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An Automated Computational Fluid Dynamics Framework for 3D Multilayer Coextrusion Simulations in Complex Die Geometries

by Dayne A. Plemmons



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14. ABSTRACT Multilayer coextrusion is a scalable manufacturing technology for producing advanced polymer composites with targeted, micro-, and nanostructured layer architectures. However, achieving precise layer fidelity requires careful optimization of processing conditions and die geometries. Due to the cost and complexity of physical prototyping, predictive computational tools are essential for evaluating layer morphologies and flow stability. We present an automated, open-source computational fluid dynamics (CFD) framework built on the OpenFOAM platform to simulate 3D, two-phase coextrusion flows. The closed-loop workflow integrates parametric CAD generation, automated meshing, generalized Newtonian transport modeling, and quantitative field analysis. Applied to layer-multiplying element (LME) dies used during multilayer coextrusion, the framework effectively captures critical flow phenomena—including viscous encapsulation, shear-thinning-induced layer distortion, and interfacial stress spikes—for both viscosity-matched and mismatched resins. Furthermore, the tool is applied to evaluate and optimize novel LME geometries, demonstrating that maintaining a constant cross-sectional area and gradual convergence angles significantly reduces interfacial shear stresses and suppresses layer asymmetry. Ultimately, this predictive framework provides an efficient, scalable tool for guiding LME die design, mitigating processing defects, and targeting exact layer morphologies in advanced polymeric composite manufacturing.					
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1. Introduction

Multilayer coextrusion is a versatile manufacturing process that enables the production of polymeric composites with unique morphologies.^{1–4} However, due to the complexities inherent in the process—such as rheology, die design, and heat transfer—various nonuniformities or instabilities may arise, making it difficult to achieve a desired morphology. Detrimental phenomena include layer rearrangement caused by viscous encapsulation,^{5–7} interfacial defects resulting from wave-like or zigzag instabilities,^{8–10} and spatially varying layer thickness profiles.¹¹ In some cases, these phenomena may be counterintuitive, arising from uneven stresses that are difficult to anticipate a priori. Consequently, a predictive tool for flow behavior under specific processing parameters is highly desirable to understand the resulting layer morphologies and associated stresses. While preliminary estimates can be made using analytical predictions for simple geometries (i.e., shear flow in a channel¹²), numerical tools are ultimately required to predict velocity profiles and interfacial stresses in the complex, real-world geometries used during multilayer coextrusion. While previous studies have laid the groundwork for the numerical treatment of laminar multilayer flows with varying rheological complexity (e.g., generalized Newtonian^{13–15} and viscoelastic fluids^{16–18}), this report outlines a general computational workflow applicable across multiple use cases in the simulation of multilayer coextrusion flows. These applications include predicting layer morphologies under specified process conditions and material properties, estimating conditions that trigger process instabilities, and iteratively optimizing design criteria using computational fluid dynamics (CFD) simulation feedback.

The key component in the numerical simulation of multilayer coextrusion is the treatment of the interface between different polymer species. When the components are immiscible (or interdiffusion is negligible within the relevant time scales), the interface acts as a phase boundary. Both implicit and explicit interface-tracking methods¹³ have been employed in both finite element method^{13,14,19,20} and finite volume method (FVM)^{5,16,21} simulations of multilayer coextrusion processes. While the exact algorithmic details are beyond the scope of this study, key developments in multilayer coextrusion enabled by numerical simulations warrant discussion. Numerical simulations of simple coextrusion flows have shed light on experimentally observed instability phenomena. These studies—frequently focusing on two-layer flows—demonstrate that instability typically arises when the shear stress at the interface exceeds a threshold level.^{8,18,22} Using the concept of a “critical interfacial shear stress,” stability criteria for varying flow-rate mismatch, viscosity mismatch, and layer count may be rationalized.^{9,10} Additionally,

computational insights have yielded key design criteria for layer-multiplying elements. First, Lee and Dooley demonstrated that decreasing the relative path length difference across different die sections improves layer uniformity¹¹; this requirement was accommodated by increasing the length of the multiplier channels. Second, dies with constant cross-sectional areas were employed to reduce pressure drops and interfacial shear stresses.^{20,23} Third, high-aspect-ratio dies were utilized to minimize the effects of radial asymmetry and secondary flows.^{19,24} Finally, dies with symmetrical flow paths minimize the skew caused by interfacial distortions.

The goal of this work is to present a generalized multilayer simulation framework built upon mature numerical techniques. This framework can simulate coextrusion across a variety of process conditions with adjustable degrees of simplification and complexity. Crucially, the tool uses existing open-source packages and can be scripted via Python for advanced customization and automated postprocessing. This enables efficient parametric sweeps across variables such as absolute and relative volumetric flow rates, rheological properties, and die geometries. Furthermore, methods are outlined for quantifying and visualizing the effects of these parameters on the resulting morphologies and flow phenomena. Insights gleaned from a few tutorial use cases are summarized in this report; most notably, feedback from CFD simulations is used to optimize the design of a layer-multiplying element (LME) die for a 2:1 aspect ratio flow channel. Ultimately, the tool offers actionable guidance for process design in multilayer coextrusion across a range of real-world applications.

2. Theory and Methods

The methods described here use the open-source FVM platform OpenFOAM as the computational engine. OpenFOAM is a mature, modular tool in which many different physics, geometries, and analytical methods can be incorporated. In addition to built-in utilities for meshing and postprocessing, its case structure and file-based field variable architecture facilitate seamless integration with external tools (e.g., Python and ParaView) for advanced visualization and quantitative analysis. Nevertheless, non-Newtonian rheological models and additional physical complexities—such as nonisothermal heat transfer—can be readily implemented. Figure 1 shows how these open-source tools work together to form a closed-loop workflow for designing, simulating, and analyzing multilayer coextrusion processes. The overall process consists of the following steps: 1) parametric geometry definition using a CAD tool such as FreeCAD; 2) hexahedral meshing of the geometry using block-fitting and edge-refinement techniques; 3) definition of the physical models, process parameters, and simulation initialization using OpenFOAM case setup (automated through the foamlib Python library); 4) running

the simulation with the OpenFOAM FVM engine; and 5) postprocessing the resulting field data using ParaView. The following sections describe the framework and methodology for each stage in detail.

