

The Presentations

Wednesday Afternoon: Modeling

A Wavelet-Galerkin Method for Simulating the Doi Model with Orientational Dependent Rotational Diffusivity

Jason K. Suen, Robert A. Brown, Robert C. Armstrong

In this talk, we present a *wavelet-Galerkin* method for simulating the dynamics of kinetic theory models of liquid crystalline polymer molecules. Wavelets are a class of basis functions which are defined based on translation and dilation. The specific class of Daubechies wavelets further possesses useful properties such as compact support and orthonormality. Moreover, they can represent exactly polynomials up to a specific order n . The compact support property allows the computation of the Jacobian matrix to be an order N operation, where N is the dimension of the solution vector; the ability to approximate exactly polynomials up to a specific order n allows a p -refinement, on top of the usual h refinement. Furthermore, the dimension of the solution vector remains the *same* with the p -refinement for a given mesh. This is due to the compact support property of the wavelets. Since the computation of the inner products of the wavelets, called the connection coefficients, can be formulated as an eigenvalue problem, the accuracy of these connection coefficients can be computed up to machine precision. This allows a quadrature-free implementation for forming the Jacobian matrix. All of these properties make the Daubechies wavelet system an attractive candidate for approximating a sharply peaked distribution function and the highly nonlinear integro-differential operators in the diffusion equation.

As an example of simulating molecular models with increasingly realistic description of complex fluid behavior, we employ the wavelet-Galerkin method to simulate the Doi model with orientational dependent diffusivity. Despite the fact that the Doi model was first derived in 1981 (*J. Polymer Sci.*) and the fact that various approximated versions of the Doi model are capable of qualitatively describing the rheological properties of lyotropic liquid crystal polymers, there

has been only very limited effort to explore the nonlinear dynamics of the original Doi model. The wavelet-Galerkin method demonstrates qualitatively different dynamics between the original Doi model and that with an orientationally averaged diffusivity. For example, at $U = 10.67$, we do not find a stable kayaking state between the transition from the log rolling state to the wagging state on the unapproximated Doi model, which is in contrast with previous observations of Larson and Öttinger (*Macromolecules*, 1993) on the orientationally averaged model.

Previous studies of the Doi model without closure approximations have been qualitative with the notable exception of a few bifurcation studies carried independently by Nayak (Ph.D. Dissertation, Massachusetts Institute of Technology, 1998) and Faraoni, *et.al.* (*J. Rheol.*, 1999). Both studies employed the Maier-Saupe intermolecular potential, which can be viewed as a first order approximation of a more rigorous Onsager potential (which was developed based on the statistical mechanics of hard ellipsoids). In this study, we simulate the unapproximated Doi model with the Onsager potential, together with an orientational dependent rotational diffusivity. By means of nonlinear simulations, we attempt to capture some of the stability properties of this model. In particular, we study and characterize the different periodic states for the family of in-plane solutions. The parameter space is two-dimensional and consists of the magnitude of the excluded volume potential, U , and that of the simple shear flow, De . At a given U or at a given De , the transition between the wagging state and the flow-aligning state is found to be a *Hopf* bifurcation. The amplitude, defined as the difference between the maximum and minimum values of the periodic orbit of a structural parameter, scales as $(De_c - De)^{\frac{1}{2}}$ for a given U or as $(U - U_c)^{\frac{1}{2}}$ for a given De , which is a signature of the Hopf bifurcation. The transition from the tumbling state to the wagging state is found to be marked by a maximum value in amplitude as De increases. As De approaches 0, we noticed that the amplitude of the periodic orbit scales linearly with De . In addition, as De goes to zero, the frequency of the orbit vanishes and the period approaches infinity. This suggests a homoclinic bifurcation. The scaling between frequency and De , on the other hand, is found to be linear and does not provide a direct evidence for a homoclinic bifurcation. Further study of the nonlinear dynamics of the Doi model in the limit of vanishing De is currently underway.

Simulation of Reptation Models using the Deformation Field Method

A.P.G. van Heel, E.A.J.F. Peters, M.A. Hulsen, B.H.A.A. van den Brule

We use the deformation field method to study the flow of reptation models for polymer melts. We consider four reptation models: the Doi-Edwards model; the model by Pearson et al., which also includes tube-stretch; the model by Marrucci, which takes into account convected constraint release; and the recent model by Mead, Larson and Doi, in which both tube-stretch and convected constraint release are present.

We consider two flow geometries: the flow between two parallel plates and the flow past a cylinder between two parallel plates.

We explain the deformation field concept and present our simulation results of the above-mentioned models.

Computational Studies of Complex Flows Based Upon "Toy-Model" Approximations of Reptation Theories for Entangled Polymer

J. Remmelgas and L. G. Leal

We report on computational studies of both one-dimensional (Channel and Couette) and two-dimensional (Two-Roll Mill) flows using "toy" models that are intended to approximate reptation theories for entangled polymer solutions or melts. We consider two types of models. The first mimics the behavior of the Marrucci- Grizzutti extension of the original Doi-Edwards theory to include chain stretching (ie it approximates the so-called DEMG model). This model (both DEMG and the "toy" approximation) shares with the original Doi-Edwards model the existence of a non- monotonic dependence of the stress on the shear rate for simple shear and flows that are close to simple shear flow. Hence, it has a local stress maximum at some critical shear rate for this class of flows. The second "toy" model incorporates a simplified version of convective constraint release, again due to Marrucci and coworkers. This model is qualitatively similar to DEMG in extensional flows, but has a monotonic dependence of stress on the shear rate for shear and non-shear flows.

Brownian Dynamics Simulations of Single Polymer Chains in Steady and Time-Varying Shear Flow Steady and Time-Varying Shear Flow

Joe S. Hur, Thomas Kwan, Eric S.G. Shaqfeh and Ronald G. Larson

Brownian dynamics simulations are playing an increasing role in elucidating the physics necessary to include in the microscopic models that are critical to the development of any numerical scheme for calculating viscoelastic flow. These simulations have been extremely useful in our understanding of polymer stretch and recoil in extensional flows, with now a growing body of literature on the subject. There is less available for understanding how shearing flows effect single chain dynamics. Moreover, the examination of single chain DNA dynamics by Chu and co-workers has given us a unique window into aspects of this phenomena and make an examination via Brownian dynamics particularly timely. In the first part of the talk, we present the results of large-scale Brownian dynamics simulations which have been used to examine the recent experimental findings of Smith et al.(Science 283(99)) who studied a single DNA molecule in steady shear flow. We have used a series of different models - the Kramer's freely jointed chain, the Wormlike chain (Larson, J. Rheol. 43(99), the Inverse Langevin chain, the Hookean dumbbell and the Rouse chain - to understand the experimental findings. The steady average molecular extension at various Weissenberg numbers is well predicted by the Kramer's chain with 150 beads whereas chains with fewer beads tend to overestimate it. Note the average molecular extension asymptotes quite surprisingly at nearly 1/2 even for extremely large Weissenberg number. We discuss this result on a physical basis. We have further examined the probability distribution of

the extension at various Weissenberg numbers using the Kramer’s chain and compared it to that of a single DNA molecule. By increasing the number of internal modes we again observe excellent agreement with the experiment. The Power spectral density (PSD) of molecular extension of three models (the Kramer’s chain, the Wormlike chain and the Inverse Langevin chain) is directly compared to that from the experiments. Both qualitative and quantitative agreement is obtained. To understand the behavior of the PSD at various Weissenberg numbers, we have derived analytic solutions for the PSD for both the Hookean dumbbell and the continuous Rouse model. This analysis shows that the characteristics of the PSD at a given Weissenberg number depend critically on the number of internal modes and a single mode model can not capture the experimental observation.

