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Optimizing Modeling the Multilayer Coextrusion Flow of Non-Newtonian Fluids Through Rectangular Ducts: Appropriate Shear Rate Definition for a Local Power Law Formulation

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Optimizing Modeling the Multilayer Coextrusion Flow of Non-Newtonian Fluids Through Rectangular Ducts: Appropriate Shear Rate Definition for a Local Power Law Formulation

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Abstract: The accuracy of viscosity predictions is a crucial aspect of polymer melt flow modeling and essential for the design of coextrusion die systems. In the field of non-Newtonian fluid modeling for coextrusion flows through rectangular ducts, significant progress has been made in understanding multilayer flow dynamics. Our fundamental research, employing numerical techniques such as the shooting method, finite element method, and finite difference method for flow evaluation, has established a critical base for the field. Our current research advances fluid dynamics by refining our existing numerical solver, specifically developed for multilayer coextrusion flows. We aim to enhance the solver's performance by implementing more sophisticated calculations of shear rates that go beyond the traditional approach. The traditional approach often relies on average flow velocities and channel heights, which can underrepresent the complexity of experimentally studied polymer multilayer flows. Our study systematically compares various definitions for characteristic shear rates to describe the local shear rate dependent viscosity behavior using, for instance, a local power law model. A thorough error analysis quantifies the accuracy of each model and its predictive limitations for industrially relevant material combinations and operating conditions. This includes CFD simulations and experimental data comparisons, employing methods aligned with our fundamental research in

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this area. Furthermore, our work paves the way for integrating these advanced fluid dynamics models into the evolving field of process digitalization, thereby contributing to the development of more efficient, digitally integrated manufacturing processes.

Introduction

Coextrusion is a pivotal technology in plastics processing that enables the creation of advanced polymeric multilayer structures, each layer imparting different functionalities within a single product. Accurate modeling of the coextrusion process is essential for fine-tuning process parameters, aiding in the design of feedblocks and dies, and preventing interfacial flow instabilities that can compromise product quality.

The numerical modeling of non-Newtonian fluid flows, particularly in the context of coextrusion, has experienced significant advancements. Traditional computational fluid dynamics (CFD) simulations, though effective, often require substantial computational resources and in-depth knowledge of the operators. Hence, our research leverages the shooting method [1], which is well-suited for such boundary value problems. Combined with a local power law formulation, coextrusion flows of non-Newtonian fluids with any number of layers can be predicted much more efficiently via the reduction of calculation time at simultaneously high accuracies.

This study specifically focuses on refining our numerical solver MultiSim [2] for multilayer flows. By implementing more sophisticated definitions of the representative shear rate for the local power law formulation, we aim to capture the rheological behavior of polymer melts more accurately. To this end, we compare various definitions of characteristic shear rates defined by: (i) the average flow velocity divided by channel height (i.e., reference shear rate), (ii) the representative shear rate as commonly employed in mono-extrusion flows to approximate the non-Newtonian flow behavior by a Newtonian one [3], and (iii) an average shear rate per layer of the flow. Through a thorough error analysis, we quantify the accuracy and limitations of each model both experimentally and by means of CFD simulation for industrially relevant material combinations and operating conditions. This research not only enhances the understanding of multilayer flow dynamics but also paves the way for integrating advanced fluid dynamics models into digitally integrated manufacturing processes, contributing to the development of more efficient production systems [1,4].

Experimental Setup

The coextrusion experiments were performed on a novel coextrusion demonstration die with a constant rectangular cross section, allowing for a well-controllable, stratified two-layer flow. To control the die temperature, heating cartridges grouped into 11 heating zones along the two die inlets, the vane-type feedblock, and the stratified flow region were used. Static mixing elements at the die inlet assured thermal homogeneity of the melt streams. Melt temperatures were determined just before the position of the junction. The pressure drop was recorded by five pressure transducers located along the stratified flow region. Furthermore, the die includes an optical viewport to assess the layer distribution by means of an optical coherence tomography (OCT) sensor. A detailed description of this experimental setup can be found in [5]. Two identical smooth-bore single-screw extruders with conventional three-zone screws with a diameter of 30 mm and an axial length of 20.2 times the diameter were used to provide the PMMA and the ABS melt streams. The rheological characteristics of the materials were determined using high shear capillary rheometry (HKR). The measured Carreau-Yasuda parameters are presented in Table 1.

