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# Prediction of extrudate swell in polymer melt extrusion using an Arbitrary Lagrangian Eulerian (ALE) based finite element method

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ABSTRACT

Accurate prediction of extrudate (die) swell in polymer melt extrusion is important as this helps in appropriate die design for profile extrusion applications. Extrudate swell prediction has shown significant difficulties due to two key reasons. The first is the appropriate representation of the constitutive behavior of the polymer melt. The second is regarding the simulation of the free surface, which requires special techniques in the traditionally used Eulerian framework. In this paper we propose a method for simulation of extrudate swell using an Arbitrary Lagrangian Eulerian (ALE) technique based finite element formulation. The ALE technique provides advantages of both Lagrangian and Eulerian frameworks by allowing the computational mesh to move in an arbitrary manner, independent of the material motion. In the present method, a fractional-step ALE technique is employed in which the Lagrangian phase of material motion and convection arising out of mesh motion are decoupled. In the first step, the relevant flow and constitutive equations are solved in Lagrangian framework. The simpler representation of polymer constitutive equations in a Lagrangian framework avoids the difficulties associated with convective terms thereby resulting in a robust numerical formulation besides allowing for natural evolution of the free surface with the flow. In the second step, mesh is moved in ALE mode and the associated convection of the variables due to relative motion of the mesh is performed using a Godunov type scheme. While the mesh is fixed in space in the die region, the nodal points of the mesh on the extrudate free surface are allowed to move normal to flow direction with special rules to facilitate the simulation of swell. A differential exponential Phan Thien Tanner (PTT) model is used to represent the constitutive behavior of the melt. Using this method we simulate extrudate swell in planar and axisymmetric extrusion with abrupt contraction ahead of the die exit. This geometry allows the extrudate to have significant memory for shorter die lengths and acts as a good test for swell predictions. We demonstrate that our predictions of extrudate swell match well with reported experimental and numerical simulations.



## 1. Introduction

Extrudate swell prediction of a polymer melt is important for appropriate die design in processes such as profile extrusion. Prediction of extrudate swell is a challenging task due to simulation of the free surface, which requires special techniques in the traditionally used Eulerian framework. The degree of swell depends on material functions such as the first normal stress difference coefficient and the coupling between the shear and extensional viscosities, which are modeled by complex constitutive equations having convective derivatives of stress tensor. This makes the simulation of polymer flow in an Eulerian framework even more difficult. A better understanding of the flow behavior and resulting swell will ultimately lead to improvements in the understanding of the extrusion process, for optimization of both die design and processing parameters. This aspect has attracted a great deal of attention from researchers working on experimental and numerical studies of extrudate swell of molten polymer.

In the 1980s, several experimental studies on extrudate swell of polymer melts were performed, [1,2] and semi-empirical correlations were established by relating the swell ratio to the first normal stress difference ($N_1$). However, with the development of numerical techniques for viscoelastic flow, several detailed investigations on the extrudate swell phenomenon have been carried out using simulations. Many of these early numerical simulations were undertaken using the upper-convected Maxwell (UCM) constitutive equation [3,4]. Later, more realistic constitutive equations such as the integral K-BKZ model [5–13] and the differential PTT model

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[14–16] were used. Different types of damping functions such as the Wagner irreversible and reversible [9–11] damping functions, the Papanastasiou–Scriven–Macosko (PSM) type damping function [5–8], the Osaki twin exponential damping function [17] and a new three-parameter damping function suggested by Huang and Lu [13], have been used in conjunction with the K-BKZ model to study the effect of rheological non-linearities on extrudate swell. Similarly, the effect of second normal stress difference was considered in addition to the dominant effect of the first normal stress difference [6,10].

Much of the work on numerical simulations of extrudate swell in 1980s has been reviewed comprehensively by Keunings [18]. A review of more recent literature on extrudate swell simulations has been given by Huang and Lu [13]. Some of the numerical studies on extrudate swell are based on the Streamline Finite Element Method (SFEM) introduced by Luo and Tanner [5]. SFEM offers a simple algorithm for integral constitutive equations and is especially suitable for extrusion operation. This technique was subsequently modified by Luo and Mitsoulis [8], who introduced a particle-tracking scheme on the streamline by using Picard iterative scheme to decouple the computation of the free surface shape from that of velocity and stress fields. They used the iterative method of Dupont and Crochet [19] in which the strain history of the material particles was calculated along streamlines. Amongst the advantages of the scheme, one can mention its high efficiency and low requirements of computer resources. Several features of the earlier numerical method [8,19] have been modified by Goublomme et al. [9] to simulate flow at high shear rates by introducing a fourth-order Runge–Kutta algorithm to calculate the pathlines and the strains within the parent element. The iterative algorithm was of the incremental loading type, where a numerical parameter controls the transformation of a Newtonian solution into a viscoelastic one. A few researchers have employed Newton iterative scheme to compute free surface shape simultaneously with velocity and stress values (coupled method) [20].