In the second part of the talk, we present similar large scale Brownian dynamics simulations of single chains in exponential shear flow with emphasis on whether the molecular configurations and mechanical/optical response of the molecule is similar to that in extensional flows. We find that for finite strains the chain unravels significantly, similar to uniaxial extensional flow, and furthermore, it undergoes an initial stress and index of refraction relaxation that is much faster than a single exponential decay upon cessation of flow. In addition, when the first normal stress difference is plotted against the corresponding component of the index of refraction tensor $n_{11}-n_{22}$ over a full startup-relaxation cycle, we observe a hysteresis effect that was also previously found in the uniaxial extensional flow. The shear component of the stress and index of refraction also exhibits hysteresis but in the opposite direction, i.e. when plotted over a full cycle, the branches for the startup and relaxation are opposite to that for the 11-22 component. To experimentally investigate the effects of transient unsteady shear flows on dilute polymer solutions, we employ both mechanical rheometry and flow birefringence. Polyisobutylene and polystyrene based Boger fluids are prepared and their viscoelastic properties are characterized on a Rheometrics RDA-II mechanical rheometer. Using the experimental chain relaxation time, we proceed to match the flow strength, i.e. the Weissenberg number, in our experiments to the simulations. Indeed we see a very dramatic stress increase during startup and a highly non-linear relaxation. Detailed comparisons between the individual components of the stress and index of refraction are then made and compared to simulation results.

The FENE-L and FENE-LS Closure Approximations to the Kinetic Theory of Finitely Extensible Dumbbells

Gregory Lielens, Roland Keunings and Vincent Legat

We address the closure problem for the Warner Finitely Extensible Non-linear Elastic (FENE) dumbbell model of a dilute polymer solution. The FENE-L closure model, introduced recently for one-dimensional elongational flows [1] is extended to general flow kinematics [2]. A simplified version of the theory, referred to as the FENE-LS model, is also proposed. Simulations of steady-state and transient rheometrical flows reveal the superiority of the FENE-L and FENE-LS constitutive equations with respect to the simpler FENE-P closure in describing the rheological response of the FENE kinetic theory. In particular, it is capable of reproducing the

hysteretic behaviour of the FENE theory in stress versus birefringence curves during start-up of flow and subsequent relaxation (see also [3]).

[1] G. Lielens, P. Halin, I. Jaumain, R. Keunings, V. Legat, J. Non-Newt. Fluid Mech., Vol. 76, 249-279 (1998)

[2] G. Lielens, R. Keunings, V. Legat, The FENE-L and FENE-LS Closure Approximations to the Kinetic Theory of Finitely Extensible Dumbbells, accepted for publication in J. Non-Newt. Fluid Mech. (1999)

[3] R. Sizaïre, G. Lielens, I. Jaumain, R. Keunings, V. Legat, J. Non-Newt. Fluid Mech., Vol. 82, 233-253 (1999)

Capitalizing on Nonequilibrium Thermodynamics. Example 3: On Models for Non-isothermal Flow Calculations

Hans Christian Öttinger

Non-isothermal flows are becoming an increasingly important issue in the numerical simulation of viscoelastic flows. Guided by various ideas, a number of authors have attempted to formulate the proper equations for non-isothermal flows, with temperature-dependent viscoelastic properties and an additional energy or temperature equation. In this contribution, we employ a recently developed framework of nonequilibrium thermodynamics (GENERIC) for producing thermodynamically admissible equations for several models with an upper-convected configuration tensor as the relevant structural variable (Maxwell, Oldroyd-B, Giesekus, FENE-P, Phan-Thien/Tanner). Our results and conclusions are compared to those of previous authors. In particular, we find the temperature equation typically used in engineering analyses of non-isothermal flows to rest on dubious assumptions, and we offer some remarks on the assumption of incompressibility for non-isothermal flows.

End-plate instability in polymeric filaments: The influence of surface tension

Henrik Koblitz Rasmussen and Ole Hassager

The 3D Lagrangian Integral Method is used to simulate the effects of surface tension on the viscoelastic end-plate instability that occurs in the rapid extension of some polymeric filaments between parallel plates. It is shown that surface tension delays the onset of the instability. Furthermore it is demonstrated that surface tension plays a key role in the selection of the most unstable mode.

Thursday Morning: Methods

Three-Dimensional Finite Element Method for Viscoelastic Fluid Flow Problems

R. Guenette and Roger Pierre

The development of efficient and robust numerical methods for the simulation of viscoelastic fluids is still a challenging problem although much progress have been done in the past few years. Indeed, successful finite element methods are currently used for 2D viscoelastic fluid flows. Among them, there is the DEVSS method which is a discrete variant of the popular Elastic-Viscous-Split-Stress (EVSS) method introduced by Rajagopalan et al. (JNNFM, 36, 159-199, 1990). This formulation uses the rate of deformation tensor as an additional variable and no change of variable is performed into the constitutive equation. Very recently, there has been a growing interest in extending the present methodology to three dimensional problems. For 3D simulations, one must solve a system of 16 variables on a large mesh which results in a very big non-linear problem. In this context, direct solver must be avoided. In our recent work, we have explored the possibility of choosing different discretizations for the stress tensor and the additional variables. This allows more flexibility.

In particular, a discontinuous approximation for the additional variable may reduce the four fields problem to a more amenable three fields problem. A simple criteria will be presented insuring the stability of the method. Mixed formulation is the appropriate framework for the theoretical analysis. Several mixed finite elements will be studied. The numerical strategy is based on the Newton method. The linearized problems are solved by a preconditioned Krylov subspaces iterative method. Sparse matrix techniques and the Schur complement approach are used to speedup the computation and reduce the number of unknowns. The performance of this iterative method will be discussed on complex flows of industrial interest.