Table 1. Carreau-Yasuda rheological parameters for PMMA and ABS melt streams used in the coextrusion experiments, characterized using high shear capillary rheometry (HKR).

Material -	η_0 Pa.s	η_∞ Pa.s	λ s	a -	n_{CY} -
ABS	16,628	0	0.1305	0.4324	0.1356
PMMA	6,211	0	0.0123	0.4164	0.0075

Numerical Methods

Predicting the stratified flow of two non-Newtonian fluids through a rectangular duct generally requires numerical solution procedures.

Shooting Method

The shooting method is a numerical technique used to solve boundary value problems by converting them into initial value problems. In the context of coextrusion flow modeling, the shooting method is used to determine both the velocity profile and the position of interface between different layers. The method involves guessing the initial conditions for the system and integrating the differential equations governing the flow. The results are then compared with the boundary conditions at the other end of the domain. If the boundary conditions are not satisfied, the initial conditions are adjusted, and the process is repeated iteratively until convergence is achieved [1].

The power law function is used to capture the shear thinning behavior of non-Newtonian fluids by relating the viscosity of the fluid to the shear rate:

$$\eta = K \cdot \dot{\gamma}^{n-1}, \tag{1}$$

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where η is the viscosity, K is the consistency index, $\dot{\gamma}$ is the shear rate, and n is the flow behavior index [6,7]. The main advantage of this rheological model is its mathematical simplicity, but it fails to describe the upper Newtonian plateau as well as the transition region to the shear thinning regime. Consequently, we aim to overcome this by employing a local power law approach, which can be interpreted by employing the tangent to the viscosity curve at a shear rate characteristic for the flow. The consistency and the flow index can then be evaluated using the parameters of more sophisticated rheological models, such as the Carreau-Yasuda model:

$$n = 1 + (\eta_0 - \eta_\infty) \cdot \left(\frac{(\lambda \cdot a_T \cdot \dot{\gamma})^a}{1 + (\lambda \cdot a_T \cdot \dot{\gamma})^a}\right) \cdot \frac{(n_{CY} - 1) - a}{a}, \quad 2)$$

$$K = \left(\eta_\infty + (\eta_0 - \eta_\infty)(1 + (\lambda \cdot a_T \cdot \dot{\gamma})^a)^{\frac{n-1}{a}}\right) \cdot a_T \cdot \dot{\gamma}^{1-n_{CY}}. \quad 3)$$

The Carreau-Yasuda model provides a detailed description of non-Newtonian fluid behavior, incorporating additional parameters: zero shear rate viscosity η_0, infinite shear rate viscosity η_∞, a time constant related to the fluid's relaxation time λ, power law index n_{BCY}, and a, a dimensionless parameter describing the broadness of the transition region between the Newtonian plateau and the power law region. Additionally, a_T is the temperature shift factor that adjusts the viscosity based on the temperature T, accounting for temperature-dependent behavior of the fluid.

Local Shear Rate Formulations

The local shear rate, determined by one of the following formulations, is used to calculate the local power law parameters. We tested different formulations for local shear rates to better represent the complex flow behavior in multilayer coextrusion.

Reference Shear Rate

The reference shear rate $\dot{\gamma}_{ref}$ is given by:

$$\dot{\gamma}_{ref} = \frac{v_{ref}}{h}, \quad 4)$$

where v_{ref} is the average flow velocity and h is the channel height. This local shear rate is used for all layers and represents the default shear rate formulation in our inhouse software [4].

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Averaged Shear Rate

In a multilayer system, each layer of the flow – depending on its height position within the layer configuration and the rheological properties of the melts – is imposed by a particular range of shear rates. In general, layers located closer to the lower or upper boundary experience higher velocity gradients (i.e., shear rates) than layers located closer to the velocity maximum of the overall flow. The average shear rate is calculated from the velocity profile, which influences the viscosity and, consequently, the velocity profile itself. Therefore, an iterative solution is required.

