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3D modeling of dual wind-up extensional rheometers

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ABSTRACT

Fully three-dimensional numerical simulations of a dual wind-up drum rheometer of the Sentmanat Extensional Rheometer (SER; Sentmanat, 2004 [1]) or the Extensional Viscosity Fixture (EVF; Garritano and Berting, 2006 [2]) type have been performed. In the SER and EVF a strip of rectangular shape is attached onto two drums, followed by a rotation of both drums in opposite direction. The numerical modeling is based on integral constitutive equations of the K-BKZ type.

Generally, to ensure a proper uni-axial extensional deformation in dual wind-up drum rheometers the simulations show that a very small initial width and initial thickness of the strip is required. In the SER it requires an initial sample width of less than 2.5 mm and a thickness of less than 0.25 mm. This is typically observed for elastomer model.

The overall picture is though more diverse, as the possibility to perform ideal uni-axial extension is very dependent of the constitutive equation. Especially the weighting between the convected relative strain tensors in the K-BKZ model seems to control the deviation from ideal behavior. Consequently, for melts or entangled liquids a proper uni-axial flow will be kept for a much wider parameter range. In fact only the appearance of a ductile necking or a large initial thickness of the sample will create a significant deviation from ideal extension. These simulations were based on MSF constitutive model.

1. Introduction

Extension of macromolecular or polymeric materials is one of the most important rheological characterizations methods. The interest is not merely restricted to the industrial community but also to more theoretical developments. In contrast to shear flow, elongational flow demands material points to separate exponentially with time so that polymer chains experience higher degrees of molecular orientation and stretching. As a matter of fact, many non-linear effects only manifest in extension. Extensional flow measurements are also very sensitive to the molecular structure of the tested polymer.

Macromolecular materials can be liquid or solid like. Examples are dough, gels, elastomers, and plastics. The question of whether any constitutive equation for a macromolecular material is of general validity can only be answered by comparing its predictions with experimental data. Well-defined extensional measurements have shown their importance in the critical evaluation of constitutive theories [3–6]. In this paper our main concern will be (soft) elastomers and entangled polymeric liquids.

The relevance of elongation flows has motivated the development of different testing platforms intended to impose well-defined elongational flows in the material. Characterizing the extensional behavior of polymeric systems has historically been quite difficult and even though several testing platforms have been presented and widely used their performance is still discussed.

Four rheometers for uni-axial extension are currently commonly used: the Münstedt Tensile Rheometer (MTR) [7], the Meissner elongational rheometer [8] (commercialize as Rheometric Scientific RME), the Sentmanat Extensional Rheometer (SER) [1] and the filament stretch rheometer (FSR) [9]. The MTR operates using translation clamps to extend a long cylindrical shaped sample suspended in an oil bath. In the case of the RME, a film of rectangular shape is held by four belt clamps that perform a counter motion between belt pairs provoking the stretch of the sample. The SER employs a wind-up technique consisting of two cylindrical drums. The sample is attached onto these drums followed by a rotation of both drums in opposite direction. The MTR, RMS as well as the SER are all based on the assumption of an overall homogeneous uni-axial extension. In the FSR the deformation of the sample in the direction of the extension is non-uniform. A short cylindrical polymer sample is held between two plates that are pulled apart to induce the extensional flow. In contrast to the other techniques the FSR relies on the assumption of a homogeneous elongation in the center of the extended sample, where the extension is

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measured locally using laser microscopy. This subject has resulted in a large amount of numerical studies of the filament stretch initiated by Kolte et al. [10] and Sizaire and Legat [11], and is still of interest [12]. These studies are the main contributions to the understanding of the flow in the FSR.

Numerical studies of the sample deformation in dual wind-up methods as the SER and EVF have according to our knowledge never been presented. It requires a fully three-dimensional, time-dependent as well as free surface viscoelastic flow scheme, with a dynamic contact line at the rotating fixtures. Only the study by Rasmussen et al. [13] on inflation of polymer melts fulfills these requirements. As a case study of dual wind-up methods we will consider the numerical modeling of the stretch of a flat sample in the SER. Please notice that the SER and the Extensional Viscosity Fixture (EVF) [2] rheometer are identical techniques from a modeling perspective. Experimental studies of the MTR, RME and SER techniques with regard to extensional deformation control and uniformity can be found in [1,14,15].

The SER (and EVF) employs a wind-up technique designed in such a manner that it can be used for materials as polymer melts and elastomers. Sentmanat [1] experimentally examined the uni-axial polymer melt extension performing series of strain validation experiments for a broad envelope of strain rates. Digital video imaging was used to monitor the evolution of the width of the sample. However, the influence of the material as well as the initial geometry of the sample remains unclear. Here the purpose is to discuss the potential deviations from ideal uni-axial deformation, based solely on numerical computations of theoretically ideal configurations.