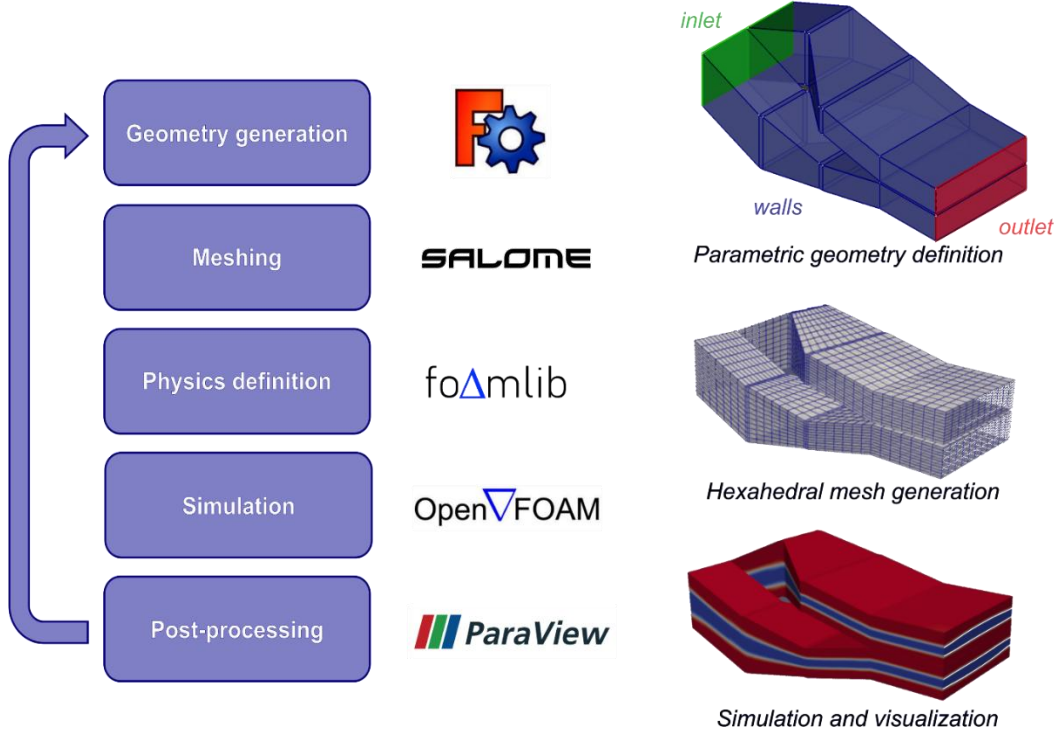


Figure 1. Schematic of the automated computational workflow for multilayer coextrusion simulations.

2.1 Two-Phase Multilayer Flow

Two-phase multilayer flow simulation relies on the volume-of-fluid (VoF) algorithm for interface capturing,²⁵ where a transport equation for a phase fraction scalar is solved simultaneously with the continuity and momentum conservation equations. Through this formulation, a single effective fluid is modeled across the computational domain, with physical properties calculated as volumetric averages based on the local phase fraction. The governing equations for continuity, momentum conservation, and phase fraction transport are expressed as

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} + \mathbf{f}_\sigma \quad (2)$$

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{u} \alpha) = 0 \quad (3)$$

where $\mathbf{u}$ represents the velocity field, ρ is the fluid density, p is the pressure field, $\mathbf{g}$ is the gravitational acceleration, and $\mathbf{f}_\sigma$ surface tension force field with surface tension coefficient σ . The deviatoric stress tensor, $\boldsymbol{\tau}$, for a generalized Newtonian fluid (e.g., purely viscous) is defined as

$$\boldsymbol{\tau} = 2\eta[\dot{\gamma}]\mathbf{D} \quad (4)$$

where $\eta[\dot{\gamma}]$ is the apparent viscosity as function of shear rate $\dot{\gamma}$, and $\mathbf{D}$ is the rate of displacement tensor. For a Newtonian fluid approximation, the apparent viscosity simplifies to a constant value, η_o . To capture the shear-thinning behavior characteristic of polymer melts, a generalized Newtonian power-law model can be employed:

$$\eta[\dot{\gamma}] = \eta_o \dot{\gamma}^{1-n} \quad (5)$$

where n is the power-law index describing the extent of shear thinning behavior.

The effective physical quantities ρ and η within the two-phase domain are evaluated as volume fraction-weighted averages as

$$\rho = \alpha\rho_1 + (1 - \alpha)\rho_2 \quad (6)$$

$$\eta[\dot{\gamma}] = \alpha\eta_1[\dot{\gamma}] + (1 - \alpha)\eta_2[\dot{\gamma}] \quad (7)$$

where ρ_i and η_i are the density and viscosity of the i th individual fluid component.

2.2 Meshing and Automated Case Scripting for Multilayer Flow in LME Geometries

The practicality of the OpenFOAM CFD workflow stems from the ability to easily script a variety of functional variables and physical approximations, rendering the simulation process highly automated. As summarized in Figure 1, the entire workflow—including parametric geometry generation, meshing, physics initialization, simulation, and postprocessing analysis—is contained within a single Python script. The foamlib Python package²⁶ is used for OpenFOAM case generation and manipulation. For a general case, the geometric parameters, material properties (e.g., viscosity model parameters and density), initial and boundary conditions, and system properties (e.g., parallel computing architecture) are passed directly into the execution script.

Geometry is programmatically generated using a Python script interfacing with FreeCAD parametric geometry software.²⁷ For various LME design variations, rectangular sketches generated in specified planes with defined dimensions are

lofted to generate a final 3D flow domain. For simple planar geometries, such as those used in standard LME designs, meshing is performed using hexahedral block fitting via a Python script within the Salome numerical simulation platform.²⁸ This approach allows for the generation of high-quality structured meshes with well-defined anisotropy. For multilayer flows, the mesh cells are typically much finer along the axis perpendicular to the layer interfaces (i.e., the y-axis as defined in Figure 1). Additionally, the appropriate granularity along the flow axis must be selected such that reasonable time steps can occur for low Courant number (e.g., $Co < 1$). Edge groups are selected in Salome for features that need refined meshing, and new 1D wire discretization hypotheses are applied in a submesh for each individual edge group. Upon computation, an efficient, structured hexahedral mesh is generated ensuring timely convergence and numerical stability in CFD simulations. In situations requiring more complex geometric curvature (e.g., a cast film exit die), the `snappyHexMesh` utility built into OpenFOAM is used. This approach relies on the refinement of an initial, simple hexahedral block mesh using the surfaces of the flow domain specified in an STL file.

Following meshing, the mesh cell centers are calculated, and a Python script initializes the field values, boundary conditions, material properties, and case system properties based on user input. For most cases reported herein, the boundary conditions consist of a fixed inlet velocity $\mathbf{u}$ and phase fraction α , a zero-gradient condition at the outlets, and no-slip conditions ($\mathbf{u} = 0$) at the walls. The inlet conditions are initialized via a script to allow for arbitrary spatial variation through interpolation onto the inlet patch cell centers. A two-layer inlet flow, for example, can be specified using piecewise functions where $\alpha = 0$ and $\alpha = 1$ for the respective spatial domains. Importantly, this framework also enables inlet values to be mapped via interpolation from the outlet values of a previous simulation. In this manner, recursive simulations representing sequential layer multiplication steps can be seamlessly performed. The cases are solved using the `incompressibleVoF` solver module in OpenFOAM v12; this solver captures a sharp fluid interface via an artificial compression term while strictly enforcing phase fraction mass conservation using the algebraic Multidimensional Universal Limiter for Explicit Solution framework.²⁵ The “PIMPLE” time-stepping algorithm—a combination of Pressure-Implicit with Splitting of Operators, or PISO, and Semi-Implicit Method for Pressure-Linked Equations, or SIMPLE—is used to manage these transient flows. To reduce computational time, simulations are parallelized across a user-defined number of cores using the “Scotch” decomposition algorithm within OpenFOAM’s `decomposePar` utility.

