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A non-Newtonian fluid model with finite stretch and rotational recovery

Donggang Yao*

School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0295, USA

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ABSTRACT

Recently, we proposed a non-Newtonian fluid model containing two separate relaxation processes to treat straining ad material rotation and demonstrated good fitting to realistic rheological functions of polymeric flow. The model described in the present paper is an extension and improvement of the previous model. Particularly, a different approach is adopted to handle the effects of finite stretch on the basis of finite chain dynamics. The resulting model shows excellent fitting to experimental results with fewer model parameters than the previous model. All model parameters are linked to corresponding physical processes and can be readily determined from standard rheological plots. This study also revealed several interesting relations between rheological functions that are worth further investigations.

1. Introduction

Flow of polymer melts and solutions typically displays the following important characteristics: (1) shear thinning, (2) normal stress differences in simple shear, (3) elongational thickening in coaxial extensions, and (4) non-indefinite growth of extensional stresses. Closed-form constitutive equations that explicitly correlate kinematic variables such as the strain rate tensor to the stress tensor are highly desired in modeling of polymeric flow of practical relevance. However, conventional fluid models of the Reiner-Rivlin type encounter a difficulty in differentiating flow types and predicting the above non-Newtonian effects in a single constitutive model [1–5].

Considerable efforts have been made in constructing closed-form non-Newtonian fluid models using kinematic variables other than the strain rate tensor. A classical approach is to expand the Lagrangian deformation history in terms of convective derivatives of the strain rate tensor and construct a constitutive model using these objective tensors [6,7]. This continuum-derived approach is mathematically rigorous; however, a long expansion is needed to model three-dimensional flow, and the resulting model coefficients in general do not carry direct physical meanings and are difficult to fit using experimental results. Schunk and Scriven [8] attributed the difference in shear and extension to material rotations and proposed to include an objective vorticity tensor in constitutive modeling. Thompson and de Souza [9,10] proposed a kinematic tensor to correlate with the persistency of strain of the material in three-dimensional flow. Inclusion of these new kinematic variables leads to differentiation of rotational flow from irrotational flow so that different softening and thickening effects in shear and extension can be modeled in a single constitutive model. Interesting results have been generated in this direction and additional research is being conducted to construct mathematically simple, physically sound models using such new kinematic tensors.

In a recent paper [5], we proposed a non-Newtonian fluid model of type $\tau = \tau(\bar{\mathbf{L}})$ for fluids containing an elastic structure, where $\bar{\mathbf{L}}$ is an objective velocity gradient. The model contains two different relaxation processes to separately tackle with rotation and straining. The base model with three parameters is able to simultaneously model shear thinning and extensional thickening as well as normal stress differences in simple shear. Additional model accuracy is achieved by incorporating finite stretch and disentanglement effects.

The model presented in this paper is an extension and improvement of the previous model [5]. In the previous model, the velocity gradient is projected onto the principle axes of the elastic strain tensor to obtain a slip velocity gradient which is used to calculate a slip stress that is added to the total stress. To fit realistic experimental results, a Carreau-type viscosity model is needed for calculating the slip stress, resulting in additional fitting parameters. In the current paper, we adopt a different approach to treat the effects of finite stretch on the basis of the dynamics of a finite chain. The new model demonstrated excellent fitting to experimental results with fewer model parameters that all can be correlated with corresponding physical processes.

* Tel.: +1 4048949076.
E-mail address: yao@gatech.edu

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2. Model development

Start with basic kinematics. A material point in the Lagrangian frame is tracked by a position vector $\mathbf{X}$ and in the Eulerian frame is represented by a position vector $\mathbf{x}$. The velocity gradient $\mathbf{L}$ at a material point is defined as $\mathbf{L} = \frac{\partial \mathbf{v}}{\partial \mathbf{x}} = \{\frac{\partial v_i}{\partial x_j}\}$, where $\mathbf{v}$ is a velocity vector defined as $\mathbf{v} = \dot{\mathbf{x}}$. The Eulerian strain rate tensor $\mathbf{D}$ is defined as $\mathbf{D} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T)$. The Finger tensor or the left Cauchy–Green deformation tensor $\mathbf{B}$ is defined as $\mathbf{B} = \mathbf{F} \cdot \mathbf{F}^T$, where $\mathbf{F}$ is a deformation gradient tensor defined as $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \{\frac{\partial x_i}{\partial X_j}\}$.

To formulate an improved model, let us first briefly review the base model developed in the previous work [5]. Finite stretch is not considered in the base model. The major assumption adopted to derive the base model is that the accumulated strain of a polymer coil suspended in a dissipative medium is equivalent to the strain accumulated in a perfectly elastic material for a time period equal to the relaxation time λ. For coaxial flow (e.g., uniaxial or planar extension), this assumption is equivalent to the adoption of the following evolution equation:

$$(\ln \mathbf{B})^{\nabla} = -\frac{1}{\lambda} \ln \mathbf{B}, \tag{1}$$

where the Finger tensor $\mathbf{B}$ here is used to represent the elastic strain accumulated in the polymer coil and λ is a relaxation time. The symbol "∇" denotes a convected time derivative for the logarithmic strain tensor, defined as $(\ln \mathbf{B})^{\nabla} = (\ln \mathbf{B})^{\bullet} - 2\mathbf{D}$ [11]. For steady-state flow with constant $\mathbf{D}$, the solution of Eq. (1) is

$$\mathbf{B} = e^{2\lambda \mathbf{D}}, \tag{2}$$

For general flow with velocity gradient $\mathbf{L}$, Eq. (2) can be extended to

$$\mathbf{B} = e^{\lambda \bar{\mathbf{L}}} \cdot e^{\lambda \bar{\mathbf{L}}^T}, \tag{3}$$

