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Extrudate swell of a high-density polyethylene melt: II. Modeling using integral and differential constitutive equations

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ABSTRACT

The extrudate swell phenomenon of a high-molecular-weight HDPE is modeled using the following viscoelastic constitutive equations: the multi-mode Kaye-Bernstein–Kearsley–Zapas (K-BKZ) integral model with the Wagner and the Papanastasiou–Scriven–Macosko (PSM) damping functions, and multi-mode Phan-Thien–Tanner (PTT), Giesekus and Double Convected Pom-Pom (DCPP) differential models. The high-molecular-weight high density polyethylene (HDPE) is rheologically characterized and the experimental data have been used to fit the parameters of the constitutive models. Experimental results on extrudate swell are compared with the numerical predictions. The simulation results showed that the integral K-BKZ model highly over-predicts and the differential PTT, Giesekus and DCPP models slightly under-predict the experimental measurements. When the capillary reservoir is excluded from the simulations, the predictions of the integral models are significantly reduced close to the experimental data, while those of the differential models remain practically unaffected. Although both integral and differential models used represent the rheological data equally well, an explanation of the dramatically different predictions of extrudate swell by the integral and differential models remains elusive.

1. Introduction

Extrudate swell is of interest to several polymer processing applications such as profile extrusion, blow molding, film blowing and fiber spinning [1]. Although it has been studied extensively both experimentally and numerically, it is not fully understood [2–9]. Precise prediction of extrudate swell is very crucial for the optimization of die design, material and operating parameters. The early numerical studies on the extrudate swell problem were mainly concerned with Newtonian fluids and showed good agreement with the experimental results [10,11]. However, no such systematic studies exist for viscoelastic fluids. The advent of advanced numerical techniques and constitutive models made extrudate swell simulation possible for viscoelastic fluids, such as polymer melts and/or solutions [12–15].

Extrudate swell simulation of a highly viscoelastic IUPAC-LDPE melt was successfully demonstrated by Luo and Tanner [13,14,16] using the integral K-BKZ model for long and short capillary dies. Luo and Tanner [13,14] have used the streamline finite element method (SFEM) with a particle tracking scheme to simulate the swell problem. This was later modified by Luo and Mitsoulis [6] to decouple the computation of free surface position. Different aspects of Luo and Mitsoulis's numerical method have been modified by Goublomme et al. [17] and Goublomme and Crochet [18] in order to simulate the flow at high shear rates (high Weissenberg numbers). In another study, Barakos and Mitsoulis [19] have simulated extrudate swell of the IUPAC-LDPE polymer melt using capillary dies of various aspect ratios, ranging from orifice dies (i.e., $L/D = 0$) to infinite length dies (i.e., $L/D \to \infty$), using the standard Galerkin weak formulation for velocities and pressure by also including the viscoelastic stress tensor as a body force in the momentum balance equations. The above described method seems to overcome the difficulties associated with SFEM and accounts for the effects of upstream contraction and recirculation on extrudate swell. However, the predictions were observed to be in agreement with experiments for short dies ($0 \leqslant L/D \leqslant 2$) only at low apparent shear rates and overpredicted the actual values for long dies. Furthermore, the extrudate swell of a HDPE melt exhibiting significant amount of slip has been studied by Ansari et al. [9], both experimentally and numerically, using capillary dies of different L/D ratios. It was observed that the model overpredicts extrudate swell even after applying the slip boundary condition. The overprediction was attributed to effects such as flow-induced crystallization, sagging/gravity, and non-isothermal effects as well as the model itself [9,19,20].

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In the case of extrudate swell simulation using differential models, most of the early efforts were mainly concerned with the high Weissenberg number (*Wi*) problem [12]. However, this problem was solved by using numerical schemes best suited for hyperbolic equations [12,21–23]. Subsequently, Elastic-Viscous Stress Split (EVSS) [24] and/or Discontinuous Elastic-Viscous Stress Split (DEVSS) [25] formulations on extra-stress tensor were introduced to obtain convergent and numerically accurate solutions. Ganvir et al. [7,26] have used an arbitrary Lagrangian–Eulerian (ALE) based finite element method and simulated transient extrudate swell of LLDPE and HDPE polymer melts. The extrudate swell is simulated for planar and axisymmetric dies with abrupt contraction. The results showed good agreement with reported experimental results on polymer melts of moderate elasticity (swell ratio of up to 1.4), however apparent shear rates as high as those used in practical applications could not be reached [7,26].

No or limited studies exist on extrudate swell using both integral and differential rheological models on the same polymer melt of high elasticity, typically used in blow molding applications. Moreover, there is no systematic study of the extrudate swell of a viscoelastic model where flow model predictions are compared with experimental results for various operating conditions relevant to polymer processing and for various geometrical parameters of capillary dies, such as diameter, D, length-to-diameter ratio, L/D, contraction angle, 2α, and the presence of the reservoir. The latter plays a significant role in the numerical predictions and their consistency with experimental results on extrudate swell as the present study attempts to demonstrate.