2.3 Field Variable Postprocessing and Visualization

Visualization and quantification of the velocity fields and phase morphology are facilitated by the ParaView large-data processing platform.²⁹ This framework allows for sampling the computed field variables along specified volumes, planes, or lines, enabling targeted calculations to be performed on discrete subsets of the data. ParaView is used for the multilayer polymer flow use case to analyze localized shear rates and stresses, evaluate the nature of phase interfaces, and trace fluid streamlines based on their initial spatial locations. To calculate interfacial shear stress, an isovolume filter spanning $\alpha = 0.5 \pm 0.01$ is first applied to isolate the phase boundary. Equation 4 is then evaluated exclusively for the mesh elements within this threshold domain. This allows for appropriate comparison of regions where interfacial shear approach may approach a critical limit. To quantify the geometric distortion of the layer interfaces, a contour filter for $\alpha = 0.5$ is applied at the outlet plane. Each individual interface is subsequently isolated using a connectivity filter, allowing the distortion to be explicitly quantified by calculating the arc length and maximum y -coordinate variance for each extracted interface layer.

3. Results and Discussion

3.1 Generalized Newtonian Simulation of Two-Component AB Flows

To aid in process design and explaining experimental observations, it is useful to have a prediction of coextrusion flow behavior and expected film morphology for given process parameters. One strategy would be to build up numerical simulations from simple approximations to increasingly realistic complexity. In this study, isothermal simulations with generalized Newtonian viscosity behavior are performed. These approximations yield simulations with tractable numerical stability and computation time such that many process conditions and designs can be explored. As an example simple study, two-layer flow behavior in an early design LME³⁰ is simulated with for varying relative flow rates (e.g., $u_A:u_B = 1:4$, $1:1$, $4:1$) and relative Newtonian viscosities (e.g., $\eta_A:\eta_B = 1:1$, $10:1$). The resulting phase morphology and velocity profile at the outlet of the LME are shown in Figures 2A and 2B, respectively.

Even in this most simple approximation, a few useful observations can be made. First, a simple prediction is obtained for the relative layer thickness of a given flow rate and viscosity ratio. Additionally, a flaw in the die design becomes apparent. There is a significantly larger shear rate gradient during layer formation for the conditions with a substantial viscosity mismatch. The shear rate maximum occurs

during the compression of the melt in the first geometric transformation in the LME (Figure 3). Figure 3C shows that during flow convergence, the shear rate at the die wall in contact with the low-viscosity material is nearly an order of magnitude larger than that at the opposite wall. This is not ideal for layer stability due to the associated increase in interfacial shear stress. Finally, the tendency for viscous encapsulation at high-viscosity mismatch initiates even for layers with nonrate-dependent viscosity.

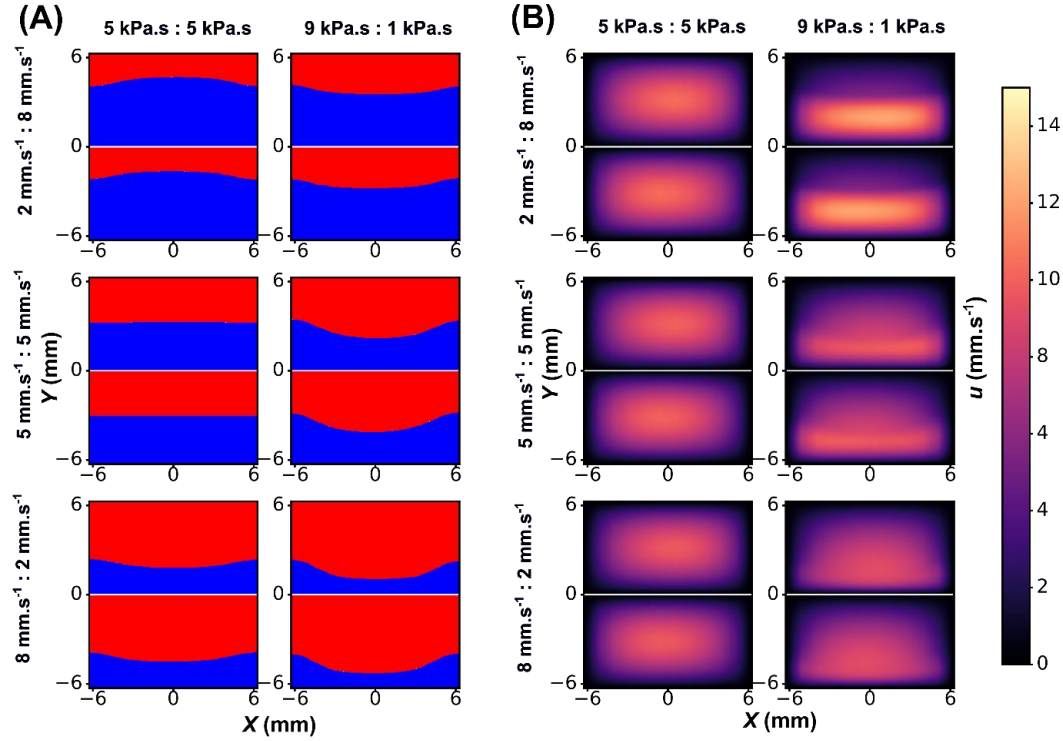


Figure 2. (A) Predicted layer morphologies and (B) velocity profiles after a single layer-multiplication stage for an AB two-layer flow. Subplots evaluate flow rate ratios of 2:8 (top), 5:5 (middle), and 8:2 (bottom) at viscosity ratios of 1:1 (left) and 9:1 (right).

