside the die is then determined by solving the advection equation [7].

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = 0 \qquad (1)$$

where $\vec{v}$ is the velocity of the polymer in the die. Since the flow in an extrusion die typically does not change with time, the time derivative term $\partial f / \partial t$ is zero in coextrusion simulation. In a region near the interface between adjacent polymer layers, where the value of f changes between its values for the two layers, the values of the material properties (density, heat capacity, thermal conductivity and viscosity) are interpolated using a Heaviside function [7].

$$H_\alpha(\varphi) = \frac{1}{2}\left(1 + \frac{\varphi}{\alpha} + \frac{1}{\pi}\sin\left(\frac{\pi\varphi}{\alpha}\right)\right) \qquad (2)$$

where, depending upon the value of *f*, the value of φ ranges from -0.5 to 0.5 between adjacent polymer layers. In the present work, $\alpha = 0.1$ was employed. With the value of H_α being -0.5 for polymer A and 0.5 for polymer B, the value of each of the material properties can be calculated using the following equation.

$$P(\varphi) = P_A + (P_A - P_B)H_\alpha(\varphi) \qquad (3)$$

where P_A is the value of the material property (density, heat capacity, thermal conductivity or viscosity) for polymer A, with P_B being the value for polymer B.

In the level-set method, the shape of the interface between adjacent polymer layers can be estimated by the surface for which the value of the polymer level (*f*) is the average of its values for the two adjacent polymers. The level-set method is much easier to implement in a software than the mesh partitioning technique, and does allow coextrusion simulation without modifying the finite element mesh during a simulation. However, as discussed later in this paper, the level-set method cannot simulate coextrusion if the layer structure is in a non-sequential order. Also, simulation of the flow in a sheet die presented later in this paper shows that interfaces which are close to each other may intersect inside the die if the level-set method is used. Such intersected interfaces are joined together to artificially form a single interface.

Resins

To simulate the flow in the coextrusion dies analyzed in this paper, 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) [8], and a polystyrene from BASF with MFR of 0.3 cm^3/min (200 ºC, 5 kg) [3] were used. The viscosities (η) of the ABS and polystyrene, shown in Fig. 1, were modeled by the Cross-WLF equation given below [9].

$$\eta = \frac{\eta_0}{1 + \left(\eta_0 \dot{\gamma} / \tau^*\right)^{1-n}} \qquad (4)$$

$$\eta_0 = D_1 \exp\left[-\frac{A_1(T - T_a)}{A_2 + (T - T_a)}\right] \qquad (5)$$

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 this paper, the values of the material parameters are given in Table 1.

Results and Discussion

For five different coextrusion dies, simulation results from the mesh partitioning technique and the level-set method are compared in this section. In each die, the same finite element mesh was used for simulating the flow using the two techniques. For all the results presented here, the polyXtrue software [10] was used to simulate the flow. The software allows the user to select either one of the two techniques for coextrusion simulation. The first two dies analyzed are sheet dies with a coat-hanger type manifold. The remaining three dies extrude a simple square cross-section with the polymer layers arranged differently in each die. Even though, a simple square extrudate shape was used to show some of the limitations of the two coextrusion techniques, these limitations were first encountered by polyXtrue users with highly complex profile dies such as those used for extruding window seals and frames. However, these proprietary die geometries cannot be included in this paper. Also, the limitations of the simulation techniques are easier to visualize in the simpler die geometries employed here.

Five-Layer Sheet Die with Five Entrances

Fig. 2 shows the geometry of a five layer sheet die with coat hanger type of manifold. ABS was used for the top, bottom, and center layers, whereas polystyrene was used for the other two intermediate layers. Since each of the five polymers have different entrances, the value of the polymer level (*f*) was initialized to different integer values at the five entrances with the value increasing sequentially from 1 for the top layer to 5 for the bottom layer. Starting from the contact line, each interface between the adjacent polymer layers was determined by the surface corresponding to the average of the polymer level values for the two adjacent polymers. Fig. 3 shows the polymer level distribution in the seven different cross-sections of the sheet die. It is evident from Fig. 3 that starting from the five entrances, the value of the polymer level is convected all the way to the die exit. For this die, the four interfaces between the five layers, defined by the surfaces with average values of the polymer level, were clearly distinct all the way from the contact lines to the die exit. The interface between the bottom layer and the layer above it is shown in Fig. 4. The finite element mesh shown in Fig. 4 was obtained by connecting the points with average value of the polymer level (4.5) along the edges of the tetrahedral elements with triangular finite elements. The flow in this five-layer die was also simulated by using the mesh partitioning technique. The interface between the bottom layer and the layer above as predicted by the mesh partitioning technique is shown in Fig. 5. As expected, the interface shape predicted by the level-set method (Fig. 4) and that by the mesh partitioning technique (Fig. 5) are almost identical.