For a system with N layers, each layer has a number of divisions N_{div} discretized shear rate values. Let $\dot{\gamma}_{i,j}$ represent the j-th shear rate value for the i-th layer, where $j = 1,2,\ldots,N_{div}$. The average shear rate for the i-th layer $\dot{\gamma}_{avg,i}$ is calculated as follows:

$$\dot{\gamma}_{avg,i} = \frac{1}{N_{div}} \sum_{j=1}^{N_{div}} \dot{\gamma}_{i,j}. \quad 5)$$

This equation provides the average shear rate for each layer by summing up the N_{div} discretized shear rate values and dividing by N_{div}. The solver is subsequently executed using the updated local shear rates. The shear profiles for each layer are then averaged using equation 5. This iterative process is repeated until convergence (precision threshold for $\dot{\gamma}_{avg,j}$ is set to 10^{-5} 1/s [2]) is achieved.

Representative Shear Rate

The representative shear rate $\dot{\gamma}_{rep}$ is well-known from monoextrusion pipe and slit flows and is designed to provide a single characteristic value that reflects the overall shear behavior of the flow. It is calculated using the volumetric flow rate and geometric parameters of the flow channel:

$$\dot{\gamma}_{rep} = \frac{6\dot{V}}{wh^2} \cdot 0.772, \quad 6)$$

where $\dot{V}$ is the volumetric flow rate, w is the width, and h is the height of the channel, whereas 0.772 is an empirical value for rectangular ducts [3].

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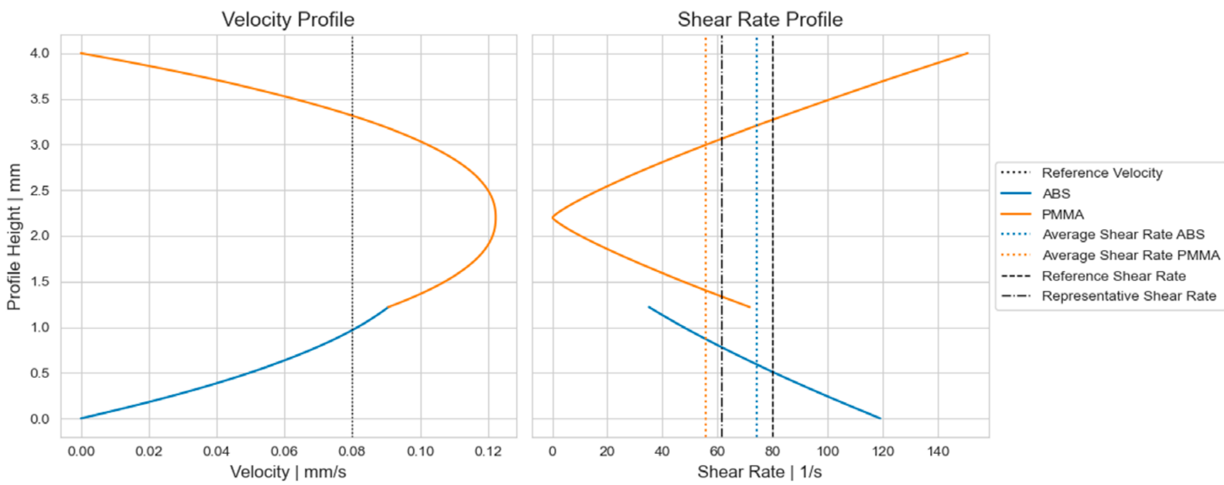

Figure 1. Velocity and shear rate profiles for ABS and PMMA two-layer coextrusion flow. The left panel shows the velocity profiles and the right panel displays the shear rate profiles. Reference, average, and representative shear rates are indicated to compare different shear rate formulations.