2. Equipment description

The SER can be mounted on any rotational rheometer and consists of two cylindrical drums, as illustrated in Fig. 1. In most cases a polymer sample shaped as a rectangular strip is attached onto these drums that are rotated in opposite directions with the same rotation rate, Ω. Further description of this equipment and operation principles can be found in Sentmanat's original paper [1]. The drive shaft rotation rate, Ω, is set to be constant, and the set or nominal Hencky strain rate applied to the sample specimen can be expressed as

$$\dot{\epsilon}_N = \frac{2\Omega R}{L_0} \tag{1}$$

R is the radius of the equally dimensioned wind-up drums, and L_0 is the length of the unsupported part of the sample being stretched, equal to the centerline distance between the two drums. The nominal Hencky strain itself is

$$\epsilon_N = \dot{\epsilon}_N t \tag{2}$$

where t is the time from the start of the extension. For a constant Hencky strain rate, the nominal tensile stress growth function, $\bar{\eta}_N^+(t)$, of the stretched sample can then be expressed as:

$$\bar{\eta}_N^+(t) = \frac{F(t)}{\dot{\epsilon}_N A_0 \exp(-\epsilon_N)} \tag{3}$$

$F(t)$ is the instantaneous extensional force at time t exerted by the sample as it resists stretch and A_0 the initial cross-sectional area of the sample. Here $A_0 = W_0 T_0$ where W_0 and T_0 are the initial width and thickness of the sample respectively. Experimentally, $F(t)$ is determined from the measured torque signal. The initially rectangular shaped sample is assumed to have uniform width and thickness.

Experimentally, the deviation between kinematic strain (based on the time-dependent sample width) and set strain with different strain rates and polymer samples has been investigated and discussed in the original SER reference [1]. To experimentally validate

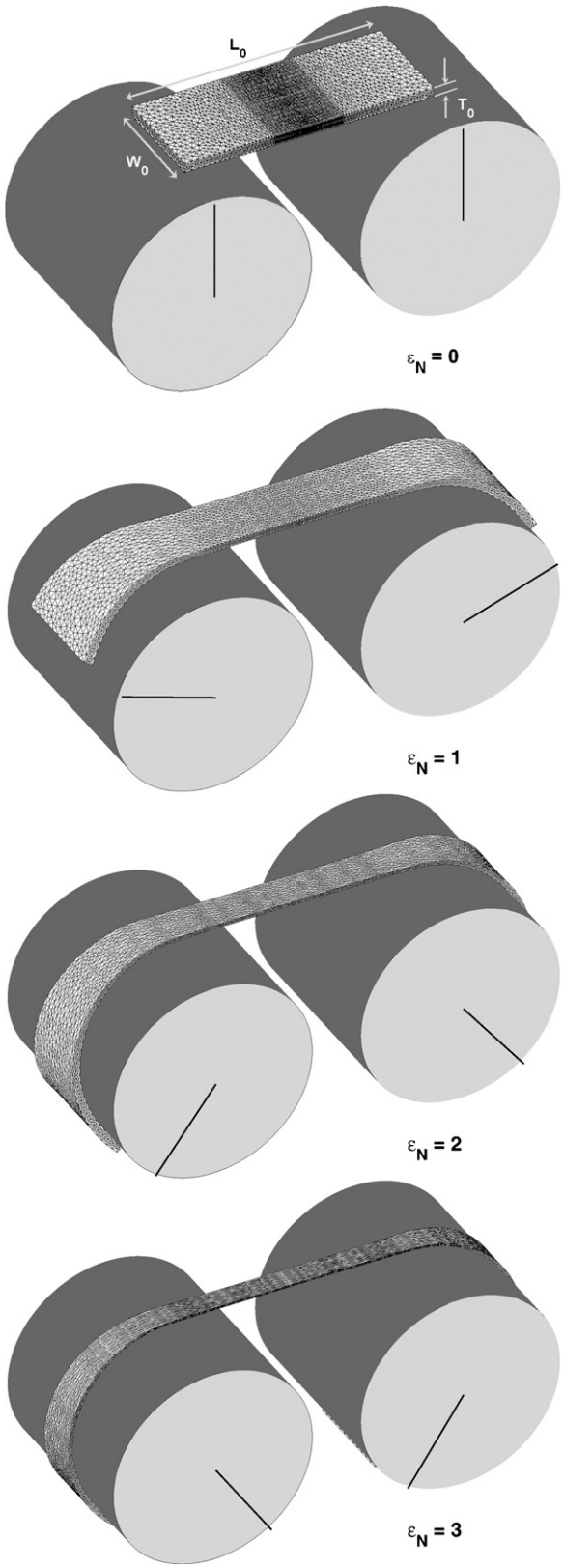

Fig. 1. Simulation of an extension in the SER. The finite element meshes at the four strains $\epsilon_N = 0$, 1.0, 2.0 and 3.0 are shown. L_0, W_0 and T_0 are the initial length, width and thickness of the specimen.