Five-Layer Sheet Die with Two Entrances

The flow in the five-layer sheet die analyzed in the last section was next simulated with a different feed block. As shown in Fig. 6 the new feed block used for the sheet die has only two entrances, with the ABS for the top, bottom and the center layers coming from the right entrance, and the polystyrene for the two other intermediate layers entering from left. The value of the polymer level was initialized to 1 at the left entrance and 2 for the right entrance. In the seven different cross-sections, the predicted polymer level is shown in Fig. 7. In Fig. 7, the blue or the red color for the polymer level is maintained in each layer as the two polymers go through the feed block. The blue and the red colors in the five layers are also retained for a short distance after the five layers meet. However, the layered structure of the blue and red colors is lost after this short distance. Beyond this short distance after the five layers meet, the color is red near the top and bottom die walls, with the yellow color in most of the region away from the die walls. Since the layered structure of blue and red colors is maintained only for a short distance after the five layers meet, as expected, the level-set method can only determine the interface between the polymer layers in this region. The interface between the bottom layer and the layer above it, as predicted by the level-set method, is shown in Fig. 8. The interface for the two bottom layers in Fig. 8 actually also include the interface above this. The two interfaces intersect each other after the region where the blue and red layered structure is maintained in Fig. 7. Once the two interfaces intersect, the distinction between the two interfaces is lost in Fig. 8. For this sheet die with only two entrances, the interface between the bottom layer and the one above it, as predicted by the mesh partitioning technique, is shown in Fig. 9. The predicted interface shape in Fig. 9 is almost the same as the interface shapes in Figs. 4 and 5 for the die with five different entrances.

Since the advection equation for calculating polymer level (Eqn. 1) has no diffusion term, theoretically the value of the polymer level for each layer should convect from entrance all the way to the exit without any change. However, in a numerical simulation, some diffusion of the polymer level values does occur across the interface. To minimize this transverse diffusion of the polymer level, an upwind discretization scheme [11] was employed in the finite element formulation of Eqn. 1. In spite of the upwind discretization, some diffusion always occurs in a numerical simulation. Therefore, if the adjacent interfaces are only a small distance apart, due to the artificial diffusion in the polymer level, as observed in Fig. 8, the two interfaces can artificially intersect in a numerical simulation by the level-set method.

To examine the effect of mesh refinement on the accuracy of the interface shape predicted by the level-set method, the flow in the five-layer sheet die with two entrances was simulated again with a finer finite element mesh with 1,019,847 tetrahedral elements. The maximum number of elements allowed for coextrusion simulation in polyXtrue is 1.15 million. The original finite element mesh used for the results presented in Figs. 7 – 9 had 458,188 elements. The polymer level and interface shape predicted with the finer finite element mesh are respectively shown in Figs. 10 and 11. Even with the finer mesh, in Fig. 10 the layered structure of blue and red colors is lost soon after the five layers meet. Unexpectedly, in Fig. 10 the distance for which the layered structure of blue and red colors is retained with the finer mesh is actually smaller than that in Fig. 7. Accordingly, in Fig. 11, the interface predicted between the two adjacent layers near the bottom intersects the interface above it immediately after the two interfaces start from the two separate contact lines. Even though, the polymer level and interface shape for the five-layer die predicted by the level-set method in this section did not improve with the finer finite element mesh, the similar predictions for a two-layer die discussed in the next section did improve when a finer mesh was employed.

Square Cross-Section Die with a Circular Core

For a two-layer die with square cross section of polystyrene outside and a circular core layer of ABS inside (Fig. 12), the polymer level and interface predicted by the level-set method are shown in Figs. 13 and 14. In Fig. 13 the polymer level for the core polymer, and in Fig. 14 the interface between the two layers, shrink sharply right after the two polymers come in contact for the first time. The streamlines for the core polymer, as predicted by the simulation using the level-set method, are shown in Fig. 15. It is evident from Figs. 14 and 15 that, due to inaccuracies in the numerical solution of Eqn. 1, the interface in Fig. 14 is crossing the streamlines. The interface between the two polymer layers in the die, as predicted by the mesh partitioning technique, is shown in Fig. 16. The interface in Fig. 16 matches well with the streamlines shown in Fig. 15.

