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Convoluted models and high-Weissenberg predictions for micellar thixotropic fluids in contraction–expansion flows

J.E. López-Aguilar[a], M.F. Webster[a,*], H.R. Tamaddon-Jahromi[a], O. Manero[b]

[a] Institute of Non-Newtonian Fluid Mechanics, College of Engineering, Swansea University, Bay Campus, Fabian Way, Swansea SA1 8EN, United Kingdom
[b] Instituto de Investigaciones en Materiales, UNAM, 04510, Mexico

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ABSTRACT

This study is concerned with finite element/volume modelling of contraction–expansion axisymmetric pipe flows for thixotropic and non-thixotropic viscoelastic models. To obtain solutions at high Weissenberg numbers (*Wi*) under a general differential form $Wi\,\overset{\nabla}{\boldsymbol{\tau}}_p = 2(1-\beta)\boldsymbol{D} - f\boldsymbol{\tau}_p$, both thixotropic Bautista–Manero micellar and non-thixotropic EPTT *f*-functionals have been investigated. Here, three key modifications have been implemented: first, that of convoluting EPTT and micellar Bautista–Manero *f*-functionals, either in a multiplicative ($Conv^*$) or additive ($Conv^+$) form; second, by adopting *f*-functionals in absolute form (ABS-*f*-correction); and third, by imposing pure uniaxial-extension velocity-gradient components at the pure-stretch flow-centreline (VGR-correction). With this combination of strategies, highly non-linear solutions have been obtained to impressively high *Wi* [=O(5000+)].

This capability permits analysis of industrial applications, typically displaying non-linear features such as thixotropy, yield stress and shear banding. The scope of applications covers enhanced oil-recovery, industrial processing of plastics and foods, as well as in biological and microfluidic flows. The impact of rheological properties across convoluted models (moderate-hardening, shear-thinning) has been observed through steady-state solutions and their excess pressure-drop (*epd*) production, stress, *f*-functional field structure, and vortex dynamics. Three phases of vortex-behaviour have been observed with rise in elasticity, along with upstream–downstream Moffatt vortices and plateauing *epd*-behaviour at high-*Wi* levels. Moreover, enhancement of positive-definiteness in stress has improved high-*Wi* solution attenuation.

1. Introduction

The *theme of this study* is particularly concerned with exploring predictive solutions for thixotropic worm-like micellar systems under medium to high elasticity conditions. To achieve this goal, convoluted hybrid constitutive models have been developed and embellished upon, utilising base Bautista–Manero (MBM) models to accommodate the dynamic micellar response, and grafting these upon exponential Phan–Thien–Tanner (EPTT) models for rubber-network response. The class of time-dependent MBM models follow those developed in [1–5]. In contrast, the time-independent network-based EPTT models were first proposed in [6], though more widely used today for many polymeric systems due to their inherently robust numerical characteristics. The work concentrates on the axisymmetric contraction–expansion flow problem, of geometric ratio 4:1:4 with rounded contraction-cap and recess-corners.

The issue of extraction of highly-elastic numerical prediction is tackled in a number of different directions. First, convolution of MBM and EPTT models is proposed, through their network-structure (*f*-) functionals, of multiplicative and additive forms. Second, and based on physical grounds, by appealing to only absolute values in structure-function dependency (ABS-*f*-correction), which controls non-linear response (see [5]). Third, through the problem approximation and its discretisation, via the imposition of consistent velocity gradient representation along the pure-stretch centreline of the flow (VGR-correction). The many relevant factors influencing the determination of particularly high elastic solutions (and their limitation in strain-hardening context) are discussed in depth in [5]. These aspects touch on: the numerical technique and discretisation for independent variables (stress, velocity, pressure, velocity-gradient); possible loss of IVP (Initial Value Problem) evolution and lack of positive definiteness retention (leading to stress-subsystem eigenvalue (s_i) analysis, s_i–N_1 centreline relationship); the complex flow problem itself (sharp stress boundary layers, flow singularities); and the particular constitutive equation of choice [5].