Figure 1 illustrates the velocity and shear rate profiles for ABS and PMMA layers in a multilayer coextrusion flow, representing one of the systems that were also experimentally examined. The left panel shows the velocity profiles, with the reference velocity v_{ref} marked by a dotted vertical line. The right panel presents the shear rate profiles, with vertical lines highlighting different shear rate formulations: the dotted orange line for the average shear rate of PMMA, the dashed line for the reference shear rate, and the dash-dot line for the representative shear rate.

Results

The results include a comparison of Ansys [8] CFD multiphase simulations (volume-of-fluid approach) with our solver calculations using the implemented shear rate formulations. The solver showed a significant reduction in computational time while maintaining accuracy (Table 2, Figure 2).

Table 2. Mean relative error (MRE) and standard deviation (in parentheses) for interface positions using different shear rate formulations in reference to the ANSYS CFD Multiphase Simulation. Pressure drop data is not included, as it was not available for the CFD simulation.

Shear Rate Formulation -	MRE Interface Positions %
Average Shear	1.12(±2.42)
Reference Shear	0.95(±2.67)
Representative Shear	1.05(±2.12)

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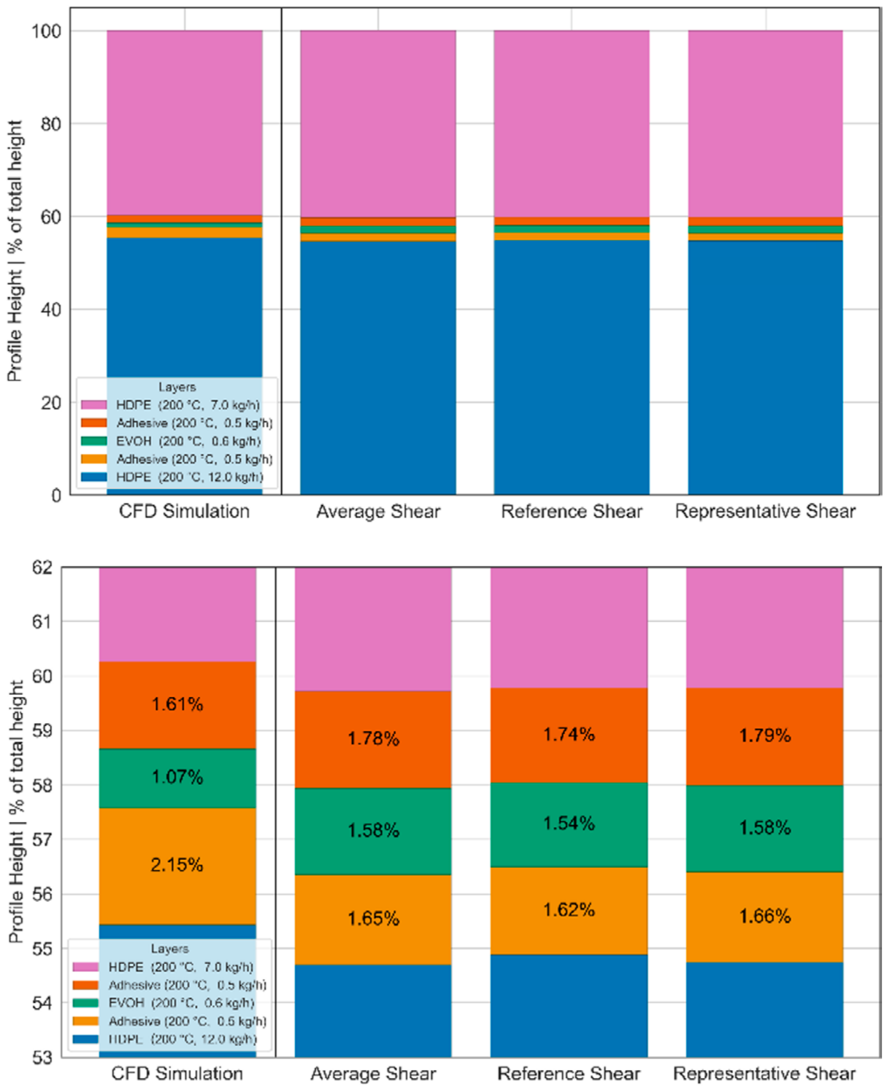

Figure 2. Comparison of numerical solver predictions and experimental results for interface positions in multilayer coextrusion. The left diagram shows the profile height percentages of different layers for the CFD simulation and the three shear rate formulations (average shear, reference shear, and representative shear). The right diagram provides a zoomed-in view of the height range from 53% to 62% of the total height, highlighting finer details of the interface positions for the different shear rate formulations.