To further explore the effect of mesh refinement on the interface shape predicted by the level-set method, the flow in this two-layer die with square cross-section was simulated again with a finer finite element mesh. The mesh originally used for the results shown in Figs. 13 – 16 had only 137,130 tetrahedral elements. The polymer level and interface shape predicted by using a finer mesh with 1,075,196 elements are shown in Figs. 17 and 18 respectively. The predicted polymer level and interface shape in Figs. 17 and 18 are significantly better than the corresponding predictions in Figs. 13 and 14. Shape of the interface at the die exit predicted by the two simulation techniques is shown in Fig. 19. It is evident from Fig. 19 that even with a finer mesh the interface shape predicted by the level-set method has significant fluctuations and the interface still crossed the streamlines.

Square Cross-Section with Non-Sequential Layer Structure

A limitation of the level-set method is that the polymer layers in the die must have a sequential layout. That is, the i^{th} layer can only be in contact with $(i - 1)^{th}$ and $(i + 1)^{th}$ layer. Therefore, the flow in the six-layer square cross-section die with non-sequential layer structure shown in Fig. 20 cannot be simulated by the level-set method. As evident by the contact lines, which are shown highlighted in yellow in Fig. 20, the die has a circular core layer, two semicircular layers on top and bottom, and two rectangular layers on the two sides. All of these five ABS layers are in contact with a common polystyrene layer. The circular core enters the die from the rear, whereas the other five layers enter the die from five side entrances. Flow in this six-layer die was simulated using the mesh partitioning technique. The predicted shapes of the five interfaces are shown in Fig. 21 (a) – (c). The layer structure at the exit of the six-layer die (red) along with contact lines where the polymers came in contact for the first time (black), are shown in Fig. 22. The flow in this die is symmetric about the horizontal plane through the center of the die. The flow is not symmetric about the vertical plane through the center of the die because the entrance for the common layer, which is in contact with the other five layers, is located on the right side. The symmetry about the horizontal center plane is maintained in the predicted interfaces in Figs. 21 (a) – (c) and also in the layer structure at the die exit in Fig. 22.

Square Cross-Section Die with a Merging Interface

Flow in a die in which two interfaces start separately, and then merge into a single interface inside the die (Fig. 23) is simulated in this section. ABS is used in the top layer, whereas the bottom layer is polystyrene. In the region near the two contact lines, shown highlighted in Fig. 23, the square cross-section of the die has a vertical slit. Therefore, the interface between the two layers in this die starts from two separate contact lines and then merges into a single interface in the region of the die beyond the vertical slit. The present implementation of the mesh partitioning technique in the polyXtrue software assumes that each of the interfaces between adjacent layers in a die does not split into multiple interfaces or merge with another interface starting from a different contact line. Consequently, the flow in the die shown in Fig. 23 could not be simulated by the current implementation of the mesh partitioning technique in the polyXtrue software. Therefore, the level-set method was used to simulate the flow in this die. The interface shape and the layer structure at the die exit predicted by the level-set method are shown in Figs. 24 and 25, respectively. It is noted that the predicted interface shape in Fig. 25 has some unexpected fluctuations near the contact lines. Also, even though the flow is symmetrical about the vertical plane passing through the center of the die, the interface shape in Fig. 24, and the layer structure at the die exit in Fig. 25, are not symmetrical about the vertical center plane. This inherent inaccuracy in the interface shape predicted by the level-set method was also evident in the two-layer square die with a circular core discussed earlier.

Conclusions

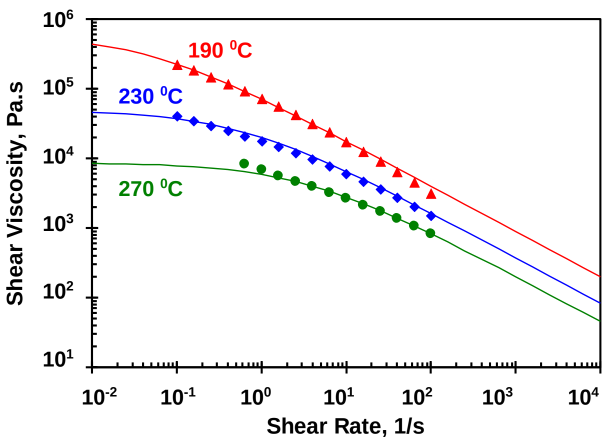
For the three dies in which the flow was simulated using both coextrusion simulation techniques, the layer structure predicted by the mesh partitioning technique was found to be more accurate than the corresponding predictions from the level-set method. In particular, it is found that if the interfaces between the layers are very close to each other, these interfaces may intersect artificially if the level-set method is used, whereas such interfaces remain separate in the mesh partitioning technique. The flow in a die with non-sequential layer structure cannot be simulated using the level-set method. The mesh partitioning technique cannot simulate a multilayer flow if an interface between the polymer layers splits into two interfaces, or if two interfaces, which start separately, merge into a single interface in the die.