Computation of Transient Flows of Dilute Polymer Solutions in Complex Geometries using the Adaptive Lagrangian Particle Method

Xavier Gallez , Roland Keunings and Vincent Legat

The Lagrangian Particle Method (LPM) has been proposed recently [1] for the computation of transient viscoelastic flows using either a constitutive equation (macroscopic approach) or a kinetic theory model (micro-macro approach). In LPM, the polymer stress is computed at discrete Lagrangian particles which are convected by the flow, while the conservation equations are solved by means of a finite element technique. The polymer stress computation is achieved

by solving along the particle trajectories either the macroscopic constitutive equation or the stochastic differential equation for a particular kinetic theory model.

In this talk, we present the Adaptive LPM (ALPM) where the Lagrangian particles are automatically and continuously created or deleted when and where needed [2]. ALPM is applied to flows in complex geometries, including a large eccentricity journal bearing, a planar 4:1 contraction, and a 4:1:4 constriction. Results are presented and compared for the FENE, FENE-P, and FENE-LS [3] fluids.

[1] P. Halin, G. Lielens, R. Keunings, V. Legat, J. Non-Newt. Fluid Mech. Vol. 79, 387-403 (1998)

[2] X. Gallez, P. Halin, G. Lielens, R. Keunings, V. Legat, The Adaptive Lagrangian Particle Method for Macroscopic and Micro-Macro Computations of Time-Dependent Viscoelastic Flows, accepted for publication in Computer Methods in Applied Mechanics and Engineering (1999)

[3] G. Lielens, R. Keunings, V. Legat, The FENE-L and FENE-LS Closure Approximations to the Kinetic Theory of Finitely Extensible Dumbbells, accepted for publication in J. Non-Newt. Fluid Mech. (1999)

Semi-Lagrangian Finite Volume Methods for Viscoelastic Flow Problems

T. N. Phillips and A. J. Williams

Standard finite volume methods for problems in computational fluid dynamics suffer from restrictions on the size of the time step due to stability considerations. This restriction is not so severe when Lagrangian methods are used. However, the unrestricted movement of the points in a Lagrangian formulation introduces difficulties associated with mesh distortion. Semi-Lagrangian methods, however, combine the advantages of fixed grids inherent in Eulerian methods with modifications to treat the convective terms using particle tracking methods.

The hyperbolic nature of the constitutive equation is responsible for many of the difficulties associated with the numerical simulation of viscoelastic flows. Many techniques introduce some form of upwinding in order to obtain numerical solutions at high values of the Weissenberg number. In some finite volume techniques artificial diffusion is added to the constitutive equation. The Semi-Lagrangian approach described here is a natural way of treating the convective terms in the constitutive equation without resorting to these techniques.

The solution algorithm is based on SIMPLER together with a semi-Lagrangian treatment of the convective terms. Numerical results are presented for the viscoelastic flow through a planar 4:1 contraction using the Oldroyd B and Phan-Thien Tanner models. Particular emphasis is given to the convergence and stability of the method and the development of vortex structure with increasing Weissenberg number.

The Backward-tracking Lagrangian Particle Method (BLPM) for Computing Transient Viscoelastic Flows

Peter Wapperom, Roland Keunings and Vincent Legat

We present a new Lagrangian particle method for solving transient viscoelastic flow for both macroscopic and microscopic stress equations. In Lagrangian particle methods [1,2], "stress-carrier" particles are distributed at some initial positions in the flow domain and are then tracked forward along flow trajectories. In BLPM, we take an opposite approach by specifying the particle positions at the current time and then calculating the particle trajectory leading to that point by tracking backward in time. The backward tracking process is stopped after a specified time (possibly only a single step), and the initial configuration for the Lagrangian integration of the stress is obtained by interpolating a stored Eulerian field at that time.

In order to demonstrate the accuracy, efficiency and stability of the method, we will consider two benchmark problems in the context of the FENE dumbbell kinetic theory of dilute polymer solutions and its FENE-P approximate constitutive equation: the high eccentricity journal bearing flow and the 4:1 contraction flow. With the help of these examples we show in which manner accurate results can be obtained, for transients of both velocity and polymer stress, with a minimum number of particles and a minimum particle path length.

[1] P. Halin, G. Lielens, R. Keunings, V. Legat, J. Non-Newt. Fluid Mech. Vol. 79, 387-403 (1998)

[2] X. Gallez, P. Halin, G. Lielens, R. Keunings, V. Legat, The Adaptive Lagrangian Particle Method for Macroscopic and Micro-Macro Computations of Time-Dependent Viscoelastic Flows, accepted for publication in Computer Methods in Applied Mechanics and Engineering (1999)

A Cell Vertex Finite Volume/Element Method for Viscoelastic Flows

M. Aboubacar and M.F. Webster

This study considers the accuracy and stability properties of a new hybrid finite element/volume scheme in its application to the numerical solution of some viscoelastic flows. Previously, a second-order scheme has been constructed that demonstrates its efficiency over finite element counterparts on model problems. The current direction of investigation focuses on highly elastic solutions, with retention of accuracy and favourable stability properties. Holding this goal in mind, results shall be presented for the benchmark problem of flow through a 4:1 planar contraction with sharp re-entrant corners for an Oldroyd-B model.

Typically, incompressible viscoelastic flows, may be classified through mixed parabolic-hyperbolic differential systems. The central ethos of the current approach is to apply finite element technology to the self-adjoint aspects of the system (optimal), and finite volume schemes

to the hyperbolic parts. Finite volume technology has advanced considerably, over the last decade, in its treatment of pure advection equations, and has matured sufficiently to offer itself to the present regime. The emergence of non-trivial source terms via the constitutive equations gives rise to some open questions for the finite volume representation, these remain to be resolved.

Features of this approach include, a hybrid time-stepping treatment of finite elements (semi-implicit Taylor-Galerkin/Pressure-Correction) for continuity and momentum equations, and a cell vertex finite volume scheme for the constitutive equation, within the context of a fractional staged formulation based upon each time-step. The positioning of finite volume nodal values and control volumes, is such that four linear finite volume triangular cells are formed as embedded subcells of each parent quadratic finite element triangular cell. This is accomplished by connecting the mid-side nodes of the parent finite element triangular cell. With stress variables located at the vertices of the finite volume cells, no interpolation is required to recover the finite element nodal stress values. The cell vertex approach is naturally associated with fluctuation distribution, an upwinding technique that distributes control volume contributions for each equation to provide nodal solution updates. The consideration of triangular cells offers the flexibility of either structured or unstructured meshing as equally viable options, without further complication.

