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Assessment of a general equilibrium assumption for development of algebraic viscoelastic models

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Abstract

The recent development of algebraic explicit stress models (AESM) for viscoelastic fluids rests upon a general equilibrium assumption, by invoking a slow variation condition on the evolution of the *viscoelastic anisotropy tensor* (the normalized de-viatoric part of the extra-stress tensor [G. Mompean, R.L. Thompson, P.R. Souza Mendes, A general transformation procedure for differential viscoelastic models, J. Non-Newtonian Fluid Mech. 111 (2003) 151–174]). This equilibrium assumption can take various forms depending on the general objective derivative which is used in the slow variation assumption. The purpose of the present paper is to assess the validity of the equilibrium hypothesis in different flow configurations.

Viscometric flows (pure shear and pure elongation) are first considered to show that the Harnoy derivative [A. Harnoy, Stress relaxation effect in elastico-viscous lubricants in gears and rollers, J. Fluid Mech. 76(3) (1976) 501–517] is a suitable choice as an objective derivative that allows the algebraic models to retain the viscometric properties of the differential model from which they are derived. A creeping flow through a 4:1 planar contraction then serves as a benchmark for testing the equilibrium assumption in a flow exhibiting complex kinematics. Results of numerical simulations with the differential Oldroyd-B constitutive model allow to evaluate a posteriori the weight of extra-stress terms in different regions of the flow. Computations show that the equilibrium assumption making use of the Harnoy derivative is globally well verified. The assumption is exactly verified in flow regions of near-viscometric kinematics, whereas some departures are observed in the very near region of the corner entrance.

Keywords: Viscoelastic flow simulation; Algebraic explicit stress models; Equilibrium assumption; 4:1 Planar contraction; Finite volume method

1. Introduction

The prediction of viscoelastic flows modeled with differential stress constitutive laws remains a numerical challenge in spite of the increasing speed and storage capacity of modern computers. For a three-dimensional flow, in addition to the momentum, mass and energy conservation equations, a set of six differential equations for the stress components has to be solved. The number of equations increases even more dramatically if multi-mode fluid models are to be considered.

Starting from this simple fact, and motivated by the numerous industrial applications, the quest for simplified viscoelastic models has been a direction of research for years. The original approach towards algebraic models known as "ordered fluids" ([1], p. 299) is based upon Taylor series expansion of Rivlin–Ericksen kinematic tensors. Such ordered fluids possess instantaneous memory ([2], p. 76).

In recent years, a different approach was proposed to derive algebraic viscoelastic models. The basic idea is to derive a unique differential equation for the first invariant (the trace) of the extra-stress tensor, and to obtain explicit expressions for the extra-stresses via a polynomial expansion [3]. This type of simplified model is named *Algebraic Explicit Stress Model* (AESM) and retains fluid memory through the transport equation for the trace of the extra-stress tensor. The transformation reduces the set of partial differential equations found in differential models into a single one, preserving their elasticity prediction capability. The reduction of the number of transport equations to be solved numerically must obviously result, especially for three-dimensional engineering applications, in a significant economy of computational time and storage memory. This technique was inspired by the analogy between viscoelastic fluids and turbu-

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lence closure mentioned by Rivlin [4]. It has been extensively employed by the turbulence modeling community since the pioneering work of Pope [5] to simplify the differential Reynolds stress equations.

In the framework of viscoelastic fluids, the first attempt towards obtaining algebraic explicit stress models based on a transport equation for the trace was due to Mompean et al. [3] for the Oldroyd-B fluid. The same method was later extended to the PTT-fluid by Mompean [6]. A general transformation procedure (GTP) for viscoelastic differential constitutive equations was recently proposed by Mompean et al. [7]. This procedure was devised to simplify any differential stress model into an algebraic stress model having just one differential equation for the evolution of the trace of the extra-stress tensor. The procedure makes use of two kinematic tensors (see Refs. [8,9]), namely (i) $\boldsymbol{\Omega}$, the rate of rotation of the principal directions of the rate-of-deformation tensor $\mathbf{S}$, and (ii) $\bar{\mathbf{W}} = \mathbf{W} - \boldsymbol{\Omega}$. The latter, which is an objective quantity, is the relative rate-of-rotation tensor, and measures the rate of rotation of a fluid particle as seen by an observer fixed to the principal axes of $\mathbf{S}$. This approach is inspired from the early work by Schunk and Scriven [10], Souza Mendes et al. [11] and Thompson et al. [12] who employed $\bar{\mathbf{W}}$ to propose algebraic constitutive models with enhanced capability for predicting rheological steady-state functions.