References

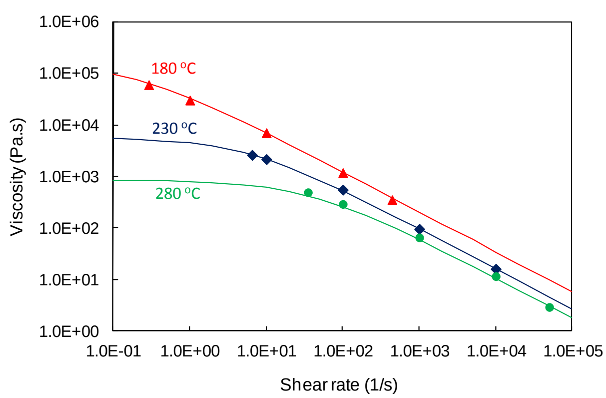
1. C. Rauwendaal, "Polymer Extrusion", 4th Edition, Hanser Publishers, (2001).
2. A. Karagiannis, A. N. Hyrmak, and J. Vlachopoulos, *Rheologica Acta*, Vol. 29, 71 – 87 (1990).
3. M. Gupta, *SPE ANTEC Technical Papers*, Vol. 58, (2012).
4. M. Gupta, *SPE ANTEC Technical Papers*, Vol. 54, 217 – 222 (2008).
5. M. Gupta, *SPE ANTEC Technical Papers*, Vol. 56, 2032 – 2036 (2010).
6. M. Gupta, *SPE ANTEC Technical Papers*, Vol. 59, 1227 – 1231 (2013).
7. J. A. Sethian, Level Set Methods and Fast Marching Methods, Cambridge University Press (1999).
8. A. Altinkaynak, M. Gupta, M. A. Spalding, and S. Crabtree, *Int. Polym. Proc. J.*, Vol. 26, 182 – 196 (2011).
9. C. W. Macosko, "*Rheology Principles, Measurements, and Applications*", Wiley-VCH, New York, (1994).
10. PolyXtrue software, Plastic Flow, LLC, Hancock, MI 49930.
11. A. N. Brooks and T. J. R. Hughes, *Comput. Meth. Appl. Mech. Engrg.*, Vol. 32, 199 – 259 (1982).

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.

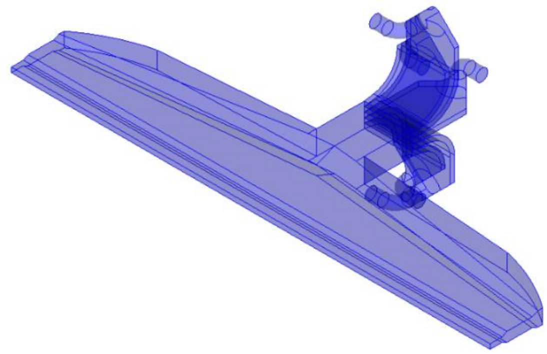


Fig. 2 Geometry of a five-layer sheet die with a separate entrance for each layer.

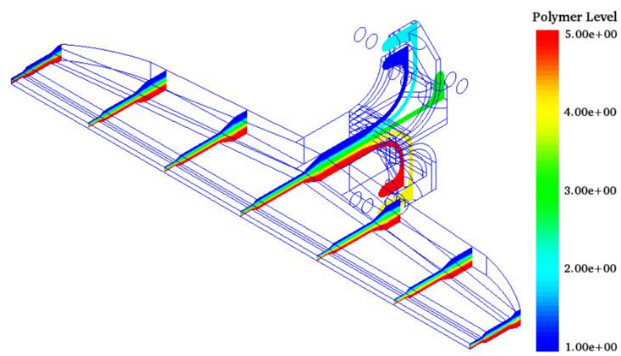


Fig. 3 Polymer level in the five-layer sheet die with five entrances.