The viscoelastic regime automatically generates problems with nontrivial source, as well as the usual advective flux terms. Infact in shear flow or in no-slip boundary vicinities, source terms dominate, with dependency on stress and velocity gradients, as flux terms vanish. The methodology proposed behind the cell vertex finite volume scheme, strives to maintain a consistent treatment for both flux and source term contributions, reminiscent of Petrov-Galerkin variational weighting. Likewise, such considerations may be extended to embrace the transient terms. Fluctuation splitting schemes may be of linear or non-linear type, and introduce such properties as positivity and linearity preservation. Various forms are considered, recognising the importance of linearity preservation in retaining high-order accuracy. In our earlier work, superior accuracy of the stress has been established, once solution representation is based upon the background parent finite element. This idea is extended in the present study. Prior studies established accuracy properties against analytical solutions for smooth flows, before addressing stability issues for complex smooth and non-smooth flows. The latter are reconsidered here.

Various different alternative treatments are considered for dealing with flux and source terms to identify their relative strengths and weaknesses. There is the contrast between the fluctuation parts and those dealt with by reference to the median dual cell, a unique non-overlapping region associated with each finite volume node. Other issues arise concerning the use of area or line integrals, the choice of stress representation, precision of quadrature, and gradient representation. Through identifying stress behaviour, as a consequence of scheme implementation, both in fully-developed exit shear flow and in the near-corner neighbourhood, the corresponding properties of such schemes may be adjudged. From this information, a localisation approach may emerge, to attract the advantages of each form.

Finite Volume Numerical Simulation of Viscoelastic Flows Trough Planar Contractions with AESM Formulation

The flow of a viscoelastic fluid through an abrupt planar contraction of ratio 4:1 is numerically solved using the AESM (Algebraic Extra-Stress Model) for an Oldroyd-B fluid. The results concerning the extra-stress components are compared with the classical differential formulation. It is shown that the AESM formulation predicts exactly the same values for extra-stresses in the case of pure shear and pure elongational flows. In order to study the applicability of the AESM formulation inside abrupt contractions a criteria based on the shear rate and on the rotation rate is proposed. Regions of pure shear, pure elongation and pure "rotation" are found inside the planar contraction. The presence of the singularity at the corner for the extra-stress components is confirmed for the Oldroyd-B fluid. The AESM formulation is valid only for steady-state flow situations. In order to solve numerically the equations, the finite volume method with a time-marching algorithm of second-order precision based on the Richardson extrapolation is employed. When using the differential formulation for Maxwell and Oldroyd-B fluids, for a given mesh, an instability is detected in the region of the sharp corner. This instability propagates inside the flow a traveling wave with a well defined frequency. The velocity and extra-stress fields become periodic just before the Deborah number limit is reached.

Thursday Afternoon: Stability

The Finite Element Analysis of Stability of Viscoelastic Flows in Two-dimensional Complex Geometries to Three-dimensional Perturbations

M.D. Smith, R.C. Armstrong, and R.A. Brown

Methods are presented for the analysis of the linear stability of spatially complex, two-dimensional steady viscoelastic flows to two- and three-dimensional disturbances. The analysis is based on finite element calculation of the steady base flow and two distinct approaches for calculation of the long time solution of the time-dependent equations formed by linearization about the base flow. In the first approach the equation set is solved by direct time integration. Here finite element discretizations in space are based on the DEVSS-G finite element discretization that is used with Newton's method to compute steady-state solutions. We investigate two different time integration schemes to compute the time evolution of general, random disturbances: a theta-method operator-splitting scheme and a fourth-order Runge-Kutta method. For both time integrators, time stepping is decoupled into a solution of a modified Stokes problem and an evaluation of the time-dependent constitutive equation. The overall efficiency of both time integrators is extremely high, as is the potential for implementation on parallel computers. Although computationally efficient, this approach has the drawback that the computation must be continued to sufficiently long time to integrate through any non-normal behavior of the linear dynamics (Sureshkumar, Smith, Armstrong, and Brown, *J. Non-Newtonian Fluid Mech.*, 82 (1999) 57-104), and the approach yields only the most dangerous disturbance and the growth rate of the disturbance. Integration to long times also is needed to separate eigenfunctions with

nearly equal eigenvalues, as is the case in the continuous portion of the spectrum for viscoelastic flows.

The second approach involves direct calculation of the most dangerous eigenvalues (those with largest real part) for the eigenvalue problem that corresponds to the long-time solution of the disturbance equations. The algorithm used combines time integration of the linearized equations with Arnoldi's method to accelerate the calculation of the eigenvalues with the largest real part. Although the hybrid time integration/Arnoldi approach does not dramatically reduce the computational cost over the use of time integration alone, it provides distinct calculation of a portion of the eigenvalue spectrum.

The stability of cylindrical Couette flow is used as a benchmark for the calculations by comparison with the results reported by Sureshkumar, Beris, and Avgousti (Proc. R. Soc. Lond. A, 447 (1994) 135-153). Both approaches are used here with three discretizations of the constitutive equation: Galerkin's method, streamwise-upwinding Petrov-Galerkin, and the discontinuous Galerkin formulation. The results of direct time integration and the hybrid time integration/Krylov method are in quantitative agreement, and all three discretizations of the constitutive equation converge with mesh refinement. Calculations also are reported for flow around a linear, periodically spaced array of cylinders confined in a channel for an Oldroyd-B fluid. Contrary to the results in our previous paper (Sureshkumar, Smith, Armstrong, and Brown, *op. cit.*), we find the closely spaced cylinder array (the distance between cylinder centers is 2.5 radii) is stable to two-dimensional perturbations. We show that the incorrect stability prediction was caused by under-resolution of the shear-like disturbance along the wall of the channel. New results show that the two-dimensional flow is unstable to three-dimensional perturbations. The three-dimensional perturbations are concentrated near the point of flow separation on the downstream side of the cylinders. Liu (Ph.D. Dissertation, Massachusetts Institute of Technology, 1997) saw a similar instability in the flow of a Boger fluid through the same geometry, and the value of the Weissenberg number predicted here for the instability is in reasonable agreement with the experimental observations. The dependence of this instability on cylinder spacing is probed as a means of connecting this instability to the observation of a three-dimensional instability in the wake of an isolated cylinder in a channel (McKinley, Armstrong, and Brown, Phil. Trans. R. Soc. Lond. A, 344 (1993) 265-304). To date, we have not computed an instability in this geometry.