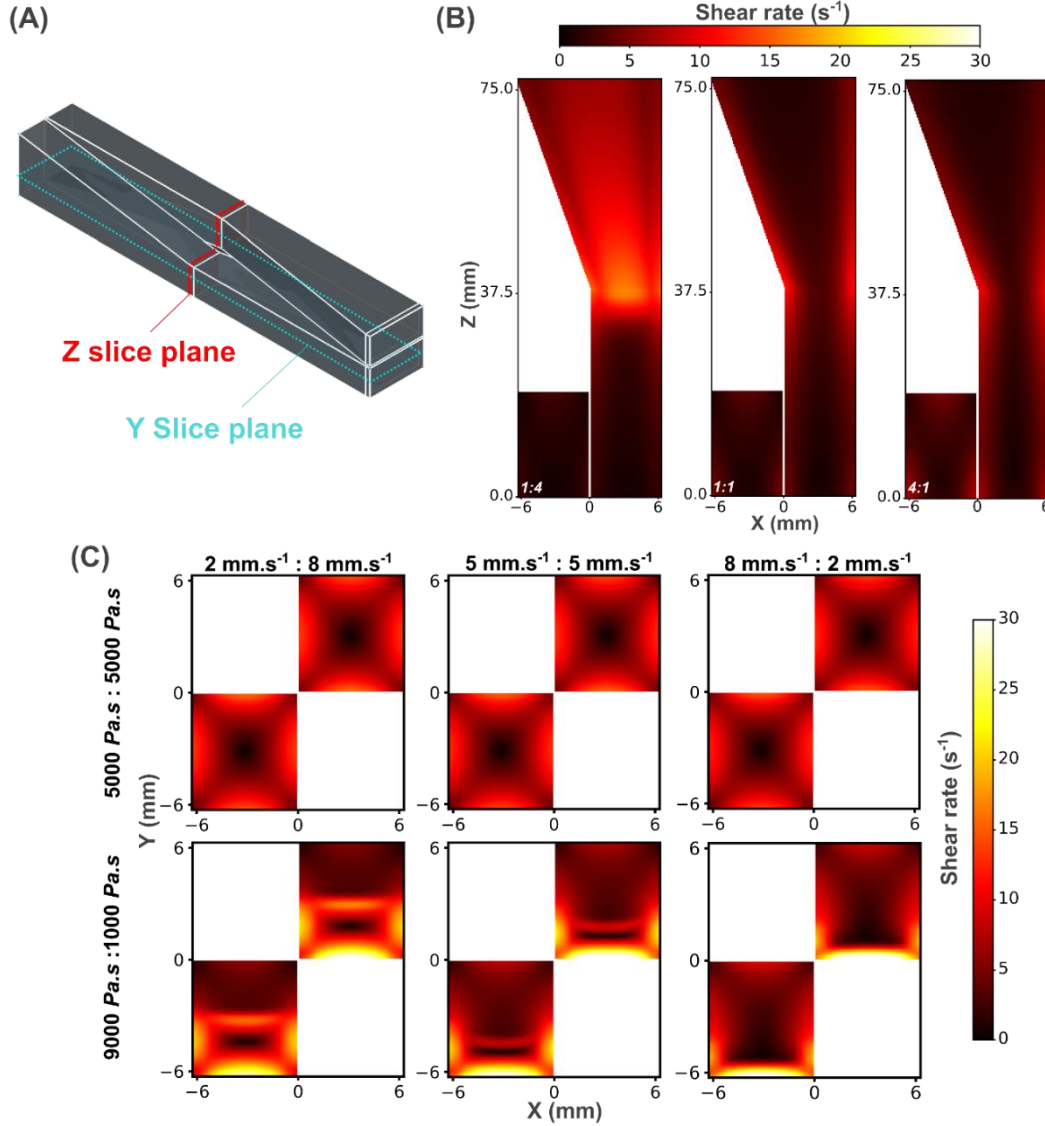


Figure 3. (A) Geometry of the LME die illustrating the associated slice planes evaluated in simulation. (B) Predicted shear rate profiles at the vertical midpoint of the bottom flow channel for a 9:1 viscosity ratio across flow rate ratios of 2:8 (left), 5:5 (middle), and 8:2 (right). (C) Predicted shear rate profiles along the z -midpoint plane of the die (plane of maximum shear rate). Subplots compare flow rate ratios of 2:8 (left column), 8:2 (middle column), and 5:5 (right column) under viscosity ratios of 1:1 (top row) and 9:1 (bottom row).

While constant viscosity simulations are a base case, it is expected that characteristic shear thinning rheology of polymer melts should result in significant distortion of layers in LME geometries with large shear gradients—for example, the low aspect-ratio channels used in early LME designs. To explore these effects, a simple power-law rheology model (Equation 5) with $n = 0.5$ was applied to explore the flow effects. Figure 4 compares the phase morphologies predicted for the Newtonian (Figure 4A) and power-law approximations (Figure 4B). Interestingly, the results are similar during the first layer multiplication process

(i.e., going from two to four layers); however, the interfacial distortions become increasingly apparent upon sequential layer multiplication processes. The interior layers become significantly thinned near the lateral die walls, while the layers bordering the top and bottom die walls become thicker. Additionally, the layers become asymmetric across the vertical midpoint line due to distortions resulting from flows being split in different directions. These layer distortions occur even when the layers exhibit the exact same viscosity behavior. These initial simulations identify the primary motivating factors for newer LME design iterations; i.e., achieving a more spatially uniform layer distribution and improving flow stability as the viscosity mismatch increases. The following sections outline simulations for varying die geometries.

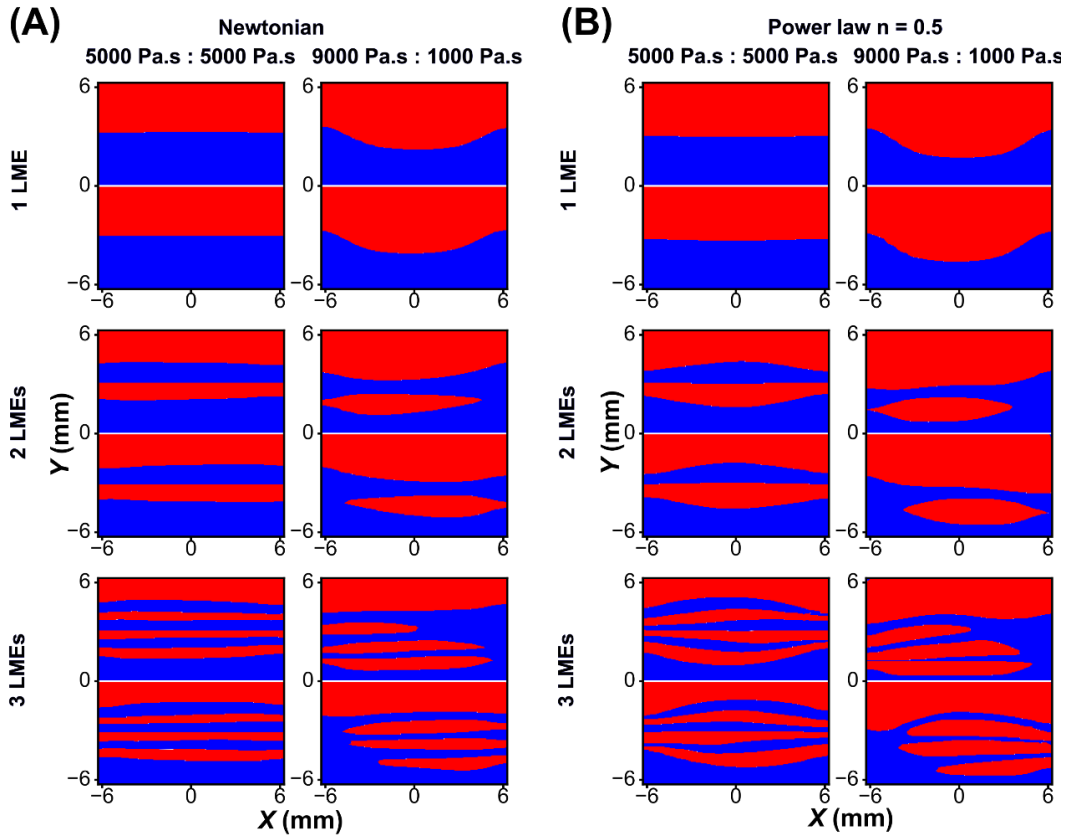


Figure 4. Predicted phase morphologies for multilayer flows after one (top row), two (middle row), and three (bottom row) LME stages under viscosity ratios of 1:1 (left column) and 9:1 (right column): (A) Newtonian fluid approximation and (B) power-law fluid approximation ($n = 0.5$).