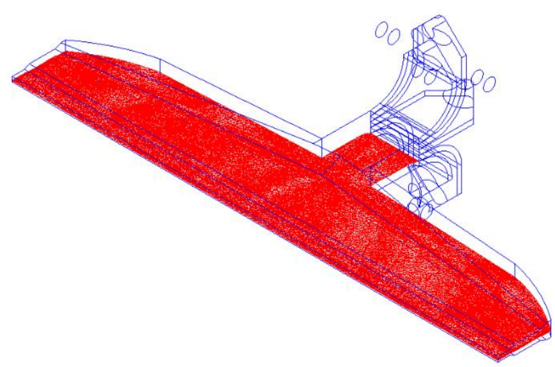


Fig. 4 Interface between the two layers near the bottom of the die as predicted by the level-set method.

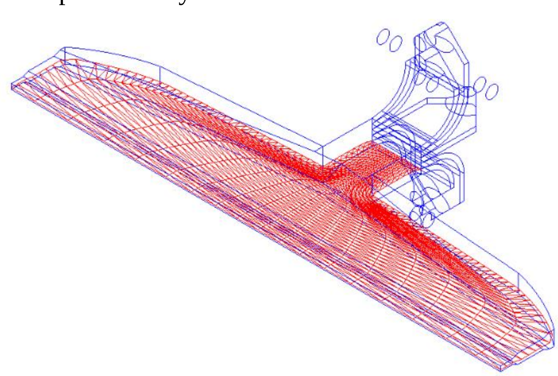


Fig. 5 Interface between the two layers near the bottom of the die as predicted by the mesh partitioning technique.

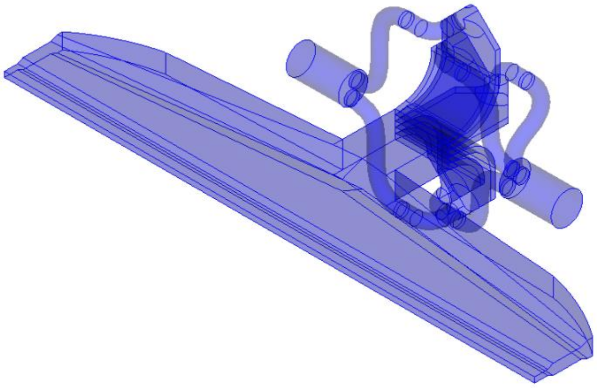


Fig. 6 Geometry of a five-layer sheet die with only two entrances.

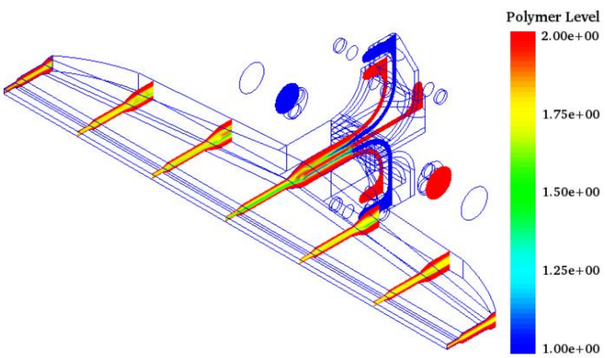


Fig. 7 Polymer level in the five-layer sheet die with only two entrances.

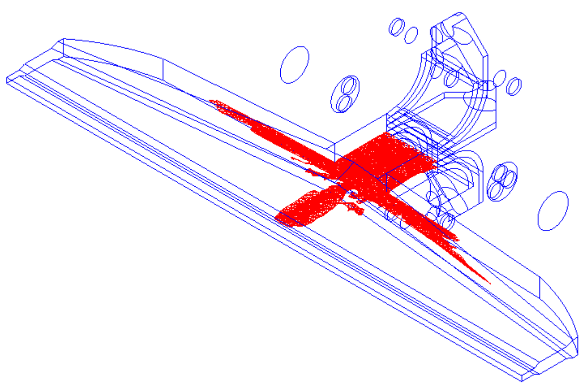


Fig. 8 Interface between the two layers near the bottom of the die as predicted by the level-set method.