Stability of Isothermal and Non-isothermal Viscoelastic Flows in Complex Geometries using Time-dependent Simulations

B. Yang, U.A. Al-Mubaiyedh, B. Khomami and R. Sureshkumar

Viscoelastic instabilities most often are the limiting factor in enhanced production of polymeric and polymeric based composite materials. To date, the analysis of viscoelastic instabilities has been mostly limited to linear stability calculations in simple rectilinear flows where direct eigenvalue solvers can be used to analyze the stability of the system. Such an approach is not feasible for analyzing the stability of 2D and 3D flows due to the tremendous cost associated with the simulations. In this study, we have used our recently developed higher order finite ele-

ment techniques for simulation of steady and transient viscoelastic flows to analyze the effect of fluid elasticity on the stability of isothermal flow past periodic arrays of cylinders to 2D periodic disturbances has been studied using quasi-linear constitutive equations such as the OLD-B and UCM models as well as the multi-mode Giesekus model. Based on these studies we have identified the critical Deborah number for the onset of the instability as well as examining the effect of multiple modes of relaxation time on the onset conditions and the full nonlinear development of the instability. In turn, the results of our analysis are compared with prior experimental results and it is shown that the simulations are capable of predicting the experimentally observed instabilities with reasonable accuracy.

Linear stability analyses of viscoelastic Taylor-Couette flow under isothermal conditions have predicted flow transitions to non-axisymmetric and time-dependent states [Shaqfeh, *Annu. Rev. Fluid. Mech.*, 1996]. Also, non-linear stability analysis has shown that the flow bifurcation is supercritical for axisymmetric disturbances [Avgousti and Beris, *Int. J. Num. Meth. Fluids*, 1993] and subcritical for the non-axisymmetric ones [Sureshkumar et al., *Proc. R. Soc. Lond.*, 1994]. In contrast, it was reported experimentally that the transition to the secondary flow is axisymmetric corresponding to a stationary state with onset Deborah number an order magnitude lower than those reported theoretically [Baumert and Muller, *Phys. of Fluids*, 1997]. Recently, Al-Mubaiyedh et al. [70th Annual Meeting of SOR, 1998] showed that energy dissipation by viscous heating in the viscoelastic Taylor-Couette flow has a significant influence on the stability characteristics of the viscoelastic Taylor-Couette flow of an Oldroyd-B liquid. First of all, for experimentally realizable values of Peclet and Brinkman numbers, the onset Deborah number predicted by the non-isothermal linear stability analysis are very close to that reported experimentally. Moreover, the most dangerous disturbance is axisymmetric and stationary. In this study, we have used time-dependent simulations to examine the non-linear stability characteristics, i.e., supercritical vs. subcritical bifurcation, of the non-isothermal Taylor-Couette flow of an Oldroyd-B liquid. The time-dependent simulations are also used to examine the non-linear evolution of the disturbance in the post-critical flow regime. We will also discuss the effect of various important parameters such as inertia, solvent viscosity, gap width, and viscous dissipation on the stability of this flow.

Non-Newtonian flow instabilities in concentrated suspensions

Aaron Avagliano and Gareth H. McKinley

We investigate the linear stability of three continuum models for concentrated suspensions of hard spheres in a steady shearing flow with a deformable free surface. We consider the diffusive flux model (Phillips et al. 1992), the suspension balance model (Nott & Brady 1993), and a model that accounts for flow induced microstructural changes (Phan-Thien 1995), giving rise to non-Newtonian stresses. We demonstrate that none of these models predict the flow instability observed experimentally by Tirumkudulu et al. 1999 (*Phys. Fluids* 11, 3). In this experiment a cylindrical Couette cell is oriented horizontally (With respect to gravity) and the inner cylinder is rotated. If the gap is completely filled with the suspension, no instability is observed. However, if the gap is only partially filled, the flow evolves from an initially uniform distribution of particles,

to form periodic bands containing high and low concentrations of particles. We show that this is a new type of flow instability and is driven solely by gradients in the non-Newtonian base state normal stresses which induce a particle flux in the presence of a free surface. A new constitutive equation, with a strong similarity to microstructural models for viscoelastic polymer solutions, is introduced that is capable of predicting the results of Tirumkudulu et al. 1999.

Fully Three-Dimensional Numerical Simulations of Vortex Breakdown in Confined Swirling Flows of a Dilute Flexible Polymer Solution

S.-C. Xue

Aiming at simulating the problems involving three dimensional, time-dependent, asymmetrical swirling flows of viscoelastic fluids in an enclosed cylindrical vessel with a rotating bottom lid, thus, testing the validation of constitutive models used to describe viscoelastic fluids, a fully three dimensional (3-D) numerical method using an implicit finite volume formulation is developed in the cylindrical coordinate system. Three difficulties arising from the coordinate transformation in a structured mesh system are removed by some simple, but effective measures. With this method, the velocity fields measured in experiments are accurately predicted, and the development of vortex breakdown processes in terms of Reynolds number Re and the height to radius ratio H/R , as well as the time, observed in experimental visualizations are exactly reproduced for Newtonian flows. The influence of elasticity on the vortex breakdown processes are investigated for the low viscosity dilute polyacrylamide(PAA) solutions described by the upper convected Maxwell (UCM) model. It is confirmed numerically that the existence domain of vortex breakdown occurred at significantly greater Re than that for Newtonian solvent of similar shear viscosity. It seems that the centrifugal force leading to vortex breakdown in Newtonian fluid is balanced by the normal stress in elastic fluid. As a results, the vortex breakdown would be significantly delayed in terms of Re or even suppressed with increasing elasticities. Steady state simulations with high viscosity elastic fluid show that an elastic ‘ring’ vortex developing at the edge of the rotating lip pushes the Newtonian vortex to the radial centre of rotating lip and finally reverses the flow with increasing elasticity. The numerical inspection of the highly unsteady spiral vortex flows of viscoelastic fluids are on the way.

Low-order continuous and discontinuous mixed finite element methods for viscoelastic fluid mechanics

Arjen C.B. Bogaerds, Gerrit W.M. Peters and Frank P.T. Baaijens

One of the key issues in simulations of viscoelastic flows remains the assessment of numerical stability of the computational method. Especially, increasing elasticity beyond critical values of the dimensionless Weissenberg number can give rise to numerical instabilities in flows

that are otherwise mathematically stable. To date, the more successful numerical methods for viscoelastic flow simulations are based upon the so called Elastic Viscous Stress Splitting (EVSS) algorithm together with a suitable form of upwinding of the hyperbolic part of the constitutive equation.

From a mathematical point of view, the inertia-less plane Couette flow of a Maxwell fluid provides an extremely useful tool for the determination of the temporal stability of a computational method. Linear stability analysis of a superimposed spatially periodic disturbance shows this flow to be stable for all values of the Weissenberg number.

However, given the smoothness of the simple shear plane Couette flow, the performance of a numerical scheme for more realistic complex flow geometries remains an open issue. Other benchmark problems are found in the flow of an Oldroyd-B fluid around a cylinder and the so-called stick-slip problem using a Maxwell model

Here, several computational methods based on the discrete EVSS scheme are benchmarked against these problems. Spatial discretizations are based on projections upon continuous and discontinuous subspaces resulting in numerical schemes ranging from fully continuous to fully discontinuous in all its variables.