3.2 Comparing Effects of LME Die Geometry

Improvements in the design of LME dies have primarily focused on two key aspects. First, maintaining a constant cross-sectional area during flow transformation helps to alleviate shear rate gradients. Second, increasing the aspect

ratio toward thinner rectangular channels reduces the relative extent of layer distortions stemming from die wall effects and secondary flows.

As shown in Figure 5A, three generalized designs are compared here. Design 1 is the 1:1 aspect ratio design evaluated in the previous section.³⁰ This die is the easiest to machine because it can be milled from a single piece (i.e., it does not require modular sections). In Design 1, the layers are split and vertically compressed in the front section, then laterally expanded and stacked in the second section. Additionally, two 2:1 aspect ratio designs with constant cross-sectional areas are considered. In Design 2, the two channels are initially offset vertically and subsequently undergo combined vertical compression, lateral expansion, and recentering to form stacked layers. This design combines geometric transformations into only two sections to simplify machining and reduce footprint. However, previous simulations have shown that combining geometric transformations can sometimes result in permanent distortion of layer interfaces.²¹ Design 3 uses a five-section modular approach in which all individual geometric transformations occur separately. The sections are 1) vertical offset, 2) horizontal recentering, 3) cross-sectional transformation, 4) vertical recentering, and 5) flow stabilization land.

Figures 5B and 5C compare the interfacial shear stresses and layer morphologies, respectively, for each of the three designs during the restructuring of a three-layer ABA flow. Table 1 summarizes the observed die pressures, maximum shear rates, and interfacial stresses for the various die geometries and process parameters. The designs are initially compared at a constant total length. The interfacial shear stress is significantly reduced by maintaining a constant cross-sectional area (Designs 2 and 3). However, the quality of the layer structure is not unequivocally improved in all cases. Some instances of viscous encapsulation remain for mismatched viscosities, while extreme asymmetric layer distortions arise (most prevalent in Design 3) even under a perfect nominal viscosity match.

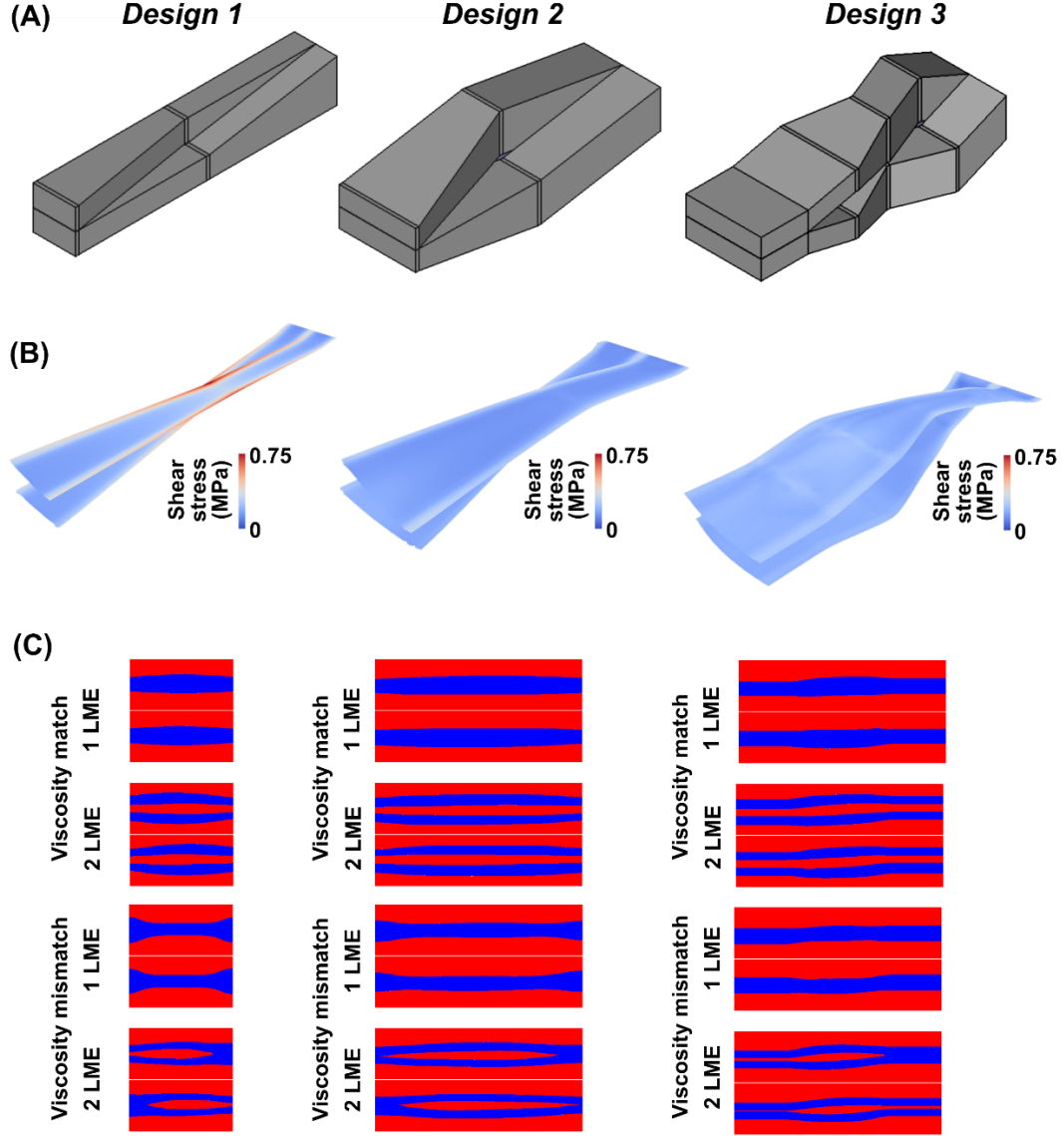


Figure 5. (A) Example CAD geometries for Designs 1 (left), 2 (middle), and 3 (right). (B) Maps of interfacial shear stress for a 9:1 viscosity ratio during the first layer-multiplication stage. Surfaces represent streamlines initiated at the phase interface at the inlet. (C) Representative phase morphologies for Designs 1 (left), 2 (middle), and 3 (right) comparing viscosity-matched conditions (rows 1 and 2) and a 9:1 viscosity ratio (rows 3 and 4) after the first (rows 1 and 3) and second (rows 2 and 4) layer-multiplication stages.

Table 1. Comparison of die pressure drops, maximum shear rates, and interfacial shear stresses across representative LME die geometries.