To arrive at explicit expressions for the extra-stresses, an equilibrium assumption applied to the normalized deviatoric part of the extra-stress tensor must be made. This assumption makes use of a general objective derivative, invoking a slow variation condition on the advection of the normalized deviatoric part of the extra-stress tensor.

The main purpose of the present paper is to derive the appropriate form of the equilibrium hypothesis for simple viscometric flows (pure shear and elongational), and assess its validity for viscoelastic complex flows. An analytical development is first conducted for viscometric flows, which permits to determine the correct form of the equilibrium assumption. For complex flows, it is necessary to solve the viscoelastic flow problem to check the equilibrium assumption a posteriori. The complex flow considered herein is a viscoelastic creeping flow through an abrupt planar 4:1 contraction. This study is carried out for the Oldroyd-B fluid model at Deborah numbers 1 and 2. The assessment of the equilibrium assumption in this geometry obviously requires a numerical solution to evaluate the weight of terms of the constitutive equation used. To solve the governing equations of the viscoelastic flow, a finite volume second-order accurate numerical method is employed and the elastic viscous split stress (EVSS) of Rajagopalan et al. [13] is implemented to improve stability.

The paper is organized as follows. In Section 2 the governing equations are presented. The theoretical developments to assess the equilibrium assumption made to derive viscoelastic algebraic stress models are described in Section 3. Although valid for any type of differential constitutive equations (Oldroyd-B, Upper-Convected Maxwell, White-Metzner, Phan-Thien-Tanner models, etc.), we shall restrict ourselves in this work to the Oldroyd-B model.

In Section 4, viscometric flows for which an analytical development is possible are first considered. The numerical simulations for the flow in the 4:1 contraction are then presented in Section 5. In this section, the geometrical configuration, the boundary conditions, the numerical method and the meshes used are first described. Results are then presented to validate the equilibrium hypothesis for this complex flow. Finally, the main conclusions are summarized in Section 6.

2. Governing equations

In order to study the isothermal laminar flow of an incompressible viscoelastic fluid, the mass and momentum conservation equations coupled with the constitutive relation for the non-Newtonian extra-stress components of an Oldroyd-B model are considered here.

The fluid density is denoted by ρ, η_s is the Newtonian solvent viscosity, η_p the polymeric viscosity and λ is the relaxation time.

The velocity vector is $\mathbf{v} = v_i\mathbf{e}_i$, where $\mathbf{e}_i$ $(i=1,\ 2)$ are orthonormal Cartesian basis vectors in the respective directions x_i $(i=1,\ 2)$. The partial differential equations to be solved in dimensional form are:

(i) mass conservation

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

(ii) momentum conservation

$$\rho \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \nabla \cdot \mathbf{T} \tag{2}$$

where

$$\mathbf{T} = \boldsymbol{\tau} - p\mathbf{I} + 2\eta_s\mathbf{S} \tag{3}$$

is the total (Cauchy) stress tensor, p the pressure and $\boldsymbol{\tau}$ is the polymeric part of the extra-stress tensor.

(iii) Oldroyd-B constitutive equation

$$\boldsymbol{\tau} + \lambda\overset{\nabla}{\boldsymbol{\tau}} = 2\eta_p\mathbf{S}, \tag{4}$$

where $\overset{\nabla}{\boldsymbol{\tau}} = \mathrm{d}\boldsymbol{\tau}/\mathrm{d}t - \nabla\mathbf{v}\boldsymbol{\tau} - \boldsymbol{\tau}\nabla\mathbf{v}^{\mathrm{T}}$ is the upper-convected invariant derivative of $\boldsymbol{\tau}$.

The operator $\mathrm{d}/\mathrm{d}t$ is the material time derivative, $\mathbf{I}$ the identity tensor and $\mathbf{S}$ is the (symmetric) rate-of-deformation tensor defined as:

$$\mathbf{S} = \frac{1}{2}(\nabla\mathbf{v} - \nabla\mathbf{v}^{\mathrm{T}}) \tag{5}$$

In Eqs. (4) and (5) the velocity gradient was defined as: $(\nabla\mathbf{v})_{ij} = \partial v_j/\partial x_i$, and $\nabla\mathbf{v}^{\mathrm{T}}$ is its transpose. For future reference, it is convenient to define the vorticity tensor as:

$$\mathbf{W} = \frac{1}{2}(\nabla\mathbf{v} - \nabla\mathbf{v}^{\mathrm{T}}) \tag{6}$$