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Micro-Macro simulation of viscoelastic free surface flows using the Brownian configuration fields method

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ABSTRACT

A micro-macro approach based on combining the Brownian configuration fields (BCF)[1] method with an Arbitrary Lagrangian-Eulerian (ALE) Galerkin finite element method is implemented to study the flow characteristics of dilute polymer solutions in coating flows. A distinct advantage of the BCF method is its ability to treat models for which no exact closed-form constitutive equations exist, such as FENE dumbbells or models with hydrodynamic and excluded volume interactions. The equations for the BCF are discretized using streamline upwinding and are coupled to the Navier-Stokes equation through the stress term. To validate the method, the results for Hookean dumbbell model are compared with those obtained from an exact closed-form macroscopic equivalent model (the Oldroyd-B liquid in the conformation tensor formulation). The conformation tensor based model is solved using the DEVSS-TG/SUPG method [2]. We find excellent agreement between the results for the BCF and the conformation tensor based model.

INTRODUCTION

Free surface flows occur when a layer of liquid meets a gas at an interface. Such flows arise in a variety of commercial applications, such as coating, ink-jet printing, fiber spinning, and micropipetting. Frequently, these applications involve liquids that are viscoelastic, because of the presence of polymer as final product (as in coating) or as rheology modifier (as in ink-jet printing). Many of these flows are time dependent; their dynamics are controlled by the elasticity and capillarity of liquid. Modeling such flows requires computational methods which can describe and predict the molecular conformation of polymers, while simultaneously capturing accurately the shape of free surfaces. The Brownian configuration fields method [1], which is an extension of the CONNFFESSIT algorithm [3], can be used to incorporate into computational models detailed information on the microstructural feature, such as stretch and orientation, of the flowing polymer molecules. The BCF method has a distinct advantage over models based on closed-form constitutive equations for the conformation tensor or the viscoelastic stress because it is able to handle directly more realistic models of the dynamics of polymer solutions.

Few time dependent calculations of viscoelastic flows with capillarity have been reported in the literature; steady calculations have been published only recently [2,4]. Here, the time-dependent flow under the downstream section of a slot coater is studied as a benchmark. The mathematical modeling of free surface flows involves solving free boundary problems in which the location of the boundary is unknown apriori and it must be a part of the solution of the problem. Several methods for handling free boundary problems have been discussed in detail in literature [5-8].

In this paper, we compute slot coating flows of viscoelastic liquids by using elliptic mesh generation equations [2,5] coupled with time dependent conservation and BCF equations. To validate this approach we present results obtained with an exact closed-form macroscopic equivalent model in conformation tensor based formulation [2].

GOVERNING EQUATIONS

Mesh generation, continuity and momentum balance equations, respectively, are:

$$0 = \nabla \cdot \tilde{\mathbf{D}} \cdot \nabla \boldsymbol{\xi} \quad (1)$$

$$0 = \nabla \cdot \mathbf{v} \quad (2)$$

$$0 = \rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v}\right) - \nabla \cdot \mathbf{T} - \boldsymbol{\Theta} \quad (3)$$

where **v** is the liquid velocity, ρ is the liquid density, $\boldsymbol{\xi}$ is the position in the computational domain, ∇ denotes the standard gradient operator in physical space **x,** and $\boldsymbol{\Theta}$ is the body force per unit volume. The dyadic $\tilde{D}$ controls the spacing of the coordinate lines [8]. **T** is the total stress tensor, which is expanded as $\mathbf{T} = -p\mathbf{I} + \boldsymbol{\tau} + \boldsymbol{\sigma}$ where p is the pressure, **I** is the identity tensor, $\boldsymbol{\tau}$ is the viscous stress tensor and $\boldsymbol{\sigma}$ is the elastic stress tensor. Further details on conformation tensor based constitutive equations are explained in Ref. [2].