Experimental Validation

The numerical results have been validated with experimental data from nine coextruded PMMA/ABS experiments. These experiments involved precise measurements of interface positions, pressure drop along the extrusion die, and comprehensive parameter studies. The mean relative error (MRE) was used to quantify the deviations between the solver predictions and experimental values,

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as shown in Table 3. This setup, consistent with previous studies [5], ensured reliable data collection and validation. The average deviation of the solver's prediction compared to the experimental data is shown in Table 3:

Table 3. Mean relative error (MRE) including standard deviation (in parentheses) for interface positions and pressure drop using different shear rate formulations compared to experimental values over nine experiments.

Shear Rate Formulation -	MRE Interface Positions %	MRE Pressure Drop %
Average Shear	11.42 (±1.69)	11.16 (±3.09)
Reference Shear	7.59 (±1.15)	12.23 (±7.76)
Representative Shear	13.74 (±9.02)	324.25 (±311.31)

Discussion

The results demonstrate that this refined numerical solver can accurately predict interface positions and shear rates in multilayer coextrusion flows. The newly implemented shear rate formulations provide a good match with experimental data and CFD simulations, enhancing the reliability and flexibility of our predictions for industrial applications.

Our results include a detailed comparison between Ansys CFD multi-phase simulations and our solver calculations using the implemented shear rate formulations. The solver demonstrated a significant reduction in computational time while maintaining accuracy. The mean relative error (MRE) for interface positions was 1.12% for the average shear rate, 0.95% for the reference shear rate, and 1.06% for the representative shear rate. These findings highlight the efficiency and effectiveness of our solver in reducing computational time without compromising on accuracy.

In our analysis of the shear rate formulations, the average shear rate generally provided better agreement with the experimental layer distribution, showing lower MRE in most cases compared to the reference shear rate. However, the representative shear rate, while sometimes showing good agreement with the kappa fraction, exhibited significantly higher MRE values for pressure drops. Specifically, the MRE for pressure drops using the representative shear rate was consistently high, indicating that this formulation may not be suitable for accurate pressure drop predictions in multilayer coextrusion flows.

These findings suggest that the average shear rate is more reliable for predicting layer thickness fractions, whereas the reference shear rate may offer a balanced performance, and the representative shear rate does not provide a benefit. The use of OCT technology has proven essential in obtaining precise interface measurements, further validating our model's accuracy.

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Overall, our refined numerical solver and improved shear rate formulations significantly enhance the predictive capabilities for multilayer coextrusion flows. This advancement not only aligns well with experimental observations but also offers a practical and efficient tool for industrial applications.

Conclusion and Outlook

Our study demonstrates that the refined numerical solver significantly reduces calculation time while maintaining precise predictions of interface positions and shear rates in multilayer coextrusion flows. The average shear rate formulation emerged as the most reliable for predicting layer thickness fractions, while the reference shear rate offered balanced performance. The representative shear rate, though useful in some scenarios, showed limitations in pressure drop predictions.

Future research should test the effectiveness of different shear rate formulations for various multilayer structures, including symmetrical, asymmetrical, and varying numbers of layers, to determine the best formulation for specific conditions. Additionally, developing and testing new shear rate formulations could enhance prediction precision.

More extensive experimental validations and CFD simulations are necessary to support these developments. Testing under diverse operating conditions and with a broader range of polymer materials will ensure the robustness and generalizability of the models. Continuous refinement of solver capabilities to handle complex geometries and multilayer dynamics will also be crucial.

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