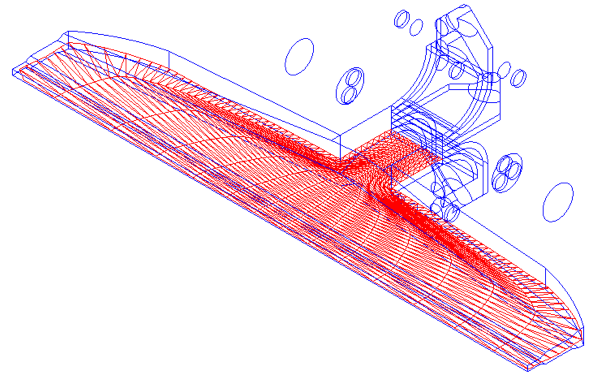


Fig. 9 Interface between the two layers near the bottom of the die as predicted by the mesh partitioning technique.

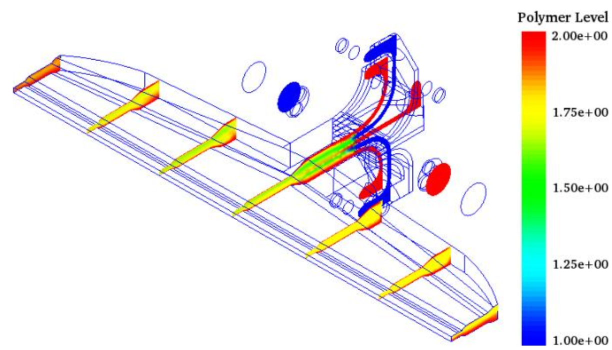


Fig. 10 Polymer level in the five-layer sheet die with only two entrances using a finer finite element mesh.

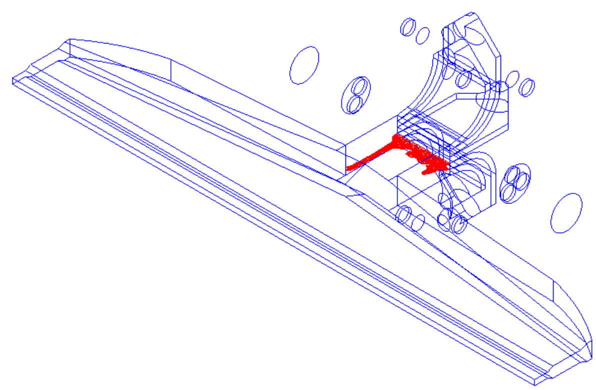


Fig. 11 Interface between the two layers near the bottom as predicted by the level-set method using a finer mesh.

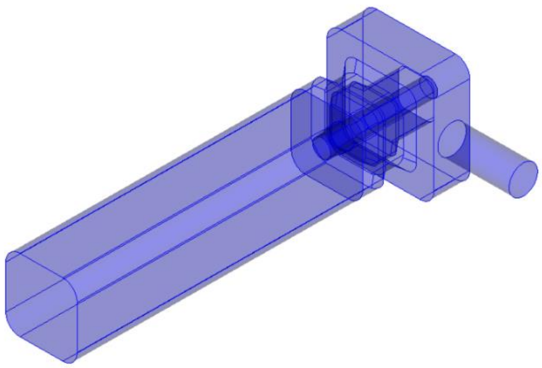


Fig. 12 Geometry of a die with square shape extrudate and a circular core layer.

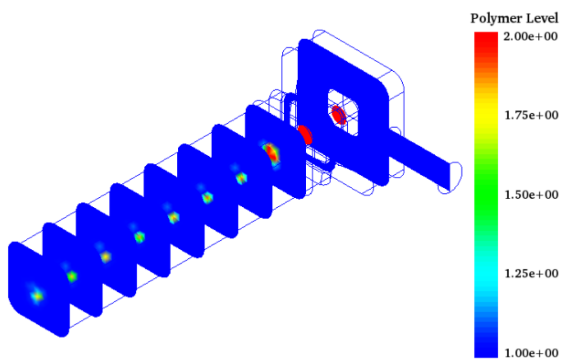


Fig. 13 Polymer level in the square die with a circular core.

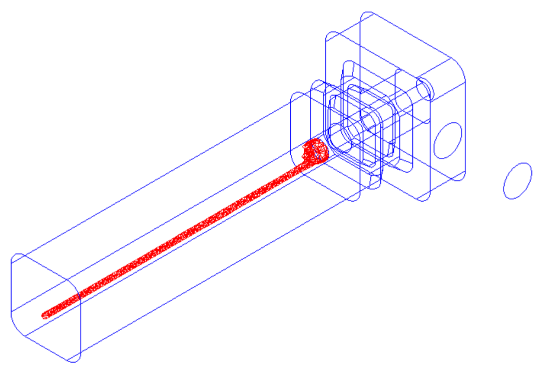


Fig. 14 Interface between the two layers as predicted by the level-set method.