The viscous stress is given by the Newton's law $\boldsymbol{\tau} = 2\mu\mathbf{D}$ where $\mathbf{D} = 1/2\ (\nabla\mathbf{v} + \nabla\mathbf{v}^{\mathrm{T}})$ and μ is the Newtonian viscosity. The elastic stress is calculated by using the BCF method. The polymer molecules are modeled as Hookean dumbbells. In this simplistic model, the polymer solution is considered to be a suspension of non-interacting dumbbells with two Brownian beads connected by a linear spring. The configuration field of a dumbbell $\mathbf{Q}(\mathbf{x},t)$ is governed by the following stochastic differential equation [1]:

$$\frac{\partial \mathbf{Q}}{\partial t} = -\mathbf{v}\cdot\nabla\mathbf{Q} + \nabla\mathbf{v}^{T}\cdot\mathbf{Q} - \frac{2H}{\zeta}\mathbf{Q} + \sqrt{\frac{4kT}{\zeta}}\mathbf{r}(t) \quad (4)$$

where $\sqrt{4kT/\zeta}\,\mathbf{r}(t)$ is a time-uncorrelated, spatially homogeneous Brownian force which accounts for the random displacement of the beads due to the thermal motion ($\mathbf{r}$ has zero mean and unit variance), H is the Hookean spring constant, and ζ is the bead friction coefficient. The elastic stress field is related to the configuration of the dumbbells,

$$\boldsymbol{\sigma} = -nkT\mathbf{I} + nH\langle\mathbf{QQ}\rangle \quad (5)$$

where n is the number density of the dumbbells and the angular brackets denote a configuration ensemble average. The microscopic Hookean dumbbell model is equivalent to the macroscopic Oldroyd-B model [9].

NUMERICAL METHOD

The partial differential equations are translated into a set of coupled, time-dependent differential algebraic equations by using finite element basis functions and Galerkin's method for the mesh, momentum, and continuity equations (1, 2, 3) and Streamline Upwind Petrov Galerkin for the configuration fields (Eq. 4) or conformation equation. Biquadratic continuous basis functions are used for velocity and position, linear discontinuous basis functions for pressure, and bilinear continuous basis functions for the configuration fields .

The time-dependent equations in the conformation tensor formulations are solved with a fully implicit second order predictor-corrector scheme for the coupled equation set [10]. In the BCF method, the evolution of the system is computed at each time step first by fixing the elastic stress and solving the continuity, momentum, and mesh equations with an implicit scheme and Newton's method; then, the velocity field is fixed and the BCF equations are updated with an explicit Euler scheme using fixed flow kinematics; finally, a new elastic stress field is computed from the updated configuration fields.

Because the physical mesh is changing with time, the time derivatives of any time-dependent quantity $\partial\Phi/\partial t$ in Equations 3 and 4 are transformed to time derivatives at fixed iso-parametric coordinates

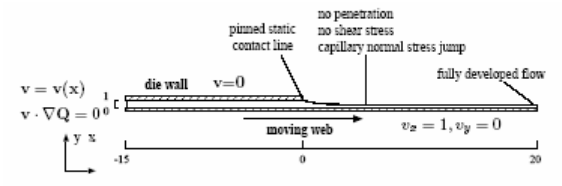

Figure 1: *Flow domain and boundary conditions used in analyzing the flow of viscoelastic liquid in the downstream section of slot coater.*

(denoted by $\mathring{\Phi}$) with the transformation

$$\frac{\partial\Phi}{\partial t} = \mathring{\Phi} - \mathring{\mathbf{x}}\cdot\nabla\Phi \quad (6)$$

where, $\mathring{\mathbf{x}}$ is the mesh velocity. In the case of free surface flows, the mass matrix in the BCF equation 4 is time-dependent and must be factorized at each time step.

RESULTS AND DISCUSSION

Here, the evolution of the molecular conformation in the downstream section of a slot coater is studied as the flow evolves from one steady state to another after a gradual change of dimensionless flow rate. Figure 1 shows the flow domain and boundary conditions used for the slot coating flow problem. The relevant dimensionless parameters for this flow are: the Reynolds number, $\mathrm{Re} = \rho vL/(\mu+\eta_p)$, the Capillary number, $\mathrm{Ca} = (\mu+\eta_p)v/\varsigma$, the Weissenberg number, $\mathrm{Wi} = \lambda v/L$ and the viscosity ratio, $\beta = \mu/(\mu+\eta_p)$ where η_p is the polymer viscosity, v is the web speed, L is the height of the gap between the web and the die, λ is the polymer relaxation time and ς is the surface tension. The dimensionless number are set to Re = 0.05, Ca = 0.1, Wi = 1.0 and β = 0.75. The finite element mesh has 550 elements with 10894 degrees of freedom for velocity and position and 1818 for each Brownian Configuration Fields. The same mesh is used in the simulation of the conformation tensor based model and the total number of degrees of freedom is 15742 in this case. 3200 dumbbell fields are used in the microscopic simulations to obtain a reasonable variance. The dimensionless time step used in the time integration is 0.02 in the macroscopic simulation and 0.0075 in the microscopic simulation.