	Viscosity ratio	Pressure drop (MPa)	Max shear rate (s ⁻¹)	Max interfacial shear stress (MPa)
Design 1	1:1	8.2	19	0.42
	9:1	10	34	0.83
Design 2	1:1	3.6	9	0.22
	9:1	4.9	11	0.4
Design 3	1:1	5.9	14	0.26
	9:1	8.6	14	0.44

To explore further die design improvements—particularly regarding layer uniformity—simulations were performed with varying section lengths. Figure 6 plots isocontours of $\alpha = 0.5$, representing the location of the interfaces in the upper die half after the first layer-multiplication stage for designs with varying total lengths. Across all designs, the mean position of the interface varies significantly from the nominal target for an ABA layer stack with a 50:50 composition ratio (i.e., Interface 1 at 0.25 and Interface 2 at 0.75). This implies that the parabolic velocity profile arising from no-slip boundary conditions at the wall increases layer thickness near the die walls and decreases layer thickness internally. In many cases, the interface position also shows significant lateral variation from its mean.

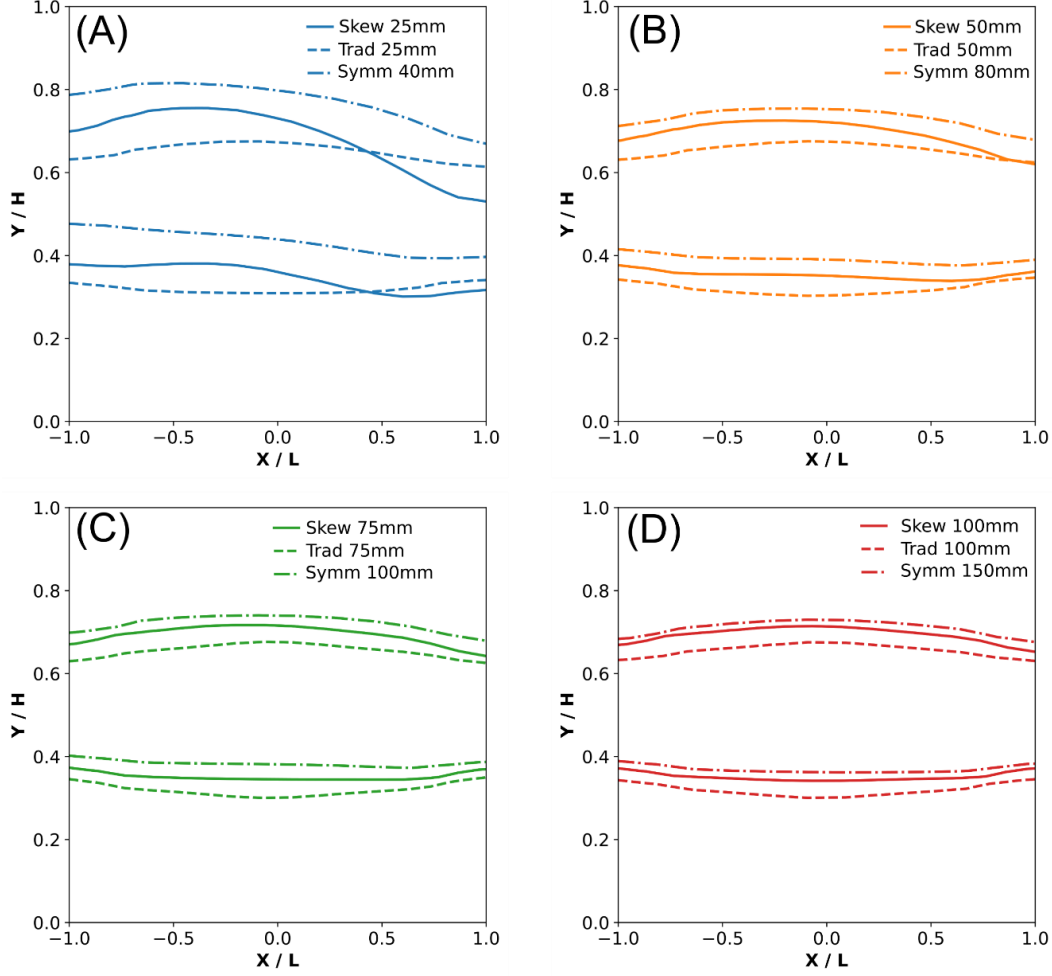


Figure 6. Predicted layer interface contours ($\alpha = 0.5$) after a single layer-multiplication stage across varying total die lengths (A–D) for Designs 1 (dashed lines), 2 (solid lines), and 3 (dash-dotted lines).

To quantify this behavior, metrics describing interface variation were defined to enable objective optimization. The root-mean-square (RMS) error of the interface position relative to the mean location describes the extent of total layer distortion. Additionally, asymmetry across the horizontal midpoint (skewness) is defined as the RMS error between the observed interface and a perfectly symmetric interface (i.e., a reflection of the left interface across the horizontal midpoint). Figure 7 illustrates how these metrics vary with total die length across the different designs. For Design 1 (Figures 7A and 7D), the metrics show little variance and largely converge for total die lengths greater than 50 mm. In comparison, Designs 2 (Figures 7B and 7E) and 3 (Figures 7C and 7F) show significantly greater variance in both RMS error and asymmetry. For Design 2, the values tend to plateau at lengths greater than 75 mm, whereas lengths of approximately 125 mm are required for Design 3. In Designs 2 and 3, layer distortions predominantly arise during the

first die section where the vertical centers are offset; irrecoverable warping and loss of vertical symmetry occur if the convergence angle is too steep. Prior simulations²¹ at constant section length yielded similar findings for vertical recentering transformations. However, contrary to those findings, the present results indicate that combined geometric transformations can be suitable, provided an appropriately small convergence angle is used. Ultimately, the simulations demonstrate that while the newer design iterations improve process stability in all cases, prudent selection of design parameters is required to maintain layer uniformity.

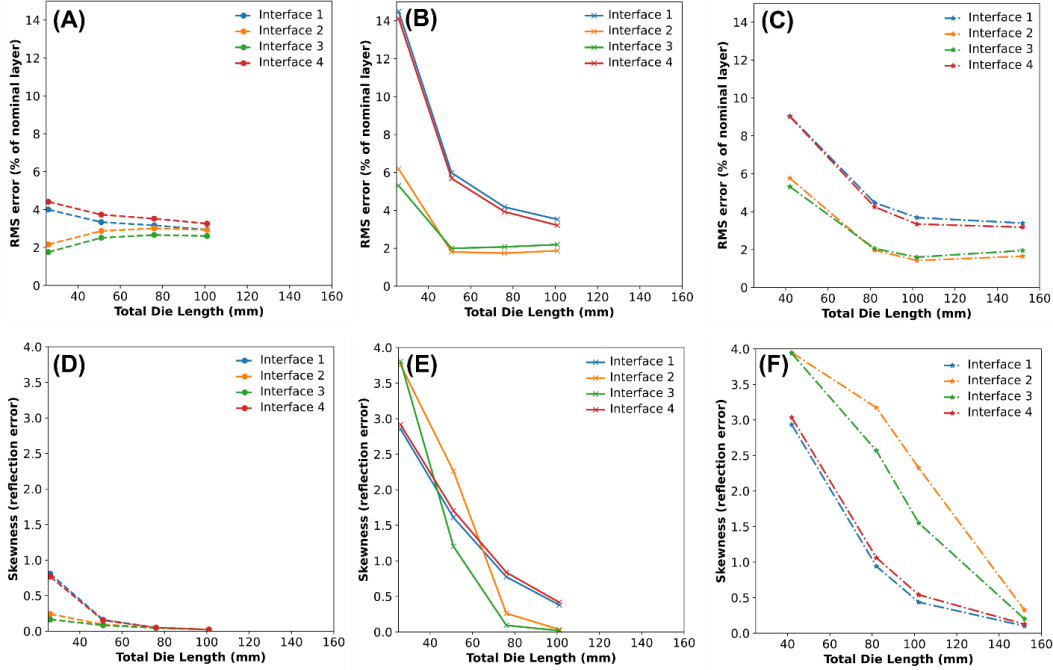


Figure 7. Quantitative metrics evaluating interfacial layer distortion after a single layer-multiplication stage: (A–C) RMS error of the interface position relative to the mean location and (D–F) interface asymmetry across the horizontal midpoint (skewness) for Designs 1 through 3, respectively.