* Corresponding author.
E-mail address: M.F.Webster@swansea.ac.uk (M.F. Webster).

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Worm-like micelle solution systems are a versatile family of fluids, composed of mixtures of surfactants and salts. Typical surfactants are cetyltrimethylamonium bromide (CTAB) or cetylpyridinium chloride (CPyCl); common salts are sodium salicylate (NaSal) in water [4,7]. These components interact physically, depending on concentration, temperature and pressure conditions, to form elongated micelles. Such elongated constructs entangle and provoke mechanical interactions, stimulating breakdown and formation of internal structure [4]. This has consequences on the material properties of viscosity and elasticity. This complex constitution spurns highly complex rheological phenomena [7], and manifests features associated with thixotropy [1], pseudo plasticity [1–5], shear banding [8–13] and yield stress [14,15]. These systems have been coined *'smart materials'*, as their rheology dynamically adjusts to conform to prevailing environmental conditions. Such features render these systems as ideal candidates for varied processing and present-day applications. Examples of such application include use as drilling fluids in enhanced oil-reservoir recovery (EOR), additives in house-hold-products, paints, cosmetics, health-care products, and as drag reducing agents [4,7].

On wormlike micellar modelling, many approaches have been pursued to describe micellar flow behaviour. The original Bautista–Manero–Puig (BMP) model [1–2] consisted of the upper-convected Maxwell constitutive equation to describe the stress evolution, coupled to a kinetic equation to account for structural flow-induced changes and, was based on the rate of energy dissipation. Subsequently, Boek et al. [3] corrected the BMP model for its unbounded extensional viscosity in simple uniaxial extension – thus producing the base-form MBM model employed in the present analysis. This model has been implemented in complex flows such as in 4:1 contraction flow [16] and 4:1:4 contraction–expansion flow [4]. Therein, inconsistency has been exposed in excess pressure drop (*epd*) predictions at the Stokesian limit. Subsequently, this anomaly has been overcome [4] by including viscoelasticity within the structure construction-destruction mechanism. Two such model-variants have appeared, with energy dissipation given: (i) by the polymer contribution exclusively (NM_τ_p model, as adopted in the present article), and (ii) by the combination of the polymer and solvent contributions (NM_T model). These considerations have introduced new physics into the material response, by explicitly coupling thixotropic and elastic properties. Moreover, new key rheological characteristics have also been introduced, such as declining first normal stress difference in simple shear flow [4].

For completeness from the micellar literature, one may cite other alternative modelling approaches, though these have largely focused on simple flows and the shear-banding phenomena. The VCM (Vasquez–Cook–McKinley) model, based on a discrete version of the *'living polymer theory'* of Cates, has been tested in simple flows, where rheological homogeneity prevails [17], and under conditions of shear-banding. VCM predictions captured the linear response of experimental shear data for CPyCl/NaSal concentrated solutions under small amplitude oscillatory shear and small amplitude step-strain experiments [18]. Moreover, Zhou et al. [19] found reasonable agreement with experimental data of Taylor–Couette and microchannel geometries and VCM predictions. Another approach consists of using the Johnson–Segalman model, modified with a diffusion term in the polymeric extra-stress equation (the so-called *d-JS* model) [20]. This model was found to predict shear-bands in cylindrical Couette flow. The Giesekus model has also been used in the representation of wormlike micelles under simple shear scenarios, whilst using the non-linear anisotropy coupling parameter to introduce shear-banding conditions [21]. Here under large amplitude oscillatory shear, a straightforward method was proposed to estimate the Giesekus non-linear parameter. Consequent Giesekus predictions were then found to lie in quantitative agreement with data for low-concentration CTAB wormlike-micellar solutions.