where $\bar{\mathbf{L}}$ is the objective velocity gradient with the rigid-body part of vorticity removed (that is, $\bar{\mathbf{L}} = \mathbf{L} - \mathbf{\Omega}$, where $\mathbf{\Omega}$ is the rigid-body vorticity). The rigid-body vorticity $\mathbf{\Omega}$ is determined through this relation

$$\dot{\mathbf{e}}_i = \mathbf{\Omega} \cdot \mathbf{e}_i, \tag{4}$$

where $\mathbf{e}_i$ (for i=1,2,3) are unit vectors along the principal axes of $\mathbf{D}$. More details on the mathematical definition of $\mathbf{\Omega}$ and $\bar{\mathbf{L}}$ can be found in the previous paper [5]. For easy presentation, we drop the bar on $\mathbf{L}$ and assume that the velocity gradients mentioned in the following text are all objective unless otherwise noted. Finally, a new parameter n is introduced to adjust the degree of rotational relaxation or recovery, resulting in the following equation

$$\mathbf{B} = \left(e^{n\lambda \mathbf{L}} \cdot e^{n\lambda \mathbf{L}^T}\right)^{1/n}. \tag{5}$$

For a Gaussian material, the stress tensor can then be written as

$$\mathbf{T} = G\left(e^{n\lambda \mathbf{L}} \cdot e^{n\lambda \mathbf{L}^T}\right)^{1/n}, \tag{6}$$

where G is the linear modulus.

The current work starts with Eqs. (5) and (6) and seeks a simpler approach to include the effects of finite stretch in the constitutive model.

Extensional experiments typically show a maximum viscosity at some value of extensional rate [12]. This is caused by the finite stretch of individual chains so that chain disentanglement or slippage occurs at large deformation. In viscoelastic models, a ceiling stretch is often incorporated to address this finite extensibility, as seen both in dumbbell-type models [13,14] and in tube models [15]. A similar idea is endorsed here by introducing a ceiling stretch S_0 and modifying the relaxation time and modulus as

$$\lambda = \lambda_0(1 - S/S_0)^{\alpha} \text{ and } G = G_0/(1 - S/S_0)^{\beta}, \tag{7}$$

where S is an equivalent stretch, defined as $S = \sqrt{\frac{1}{6} \ln \mathbf{B} : \ln \mathbf{B}}$ so that S is equal to $\lambda\dot{\varepsilon}$ in the case of uniaxial extension. The function $f(S) = (1 - S/S_0)^{\alpha}$ involved in Eq. (7) has a similar mathematical structure as that of the Warner approximation [16] to the inverse Langevin function, but is simpler for mathematical handling in the present case.

The final model can be written by the following equations

$$\mathbf{B} = \left[e^{n\lambda_0(1-S/S_0)^{\alpha}\mathbf{L}} \cdot e^{n\lambda_0(1-S/S_0)^{\alpha}\mathbf{L}^T}\right]^{1/n}, \tag{8a}$$

$$\mathbf{T} = \frac{\eta_0/\lambda_0}{(1 - S/S_0)^{\beta}} \mathbf{B}, \tag{8b}$$

where $\eta_0 = \lambda_0 G_0$ is the zero shear viscosity. It can be shown that both in shear and in coaxial extension, the two parameters α and β have a similar influence on finite stretch. Therefore, one can simply set α to 1 and leave β as a single exponent to adjust the effect of finite stretch.

It is noted that Eq. (8a) is in an implicit form because S is a function of $\mathbf{B}$. However, since S is a monotonic function of $\mathbf{B}$, this equation can be easily solved using a numerical equation-solving method, such as the well-known bisection method.

For coaxial deformation, Eq. (8a) simplifies to

$$\ln \mathbf{B} = 2\lambda_0(1 - S/S_0)\mathbf{L}. \tag{9}$$

An analytical solution to Eq. (9) can be readily obtained given an irrotational $\mathbf{L}$.

It should be noted that although the model represented by Eq. (8) is mainly derived using continuum mechanics, it does carry a physical connotation related to the basic structure of a polymer coil. The overall shape of a polymer coil can be represented by an ellipsoid. In the undeformed state, the polymer coil mimics a sphere while in the deformed state it is like an ellipsoid with different lengths of major axes. The Finger tensor $\mathbf{B}$ is an ellipsoidal tensor and therefore can be used to model such shape changes. In the current model, we essentially use the Finger $\mathbf{B}$ to quantitatively represent the conformation of the polymer coil. This seems to be reasonable for both polymer melts and polymer solutions especially when the polymer molecule is long and nearly linear. The additional effects introduced by the parameters α and β for accounting for finite stretch are also aligned with the basic dynamics of the polymer coil. Particularly, the ceiling stretch for $\mathbf{B}$ corresponds to the maximum stretch of the polymer coil. As the maximum stretch is approached, the elastic stress in the polymer coil has to be rapidly increased. This behavior is modeled by the exponent β. At the same time, the relaxation process of the polymer coil should be sped up, as adjusted by the exponent α.

3. Model testing

The following case studies are presented to show that the proposed non-Newtonian fluid model as represented by Eq. (8) with 5 model parameters is able to simultaneously predict (1) shear thinning, (2) first and second normal stress differences in simple shear, (3) elongational thickening in coaxial extensions, and (4) non-indefinite growth of extensional stresses. Fitting to representative experimental results demonstrates that the proposed model is able to predict realistic material functions in shear and extension.