Modeling and Stability Analysis of Viscoelastic Flows in Complex Geometries using Stochastic Simulation Techniques

Madan Somasi and Bamin Khomami

Modeling dilute polymeric solutions in complex flows has attracted considerable attention in recent years. Researchers [1,2] have used macroscopic constitutive equations based on elastic dumbbell models to perform simulations. Although qualitatively representative, the predictions by these models have not been able to quantitatively describe the experimental measurements. One of the main reasons put forward for this shortcoming is the closure approximation used to derive these constitutive equations. To put this issue to rest, we have performed simulations using models without closures, like the single and multimode FENE models. Since there is no corresponding macroscopic equation for the FENE model, we have used Brownian Dynamics Simulations in conjunction with adaptive Finite Element techniques to investigate the effect of the 'closure' approximation on the predictions. Our technique is based on the concept of 'Brownian Configuration Fields' recently introduced by van den Brule et al. [3]. Simulations have been performed for an axisymmetric stagnation flow as well as a sphere falling in a tube. On comparison with experiments however, we see that the discrepancies are not solely due to the closure approximation. Incorporating factors like viscous stress and conformation dependent drag into the model also does not seem to bridge the gap between experiments and simulations. It is clear that other factors such as the accuracy of the entropic spring law and inter-molecular interactions need to be considered. The next step therefore, is to consider bead-spring chain models, which can capture a better picture of the various conformations of a polymer molecule in a complex flow. We have conducted simulations with various chain models and the predictive

capabilities of these models shall be presented in detail.

Using a modified form of the concept of 'Brownian Configuration Fields'[3], we have constructed a method to study the linear stability of viscoelastic flows without resorting to a CE for polymer stress. Our approach is based on combining Brownian Dynamics simulations with time dependent adaptive Finite Element methods (BDS/A-FEM) to study the linear stability of two-dimensional flows. As an exercise of benchmarking our code, we have performed linear stability analysis of the Plane Couette Flow (PCF) using Hookean dumbbells. We have compared our results with the corresponding continuum eigenvalue analyses with the Upper Convected Maxwell (UCM) and the Oldroyd-B models and the agreement has been very encouraging [4]. We have also carried out a stability analysis of PCF using the FENE dumbbell model, for which no closed form CE is possible. Moreover, to examine the feasibility of our approach in more complex flows, we have studied the stability of the viscoelastic flow past a periodic array of cylinders. The stability and dynamics of this flow has been recently reported by independent groups [5,6] using closed form CEs and as such is an ideal candidate for our study. Our stochastic simulation results using various dumbbell models and their comparison to the continuum based simulation results shall be presented.

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Friday Morning: Experiments and Applications

Non-Newtonian Flows of Complex Interfaces

Gerry Fueller

Many interfaces containing amphiphilic species are characterized by a nonNewtonian rheology. Consequently, these two dimensional systems respond to flow by producing highly nonlinear phenomena that are reminiscent of their three dimensional counterparts. This paper presents data on several monolayers systems residing at the air/water interface that show such effects. For example, monolayers consisting of amphiphilic polymer chains are demonstrated to produce large corner vortices when forced to flow through a two-dimensional, 4:1 contraction. Likewise, when issued into an expansion, the same monolayers show evidence of two-dimensional normal stress differences. Aside from their interesting behavior in their own right, these two dimensional systems can provide model systems with which to test two-dimensional numerical simulations. In addition to data on nonNewtonian fluid mechanics, this paper also presents a summary of experimental methods that can be used to properly characterize nonNewtonian, interfacial rheology.

The Role of the Transient Extensional Rheology in Complex Viscoelastic Flows (or "An Update from the Experimental Trenches")

Gareth H. McKinley, A.Tripathi, S.L. Anna and J.P. Rothstein

In this talk we survey the importance of quantifying the transient extensional rheology of a polymeric fluid and the important role it plays in controlling the dynamics of complex viscoelastic flows. Recent experimental measurements in three prototypical flows of varying complexity will be discussed. In the filament stretching rheometer, the kinematics can now be well controlled and the true extensional stress growth of the fluid subsequently measured. Conversely, in the microfilament rheometer developed by Entov and coworkers, a slender viscoelastic filament undergoes elastocapillary thinning and ultimate breakup. The kinematics here are not imposed but selected by a balance between viscosity, elasticity and capillarity. Material properties for both Newtonian and viscoelastic fluids, can still be extracted from the observations provided one does not oversimplify the analysis. The device can also be used to explore poorly understood and heuristically characterized phenomena such as tackiness and 'stringiness' in materials such as pressure-sensitive adhesives containing volatile components. Finally, in the 4:1:4 abrupt contraction/expansion geometry, knowledge of the extensional viscosity can be used in combination with pressure-drop data plus DPIV and LDV measurements to rationalize the evolution in vortex structure and stability of the flow. However, these measurements also indicate that understanding the complex evolution in the internal macromolecular structure is important, and the interplay of the shearing and extensional components of the flow is critical. Preliminary data in a new filament stretching rheometer design will be presented in an attempt to quantify this. In each of the experiments discussed above, both numerical analysis and constitutive modeling can play an important role in guiding experimental design and interpretation of results.

Numerical Simulation of the Flow of Branched

Polymer Melts using a Multi-mode "Pom-pom" Model

Nicolson

The transient flow of a branched polymer melt through various contraction geometries has been modelled using a molecularly based constitutive equation together with a Lagrangian finite element method.

The constitutive equation, developed by McLeish and Larson [1], models the polymer as a suspension of idealised "pom-pom" molecules consisting of a cross-bar connecting two identical stars. The constitutive parameters directly relate to features in this structure.

The flow of the polymer was calculated using a finite element method with a moving triangular grid. At each time step the velocity and pressure were calculated from the current values of the constitutive parameters. The constitutive parameters, and positions of the grid vertices were then updated using the calculated data. This "flowSolve" program can produce various outputs, including the visualisation of the development of vortices upstream of the contraction and of the birefringence - both of which may be compared with direct experimental observations.

Initial simulations used a set of parameters corresponding to mono-disperse pom-pom molecules and showed results of a similar nature to those observed experimentally. These included vortex enhancement as a function of Weissenberg number and degree of branching. We have now developed the flow solver to use a multi-mode extension of the pom-pom model, with parameters that vary with the degree of branching. This constitutes a quantitative rheological model of LDPE. The parameters are obtained from a simultaneous quantitative fit to transient shear and extension data. This procedure permits quantitative prediction and comparison of real 2-D complex flows of commercial branched polymers.