Paper overview – in this article, convoluted equations of state are proposed based on the non-thixotropic network-based PTT and thixotropic micellar MBM parent models. Here, two convolution options have been devised, with additive ($Conv^+$) and multiplicative ($Conv^*$) *f*-functionals. Their *rheometric response*, via shear and extensional data, has been correlated to that within axisymmetric 4:1:4 contraction–expansion complex flow solutions. In this respect, streamline patterns, N_1-fields, *f*-functional and pressure-drops have been analysed. Moreover, *High-Wi solutions* [$Wi = O(5000+)$] are reported, achieved via ABS-*f*-correction and VGR-correction. Vortex activity has revealed a number of independent phases of interest. In this, upstream vortex enhancement has been identified at low elasticity levels, followed by complete suppression, somewhat reflecting strain-hardening/softening response. At high elasticity levels, a second stage of upstream–downstream vortex enhancement has been observed, along with secondary Moffatt vortices, of form suppressive-upstream and enhancing-downstream. The ABS-VGR correction (implying the simultaneous use of both ABS-*f* and VGR-corrections) delays any loss of positive definiteness, observed through reduced negativity of the *second eigenvalue* of the stress-subsystem, corresponding to the conformation tensor at the centreline. This has been correlated with *f-functional* values across the flow-field (now, $f \geq 1$), which grow as elasticity rises, thus ensuring positive viscosity estimation. *Excess pressure-drop* (*epd*) data asymptote to a plateau at high-*Wi* [$Wi = O(10^3)$]. At very high-*Wi* ($Wi > 10^3$), *epd*-data degenerate due to inconsistencies in inner-field to flow-outlet conditions. These inconsistencies are dealt with by imposing periodic boundary conditions at the inlet and outlet regions.

2. Governing equations, constitutive modelling and theoretical framework

2.1. Governing equations and constitutive models

The present flow context of interest is that of steady flow, under incompressible and isothermal conditions. In a non-dimensional framework, whilst assuming implied *notation on dimensionless variables (see on), the governing equations for mass conservation and momentum transport equations for viscoelastic flow become:

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

$$\mathrm{Re}\frac{\partial \boldsymbol{u}}{\partial t} = \nabla \cdot \boldsymbol{T} - Re\boldsymbol{u} \cdot \nabla \boldsymbol{u} - \nabla p. \tag{2}$$

Here, t represents time, an independent variable; the spatial gradient and divergence operators apply over the problem domain; field variables $\boldsymbol{u}$, p and $\boldsymbol{T}$ represent fluid velocity, hydrodynamic pressure and stress contributions, respectively. Moreover, the total stress ($\boldsymbol{T}$) is split into two parts: identifying, a solvent component $\boldsymbol{\tau}_s$(viscous-inelastic $\boldsymbol{\tau}_s = 2\beta\boldsymbol{D}$) and a polymeric component $\boldsymbol{\tau}_p$. Then, $\boldsymbol{D} = (\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^{\mathrm{T}})/2$ is the rate of deformation tensor, where the superscript 'T' denotes tensor transpose. Adopting appropriate scales below, corresponding dimensionless variables are defined as:

$$\boldsymbol{x}^* = \frac{\boldsymbol{x}}{L}, \quad \boldsymbol{u}^* = \frac{\boldsymbol{u}}{U}, \quad t^* = \frac{U}{L}t, \quad \boldsymbol{D}^* = \frac{L}{U}\boldsymbol{D},$$
$$\boldsymbol{\tau}_p{}^* = \frac{\boldsymbol{\tau}_p}{(\eta_{p0} + \eta_s)\frac{U}{L}}, \quad p^* = \frac{p}{(\eta_{p0} + \eta_s)\frac{U}{L}}.$$

A reference viscosity may be taken as the zero shear-rate viscosity ($\eta_{p0} + \eta_s$). Here, η_{p0} is the zero-rate polymeric-viscosity and η_s is the solvent-viscosity. Then, from this the solvent-fraction can