In this study, a high-molecular-weight HDPE is rheologically characterized using multimode integral (Kaye-Bernstein–Kearsley–Zapas referred to as the K-BKZ) and differential Phan-Thien–Tanner (referred to as the PTT), Giesekus and Double Convected POM-POM (referred to as the DCPP) models. The simulation results using ANSYS POLYFLOW® are compared with experimental extrudate swell measurements studying the effects of apparent shear rate, temperature, L/D, 2α, and the presence of reservoir. In addition, various rheological/material functions of the polymer melt under different types of deformation are computed using both K-BKZ and PTT constitutive equations to understand the origin of significant differences on the extrudate swell predictions between these two different classes of models (integral versus differential).

2. Experimental

2.1. Rheological measurements

The viscoelastic properties of a high-molecular-weight HDPE used in this work have been determined using a stress/strain controlled rotational rheometer (Anton Paar MCR501), and the details are discussed in Ansari et al. [27]. Briefly, the results from three types of tests have been used to fit the rheological parameters of the constitutive equations used; small-amplitude oscillatory shear (SAOS), start-up of steady shear, and uniaxial extension. The frequency sweep (SAOS) tests were carried out at different temperatures ranging from 160° to 220 °C with the 25-mm parallel disk geometry and a gap of about 1 mm. Further, the time-temperature superposition (TTS) principle was applied to obtain the master curves at the reference temperature of 200 °C. The steady shear experiments have also been done using the 25-mm parallel disk geometry with a gap of 1 mm at the reference temperature of 200 °C, at various shear rates ranging from 0.05 to 1 s^{-1}. The polymer was also characterized in uniaxial extension using the SER-2 universal testing platform fixture suitable for the Anton Paar MCR501 rheometer. The SER measurements were performed at different Hencky strain rates ranging from 0.05 to 5 s^{-1} also at 200 °C.

2.2. Extrudate swell measurements

A pressure-driven Instron capillary rheometer of constant piston speed has been used to study the extrudate swell and processing/slip behavior of the present polymer melt at 200 °C. More details on the swell measurements can be found elsewhere [27]. Capillary extrusion experiments using dies of various length-to-diameter ratios (L/D = 5, 16, and 33, with $D = 0.79$ mm) and diameters (such as $D = 0.43$, 0.79, and 2.11 mm with $L/D = 16$) were carried out to apply all the necessary corrections such as *Bagley*, *Rabinowitsch*, and *slip* (Mooney analysis) to the raw data [28,29]. The extrudate swell measurements were carried out by using a Keyence® LS-7030 M optical micrometer placed at the die exit. The experimental set-up is devised such that the optical micrometers can be moved up and down to capture the complete extrudate swell profile, allowing us to measure the time dependency of the extrudate swell phenomenon [27]. Moreover, a set of radiation heaters keeps the ambient temperature the same as that of the die and therefore these measurements are isothermal.

3. Mathematical modeling

3.1. Governing equations

The governing equations for the flow of incompressible fluids such as polymer melts under isothermal, creeping and steady flow conditions are given as [30,31]:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$-\nabla p + \nabla \cdot \boldsymbol{\tau} = 0 \tag{2}$$

where $\boldsymbol{u}$ is the velocity vector, p is the pressure, $\boldsymbol{\tau}$ is the extra stress tensor of the polymer melt. For viscoelastic fluids, such as polymer melts, constitutive equations that relate the stress tensor in terms of velocity/velocity gradients are required to complete the system of equations.

3.2. Constitutive equations

In the present work, mainly the integral K-BKZ (with Wagner and PSM damping functions) [32,33] and the differential Phan-Thien Tanner (PTT) [34] models were used for the extrudate swell simulations. In addition, the differential Giesekus and DCPP models were also used for few computations to evaluate their ability in predicting extrudate swell in comparison with the K-BKZ and PTT constitutive equations. A detailed review comparing various constitutive equations for representing the rheological data of polymer melts has been reported by Larson [35], which provides useful insights on selecting appropriate viscoelastic rheological models.

The K-BKZ model proposed by Papanastasiou et al. [32] and modified by Luo and Tanner [16] used in the simulations, is given by:

$$\boldsymbol{\tau} = \frac{1}{1-\theta}\int_{-\infty}^{t}\sum_{n=1}^{N}\frac{g_i}{\lambda_i}e^{(-(t-t')/\lambda_i)}h(I_{C^{-1}}, I_C) \times \left[\mathbf{C_t^{-1}}(t') + \theta\mathbf{C_t}(t')\right]dt' \tag{3}$$

where λ_i and g_i are the relaxation times and relaxation moduli, respectively, N is the number of relaxation modes, I_C and $I_C{}^{-1}$ are the first invariants of the Cauchy–Green tensor $\mathbf{C_t}$, and its inverse Finger strain tensor $\mathbf{C_t}^{-1}$, θ is a material constant given by $N_2/N_1 = \theta/(1-\theta)$, N_1 ($\equiv\tau_{11} - \tau_{22}$) and N_2 ($\equiv\tau_{22} - \tau_{33}$) are first and