The initial condition for the transient simulations is Newtonian creeping flow with a dimensionless flow rate of 0.27. A new steady state with Re = 0.05 and Wi = 1.0 is obtained from the initial condition by integrating the equations of motion (in conformation or BCF form) from time, t = 0 to 14. The flow rate is then gradually changed from 0.27 to 0.3 over the period t = 14 to 20 while keeping all other parameters fixed. The flow rate is changed gradually so as to have a divergence-free velocity field to calculate the flow field at a subsequent time step [10].

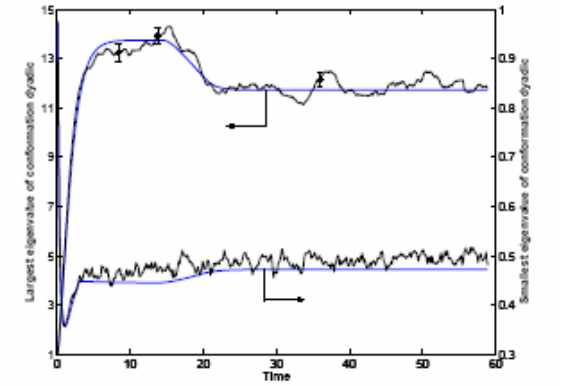

Figure 2: *Eigenvalues of the conformation dyadic as a function of time. BCF results are depicted in black color.*

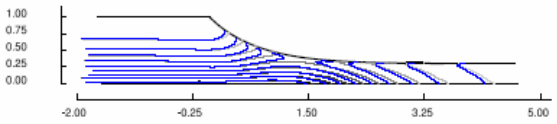

Figure 3: *Steady state contour lines of the largest eigenvalue of conformation dyadic. BCF results are depicted in gray color.*

The eigenvalues of the conformation dyadic can be used to represent the microstructural state of an ensemble of polymer molecules in a flow field [2]. Figure 2 shows the largest and the smallest eigenvalues of the conformation dyadic in the flow plane computed using both the BCF and the macroscopic Oldroyd-B models. Figures 3 and 4 show the steady state contour plots of these eigenvalues. Steady state contour lines were obtained by doing a time and ensemble-average over all Brownian Configuration Fields after the system reached a stochastic steady state (this is justified by ergodicity). Both transient and steady results computed with the closed-form model and BCF method agree well.

A typical transient simulation of the slot coater requires roughly 115 CPU hours on a single 900 MHz Itanium 2 processor using 3200 configuration fields, for 3000 time steps. The same simulation takes about 12 CPU hours for the macroscopic conformation tensor based method. However, the BCF method can be easily parallelized and the clock time drops to about 24 hours on 8 processors in a distributed memory configuration. This scalability on Beowulf-class parallel clusters makes the BCF method viable for computation of industrially relevant flows.

CONCLUSIONS

We have developed a micro-macro numerical algorithm to simulate viscoelastic free surface flows using the BCF method. To the best of our knowledge this is the first extension to complex free surface flows of the BCF method. We have validated this method by showing that the BCF results agree with those computed with the equivalent macroscopic conformation tensor based model in a sample slot coating flow problem. The

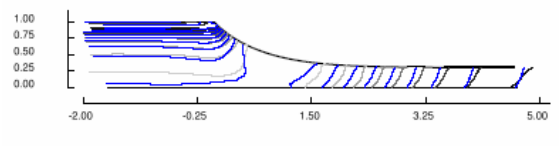

Figure 4: *Steady state contour lines of the smallest eigenvalue of conformation dyadic. BCF results are depicted in gray color.*

BCF method can be used to solve flow problems with more realistic polymer models; moreover, the BCF method may circumvent the high Weissenberg number limit in flow domains with singularities such as contact lines [2] because the BCF method preserves the inherent positive definiteness of the conformation tensor [1].

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