3.3 Reconciling Experimental Observations

3.3.1 Predicting Interfacial Instability

Several additional example simulations were performed and analyzed to further illustrate the utility of the multilayer simulations in describing observed experimental phenomena. It is desirable to predict the conditions under which interfacial flow instabilities arise for resins with mismatched viscosities. While simulating the exact physical nature of these flow instabilities would require a full viscoelastic constitutive model and highly robust numerical methods, predicting the interfacial shear stress at the layer interfaces is feasible using the methods described here.

As suggested in the literature,^{8–10} interfacial instability tends to arise when a critical interfacial shear stress is exceeded at the layer boundaries. Figure 8 shows a top-down view of the predicted shear stresses at the layer interfaces (i.e., at $\alpha = 0.5$) for increasing layer counts and a 9:1 viscosity ratio, comparing a 75-mm Design 1 die (Figures 8A–C) and a 75-mm Design 2 die (Figures 8D–F). The color map is thresholded such that saturated areas (dark red) represent positions where the critical shear stress has been exceeded. Saturation is significantly more prevalent for the Design 1 die. During a single multiplication stage, the critical shear stress (e.g., 0.75 MPa) is exceeded only near the side walls during flow convergence. However, during the second and third layer-multiplication stages, the regions exceeding critical shear become progressively larger. This occurs primarily because the additional multiplication stages position the layer interfaces closer to the die walls, where the shear rates are substantially higher. In Design 2, despite an overall increase in shear stress with higher layer counts, no regions exceed the benchmark critical shear stress. This highlights the primary advantage of LME dies designed with a constant cross-sectional area: superior flow stability under viscosity-mismatched conditions.

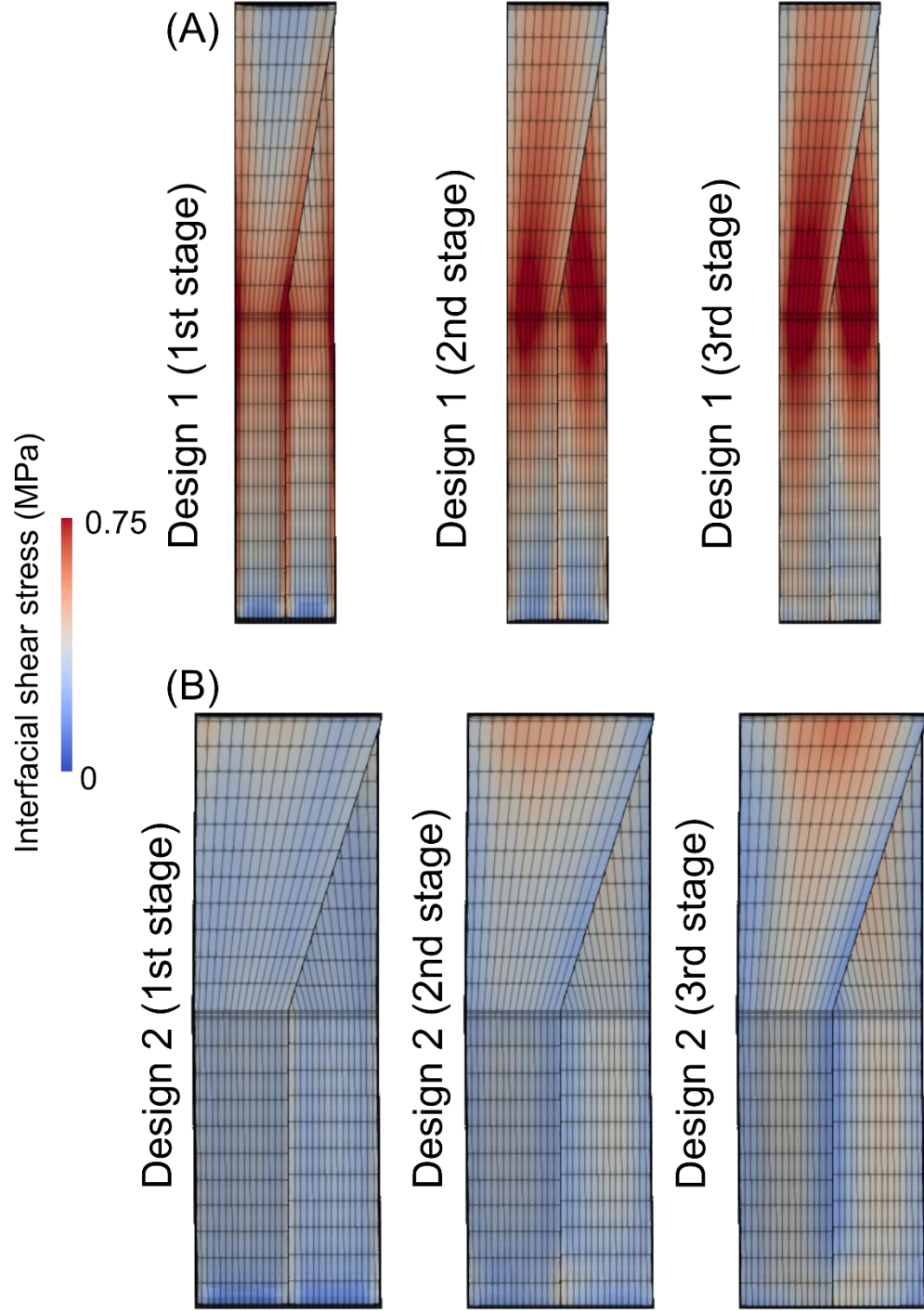


Figure 8. Top-down view of predicted interfacial shear stress distributions for 75-mm total length dies: Designs (A) 1 and (B) 2 after the first (left column), second (middle column), and third (right column) layer-multiplication stages.

3.3.2 Predicting Layer Thickness Variation

Predicting layer thicknesses based on process parameters and die design is critical for applications requiring a precise layer-thickness profile (e.g., dielectric mirror films^{31,32}). To illustrate the utility of computational tools in predicting layer thickness, multilayer simulations for up to four sequential multipliers were performed using an optimized Design 2 die geometry.