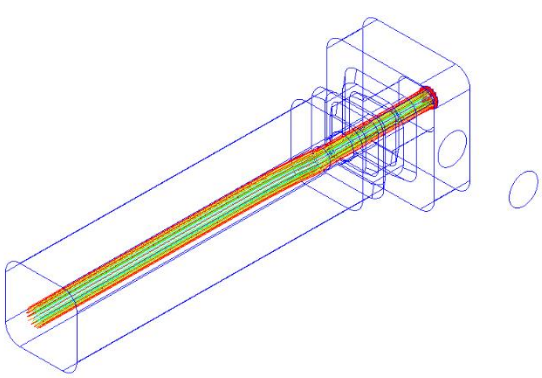


Fig. 15 Streamlines in the core layer as predicted by the level-set method.

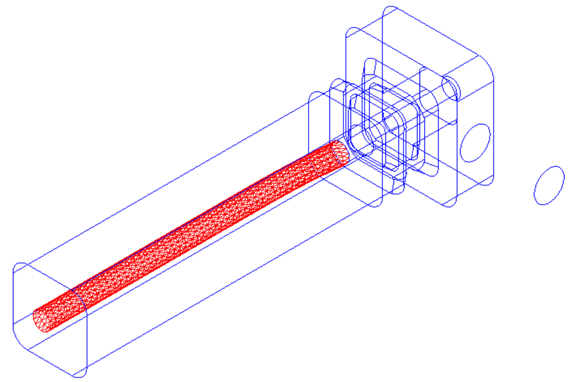


Fig. 16 Interface between the two layers as predicted by the mesh partitioning technique.

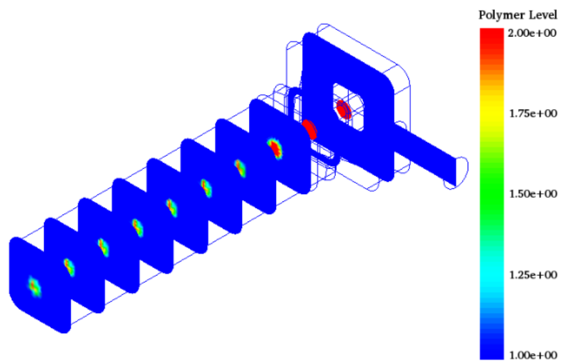


Fig. 17 Polymer level predicted using a finer finite element mesh.

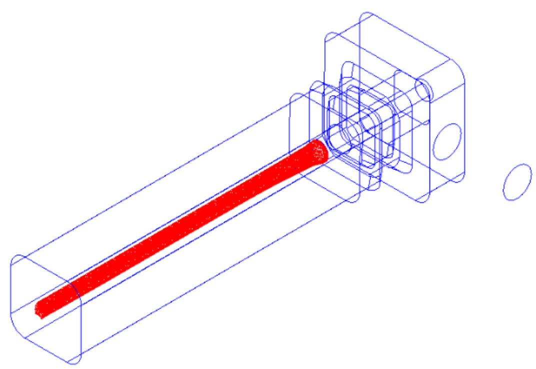


Fig. 18 Interface shape predicted by level-set method using a finer finite element mesh.

Fig. 19 Interface shape at the die exit predicted by the mesh partitioning technique and the level set method.

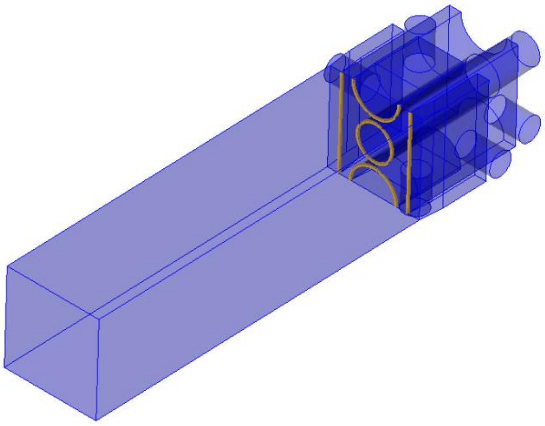


Fig. 20 Geometry of a six-layer square die with a non-sequential layer configuration.