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Generalised Differential Constitutive Equation for Polymer Melts

Wilco Verbeeten, Gerrit Peters and Frank Baaijens

Numerical simulation of visco-elastic flows remains a topic of extensive investigations, for example, in regard to polymeric melt flows in industrial applications. Eventually, the objective is to perform simulations of visco-elastic flows in characteristic geometries under industrial processing conditions. This means, flows with a realistically rheological behaviour at high elasticity rates in three dimensional geometries.

In general, visco-elastic fluids are characterised in shear, and, to a lesser extent, also in

elongation. To discriminate between different constitutive equations, predictive capabilities for shear (viscosity and first normal stress coefficient) and elongation (planar, uniaxial and biaxial), both in steady state and transient behaviour, have to be investigated simultaneously.

The 'conventional' differential constitutive equations, like the Giesekus and Phan-Thien Tanner (PTT) models, are performing well in transient and steady state shear. However, the performance of these models in elongation show deficiencies, as for example underpredictions of the elongational thickening observed for many polymer melts.

Two recent developments show strong improvement with respect to the above mentioned problems. A phenomenological method for differential constitutive equations was introduced by Peters et al. (JNNFM 82, 1999). The Feta model used in this paper is based on the exponential PTT model, where the shear viscosity is fixed to experimental data, while still allowing for flexibility in describing extensional properties. A drawback of this model is, that it overpredicts the steady state first normal stress difference when extensional properties are satisfied.

A new molecular constitutive equation for a class of branched polymers has been introduced by McLeish and Larson (J.Rheol. 42(1), 1998), the Pom-Pom model. Incorporating the Giesekus model and writing it in a closed differential form for the stress tensor, results in a generalised differential constitutive equation. By fitting the linear parameters to dynamic measurements, and most of the non-linear parameters to the transient uniaxial elongational data, a good quantitative agreement is obtained for both shear and elongation, transient and steady state data. The non-linear parameter related to the Giesekus part of the model can be adjusted to result in a qualitative agreement with second normal stress difference experiments of Kalogrianitis and Van Egmond (J.Rheol. 41(2), 1997).

An important next step is to see how this model is performing in complex flow geometries.

Flow induced birefringence in injection molded Magneto-Optical Disks

Aaron Avagliano, Mark D. Smith, Gareth H. McKinley, Robert A. Brown, Robert C. Armstrong

We model the time-dependent non-isothermal viscoelastic flow phase of the injection molding process of compact disks and digital video discs. The magnitude of the 'inplane' and 'vertical' flow induced birefringence can be calculated from the residual stress distribution that remains at the end of the filling process. These residual stresses are determined by examining the radial flow of a non-isothermal formulation of the Carreau and Giesekus models in a disk geometry. Viscoelastic effects become dominant in the narrow thermal boundary layers that form as the hot melt contacts the cold mold walls and vitrifies. The numerical simulation incorporates a treatment of the moving contact line, together with the fountain flow at the free surface in order to determine to what extent the elongational deformation history is 'frozen in' to the ultimate product. The finite element model employs the DEVSS-G formulation of the governing equations with streamline upwinding in the energy (SU) and stress (SUPG) equations. The time-dependent nature of the flow is captured using a deformable mesh, together with either (i) an implicit Euler time stepping scheme for the Carreau model, or (ii) the theta-method time

stepping scheme for the Giesekus model.

Flow of LDPE through Contractions: Comparison of Simulations with Experiments

E. Mitsoulis

Recent experiments [1] on the flow of the IUPAC-LDPE melt X in planar contractions has shown that this melt exhibits large growing vortices in the reservoir, as is also the case when flowing through axisymmetric contractions. Detailed LDV measurements have been made and the streamlines have been obtained a posteriori through integration of the velocity field. Numerical simulations with the K-BKZ integral constitutive equation show that when the planar extensional viscosity follows the shear viscosity in its shear- (and hence strain-) thinning behaviour, the model is incapable of predicting the vortex growth for the corresponding apparent shear rates used in the experiments. This defect has been corrected by using multiple strain-memory functions in the K-BKZ model with multiple parameters [2]. The model then predicts strain-thickening behaviour of the planar extensional viscosity without affecting the shear-thinning viscosity. The simulations with the so-corrected kernel are then in qualitative agreement with the experimental flow patterns, regarding the growth of vortices in the reservoir.

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Friday Afternoon: Extensional Flows

A New One Mode Molecular Model Suitable for Flows with Strong Elongational Components

I. Ghosh, G.H. McKinley, R.A. Brown and R.C. Armstrong

Several recent studies of complex flows with important elongational components, such as the 4:1 contraction (Coates et al, J.N.N.F.M, 1992) and the periodic array of widely spaced cylinders (Liu et al, J.N.N.F.M, 1998), have been unable to achieve good agreement between experiment and numerical simulation. An inadequacy common to all the above work is that the single mode constitutive equations that are used can only capture physics on the coarsest length and time scales.

Through Brownian dynamics simulations, this work demonstrates that a fine scale model

such as the Kramers chain gives excellent agreement with experiments for stress and birefringence growth following the inception of an uniaxial elongational flow. However, coarse scale models such as the FENE dumbbell underpredict these quantities by up to two orders of magnitude during the startup period. Although the need for finer scale physics is unquestionable, the use of Kramers chains in complex flow calculations is far beyond current computational limits. Polymer models that capture the physics of a Kramers chain in a few, or preferably one, mode are greatly needed.

We address this need by developing a molecular model that views a polymer molecule as a set of identical segments that are each small enough to be stretching reversibly. Since the stretching is reversible on the segment length scale, a segment can be modeled as a FENE spring. As the flow strength (Tanner, *AIChE Journal*, 1976) increases, the length of a segment decreases, but the number of segments increases so that the model always represents a molecule with a fixed contour length. As well as requiring less computation time than multiple mode spring models, a major advantage of the new model is that length scale of the model dynamically adjusts to the underlying flow. There is no need to guess the number of modes that are required a priori. As the molecule unravels, segments combine so that the length of a segment increases, but the number of segments is reduced. The modeling of the segment recombination is inspired by analyzing the unraveling of individual molecules and accounting for the importance of initial configuration on the eventual dynamics. We show that the new model gives predictions of stress and birefringence growth in uniaxial elongation that agree very well with Kramers chains. Consequently, predictions of stress-birefringence hysteresis are also well modeled.

Since the length of a segment is determined by the strength of a flow, the model can easily be extended to more general flows than pure elongation. As vorticity is added to a pure elongation, the strength of the flow decreases and length of the segments increases. In the limit of shear, the model reduces to a FENE dumbbell. We illustrate the generality of the model by examining some mixed shear and elongational flows.