Figure 9 shows the predicted phase morphology for a three-layer ABA flow with a 50:50 composition ratio after one (Figure 9A), two (Figure 9B), three (Figure 9C), and four (Figure 9D) LME stages. All 33 nominal layers are clearly resolved under viscosity-matched conditions through four LME stages. Figure 9E shows the extracted layer thicknesses normalized by their expected nominal values (d/d_{nom}) as a function of their relative vertical position within the film (y_i/L). The observed layer thicknesses inversely track the velocity profile within the die sections; i.e., layers near the die walls (where velocity approaches zero) are thicker, while internal layers (where velocity is at a maximum) are significantly thinned. Consequently, the majority of internal layers are 20% to 30% thinner than nominally expected, whereas the outer layers bordering the die walls are substantially thicker than desired.

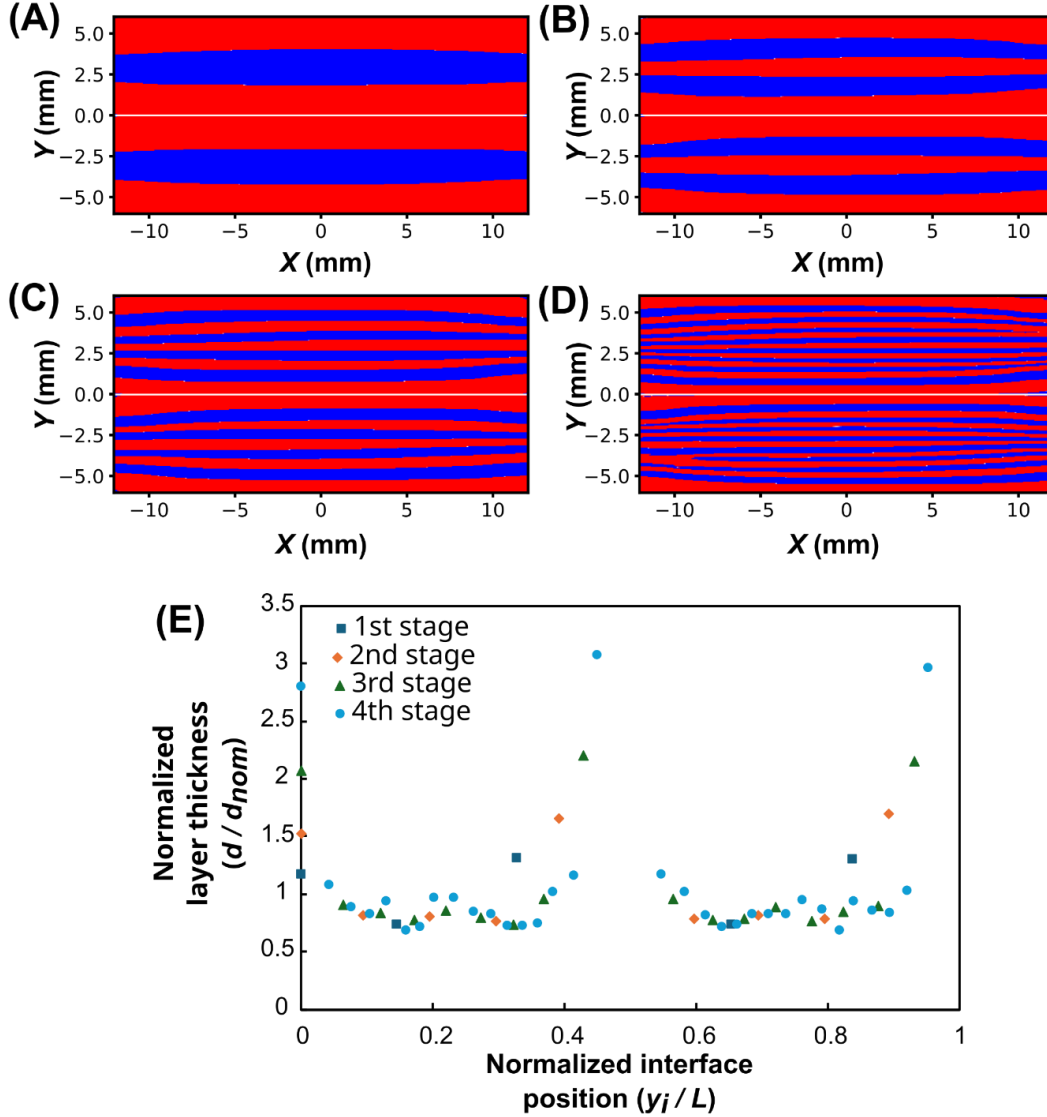


Figure 9. Predicted phase morphologies and layer-thickness distributions for an optimized Design 2 die using a three-layer ABA inlet flow: (A–D) Phase morphologies after (A) one, (B) two, (C) three, and (D) four sequential LME stages. (E) Extracted layer thicknesses normalized by their nominal expected values (d/d_{nom}) as a function of relative position across the film thickness (y_j/L).

These simulations represent layer profiles prior to entering the cast-film drawdown and take-up equipment. Complex postdie phenomena—such as transverse spreading in the exit die, nonisothermal cooling, and uniaxial drawdown—likely exert a strong influence on the final layer thicknesses near the walls. Nonetheless, this phenomenon is clearly observed in reported measurements of layer thicknesses within LME dies.^{24,33} For applications where layer thickness variation must be minimized, targeted measures—such as engineering wall slip or introducing sacrificial skin layers—should be used to mitigate the impact of velocity gradients.

4. Conclusions

In summary, this work demonstrates a comprehensive, automated computational framework for simulating multilayer coextrusion flows using the open-source OpenFOAM platform. By integrating parametric CAD generation, automated mesh discretization, and flexible Python scripting, the presented methodology enables efficient evaluation of complex, 3D, two-phase flows across a broad parameter space. Although the current model falls short of a full viscoelastic treatment, the generalized Newtonian simulations effectively capture critical flow phenomena—such as viscous encapsulation, shear-thinning-induced layer distortion, and interfacial stress spikes—while providing actionable design insights for LME dies.

A logical next extension of this framework will be incorporating fully viscoelastic constitutive models to capture secondary flows driven by second normal stress difference gradients. Additionally, expanding capability to accommodate more complex exit die geometries—such as coat-hanger and whale-tail dies—would enable visualization of layer uniformity across both the width and thickness of a final cast-film product.

Nonetheless, the numerical results presented here demonstrate that maintaining a constant cross-sectional area and optimizing section lengths with gradual convergence angles are essential to suppressing interfacial instabilities and minimizing layer asymmetry. While postdie drawdown and thermal effects will further shape the final layer architectures, this predictive CFD framework serves as a robust tool for guiding LME die design, mitigating processing defects, and targeting precise layer morphologies in advanced polymer composite manufacturing.

5. References

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List of Symbols, Abbreviations, and Acronyms

1/3D	One-/Three-Dimensional
CAD	Computer-Aided Design
CFD	Computational Fluid Dynamics
FVM	Finite Volume Method
LME	Layer-Multiplying Element
MULES	Multidimensional Universal Limiter for Explicit Solution
PISO	Pressure-Implicit with Splitting of Operators
RMS	Root Mean Square
SIMPLE	Semi-Implicit Method for Pressure-Linked Equations
VoF	Volume of Fluid

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