Most of the reported simulation studies over-predict extrudate swell at high shear rates. An example of a detailed study is that of Béraudo et al. [16], who addressed the issue of over-prediction of extrudate swell by using a multi-mode PTT model containing a slip parameter ($\xi$). The model parameters were obtained from fitting to shear and extensional data for LLDPE and LDPE melts. For LLDPE melt, they showed quantitative agreement with available experimental data. In addition to viscometric data, they also generated flow birefringence data in 2D slit flows. For LDPE melt, W-shaped fringes were observed right after the downstream channel entrance. Béraudo et al. [16] simulated the 2D flow using a finite element method based on Newton's iterative scheme and discontinuous approximations of the extra-stress tensor. The discontinuous interpolation allows elimination of stress variable at element level by means of a static condensation technique. The predicted principle stress difference along the centerline was in quantitative agreement with the birefringence data of Guillet et al. [21]. They also qualitatively predicted the W-shaped fringes for LDPE. Further for extrudate swell predictions of LLDPE, they used simple computation of the stream function which allows the determination of the free surface. While they observed good agreement with experiments for long dies it was less satisfactory for short dies, especially at high flow rates.

Another example of a detailed study on extrudate swell is that of Ahmed et al. [11]. They presented experimental observations and numerical simulations for planar entry flow and extrudate swell of two HDPE and one LDPE polymer melts. Numerical simulation was carried out using POLYFLOW a finite element software package to simulate polymeric flows [20]. Experimental rheological data was generated and fitted using the K-BKZ integral model with a single parameter Wagner damping function. Flow birefringence data was also generated in the planar flow and a quantitative comparison between the predicted centerline stress profile and that obtained experimentally was made. The comparison was excellent for HDPE, but not for LDPE. Comparison between the measured and simulated extrudate swell was done only for HDPE melts. They also predicted higher extrudate swell values than those observed experimentally.

Most of the reported numerical methods for predicting extrudate swell are based on finite element technique in an Eulerian framework and use streamlines/steamtube to compute the swell. The free surface is computed by the predictor corrector technique based on streamline method, and only steady state extrudate swell simulation is possible. In view of this, extrudate swell simulations in Lagrangian framework would be more appropriate since the surface evolves naturally with the material flow. But there are problems associated with mesh distortion, and frequent resmeshing is required [22]. This calls for alternative simulation techniques. In this paper, we present an Arbitrary Lagrangian Eulerian (ALE) formulation for the simulation of extrudate swell. ALE has advantages of both Lagrangian and Eulerian frameworks. Formulations based on ALE methods can be of immense utility since the mesh can move independent of the material thereby leading to numerous variations that can be tailored for specific needs. Keunings and coworkers [23–25] have demonstrated the utility of Eulerian–Lagrangian technique based finite element method for transient free surface simulations. The motion of internal nodes was anchored to the displacement of free surface whereby the mesh velocity becomes different from the fluid velocity. They added an additional kinematic equation with a height function to represent the free surface and solved coupled equations for material and mesh motions. They also suggested that computation of free surface can be decoupled from other unknowns and solved using predictor-corrector scheme [23].

In the present study, we use a fractional-step ALE based finite element method incorporating the differential exponential Phan Thien Tanner (PTT) polymer constitutive model to capture melt flow and extrudate swell. In our technique, the material motion and mesh motions are decoupled and solved in two separate steps; this technique is easy to implement and can accurately simulate the complex viscoelastic behavior of transient polymer flow through complex geometries. The details of the technique and its validation for a viscoelastic flow through converging geometry can be found in Ganvir et al. [26]. In the next section, the formulation and implementation of ALE based method is described. In the Section 3 of this paper, the present method is compared with numerical and experimental studies reported in the literature.

## 2. ALE formulation

The Arbitrary Lagrangian Eulerian (ALE) formulation of continuum mechanics was developed to overcome the limitations of the Lagrangian and Eulerian formulations. The central idea is to allow the computational mesh to move in an arbitrary manner, independent of the material motion [27]. This arbitrariness can be used to reduce the extent of convection between mesh and material. For the ALE formulation a one to one transformation between the material and mesh domains is required. The material velocity $\mathbf{v}$ and mesh velocity $\mathbf{v}_{\mathrm{m}}$ are given by

$$\mathbf{v} = \left.\frac{\partial \mathbf{x}(\mathbf{X}, t)}{\partial t}\right|_{\mathbf{X}}, \quad \mathbf{v}_{\mathrm{m}} = \left.\frac{\partial \mathbf{x}(\boldsymbol{\chi}, t)}{\partial t}\right|_{\chi} \tag{1}$$

where $\mathbf{X}$ is the material domain frame and $\chi$ is the referential (mesh) domain. The convective velocity $\mathbf{c}$, which is the relative