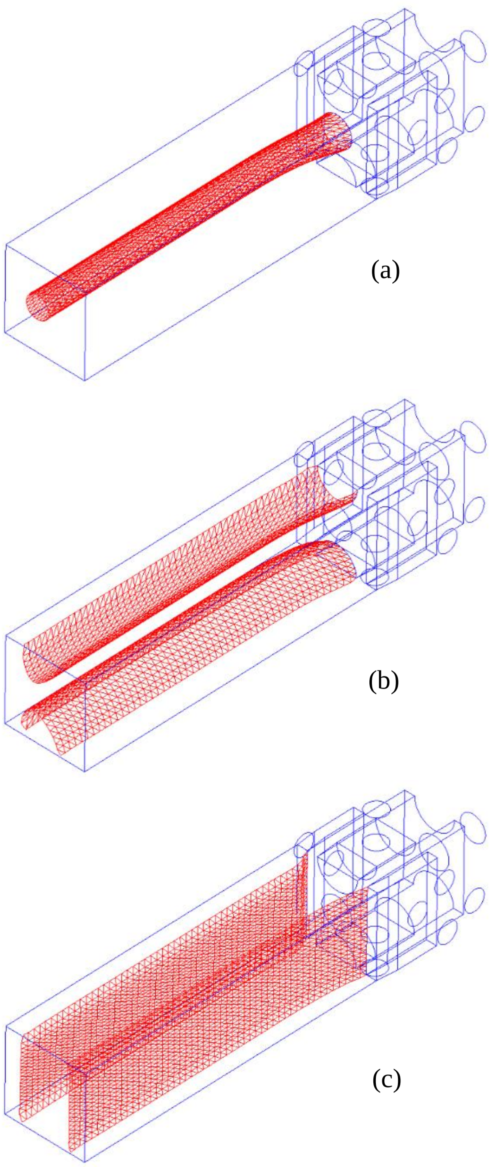


Fig. 21 Interfaces predicted by the mesh partitioning technique for the circular core (a), semicircular layers on top and bottom (b), rectangular layers on sides (c).

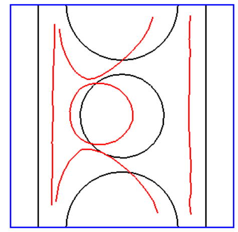


Fig. 22 Predicted layer structure (red) at the exit of the die as predicted by the mesh partitioning technique. Lines of first contact between the layers are shown in black.

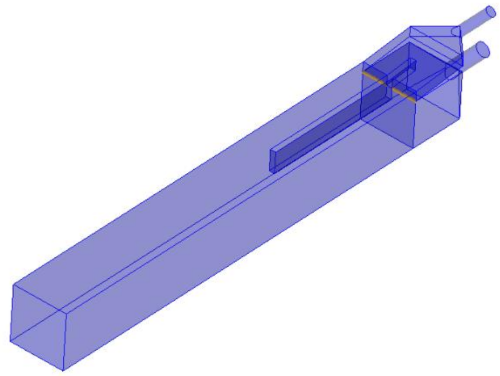


Fig. 23 Geometry of a die with an interface starting as two separate interfaces which merge into one interface before exiting the die.

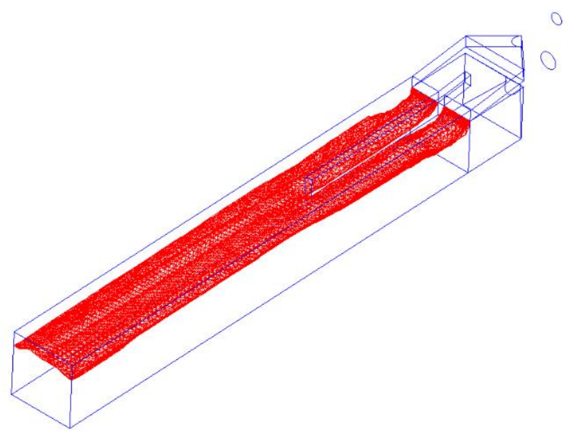


Fig. 24 Interface between the two layers as predicted by the level-set method.

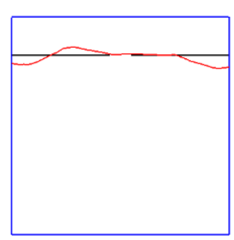


Fig. 25 Predicted layer structure (red) at the exit of the die as predicted by the level-set method. Line of first contact between the layers is shown in black.