Computational Analysis of Techniques to Determine Extensional Viscosity from Entrance Flows

Dilip Rajagopalan

Recent computational analysis of entrance flows (Mitsoulis et al, 1998) suggests that the entrance pressure drop is insensitive to large changes in steady extensional viscosity - a result that directly contradicts a large body of experimental work in this area. A re-examination of entrance flows using numerical simulations is presented in this work which shows that entrance pressure drops do depend on the steady extensional viscosity, provided the extension rate in the entrance flow is large enough. Numerical simulations are presented using both the strain thinning and thickening versions of the Phan-Thien Tanner (PTT) constitutive model. Techniques developed by Cogswell (1972), Gibson (1989) and Binding (1988,1991) for extracting extensional viscosity from entrance pressure are applied to the results of these simulations. The resulting predictions of extensional viscosity are compared to each other, and to the steady extensional viscosity curves predicted by the PTT constitutive model used to generate the simulated pressure drop

curves. These comparisons highlight the advantage of relaxing the power law assumptions for rheological properties used in the analyses, especially at low strain rates.

Influence of Extensional Properties on the Flow Stability of Polymer Melts

Donald G. Baird

The extensional flow behavior of polymer melts may play a significant role in their flow stability. First, we look at the extrusion behavior of three LLDPE's of narrow MWD ($M_w/M_n = 2.2$), two of which contain long chain branching of various degrees (e.g. 1 branch per 5 chains) and one which contains no long chain branching (LLDPE-UB). The two branched samples (LLDPE-B) have identical steady and dynamic oscillatory shear flow properties, but different degrees of extensional strain hardening. The LLDPE-UB sample exhibits no extensional strain hardening and slightly different shear properties. The onset of surface (i.e. sharkskin) and slip-stick fractures occur at higher shear rates and stresses for the branched samples. However, as the flow rate is increased the linear samples become smooth and devoid of any signs of fracture whereas the branched samples exhibit gross fracture reminiscent of highly branched LDPE. Flow birefringence was used to investigate the entry flow behavior of the materials. The effects of the strain hardening extensional behavior were evident on these patterns and consistent with the onset of an entry flow instability. Second, the film blowing stability of two polyethylene samples with and without long chain branching was also investigated. It was found that the PE with significant strain hardening was not subject to the instabilities observed for LLDPE (i.e. no long chain branching). The nature of the instabilities observed here involves the oscillation of the bubble at a critical draw-down ratio. The branched PE did not exhibit bubble oscillations but would only undergo cohesive failure when a critical draw-down ratio was reached. Although viscoelastic relaxation times are important, they do not account for the instabilities recorded here, which are apparently related to the extensional strain hardening.

Modeling Viscoelastic Drop Deformations in Start-Up Uniaxial Extension and Simple Shear Flows

Russell Hooper, Jeffrey Derby and Christopher Macosko

In this study, we seek to extend the current understanding of morphology development during processing of polymer blends by rigorously modeling via FEM the response of a single drop suspended in another immiscible fluid subjected to an ideal start-up flow. Both uniaxial extension and simple shear flows are considered since processing flows involve some combination of both and often are dominated by one or the other. The primary contribution of this work is a detailed numerical assessment of the effects on drop deformation of viscoelasticity in one or both fluid phases.

For start-up uniaxial extensional flow, viscoelasticity is implemented by using the Oldroyd-

B constitutive with a single relaxation time. This along with conservation of mass and momentum are solved fully coupled using the DEVSS-G FEM and implicit time integration. Both subcritical and supercritical flow strengths (Capillary numbers) are considered so that deformation rates as well as steady state deformations can be compared. As will be discussed in detail, viscoelasticity in the drop allows faster initial deformation rates but less steady state deformations (drop strains) relative to Newtonian drops of the same viscosity. Viscoelasticity in the suspending fluid produces more sluggish transients, but greater drop strains are predicted due to a squeezing effect associated with first normal stresses. In addition to drop deformation, the retraction of extended drops back to spherical shape once the externally imposed flow is removed is modeled. Deviations from Newtonian behavior are again observed when viscoelasticity is present. Viscoelastic drops are found to retract faster due to the release of stored elastic energy. When the matrix is made viscoelastic, a distinction must be made between constrained retraction in which the total sample length remains fixed and unconstrained retraction in which the sample ends are free to move. For the former, release of stored elastic energy can overcome interfacial tension and produce additional drop strain. In the latter, the released energy serves to decrease the total sample length. These are in contrast to retraction in Newtonian systems which exhibit a monotonic decrease in drop strain driven by interfacial tension and constant total sample length regardless of whether the retraction is constrained or unconstrained.

As opposed to the axisymmetry of uniaxial extension, simple shear flow is fully three-dimensional. Incorporating viscoelasticity is a work in progress. Currently, a pressure stabilized Galerkin FEM is applied which allows velocities, pressures and displacements to be approximated using the same set of basis functions. Results are presented for flows dominated by hydrodynamic forces in which interfacial tension plays a negligible role. First, FEM results for Newtonian systems are compared to those obtained by other methods, e.g. boundary element methods, to establish the credibility of the method. Then preliminary results for viscoelastic fluids treated using the second order fluid constitutive relation are presented. This allows the first order effects of viscoelasticity from both first and second normal stresses to be investigated.

Spectral Calculations of Time-Dependent Viscoelastic Flows

C.G. Dimitropoulos and A.N. Beris

In this work we will present the most recent advances related to the application of spectral simulations to time-dependent viscoelastic flows. In particular, we will examine the most recent developments in the simulation of turbulent viscoelastic flow in a channel and the investigations on time-dependent instabilities in a wavy channel.

Our previous work in direct numerical simulations of turbulent channel viscoelastic flow, has already shown the extensional viscosity as the most important rheological property controlling drag reduction. In this presentation, we will focus on the convergence characteristics of the spectral method and the role of artificial (numerical) viscosity.

For the investigation of 2d and 3d time-dependent viscoelastic flow in a wavy channel,

a pseudo-conformal mapping is utilized together with an efficient Poisson and Helmholtz solver based on a Preconditioned, Biconjugate Gradient method. The performance of the method is discussed, along with illustrative results, for a variety of constitutive models involving the FENE-P and the Giesekus.

Saturday Morning: Mathematical and Theoretical Models

A Posteriori Error Estimates for Spectral Element Solutions to Viscoelastic Flow Problems

Cédric Chauvière Robert G. Owens

The present work is an extension of earlier results of Owens [1] and is an attempt to provide some theoretical undergirding to the question of appropriate error estimators for numerical solutions to viscoelastic flow problems. The first result is a demonstration, that for numerical simulations of flows of a slightly elastic UCM or Oldroyd B fluid the square of the norm proposed by Warichet and Legat [2,3] for our estimated errors is equivalent to the sum of the squares of norms of the exact error for the velocity, pressure and stress. An improved error estimator is then proposed which takes account of the transmitted error. Acknowledging that the stress errors form the major contribution to our error estimators for sufficiently large Deborah numbers we have devised a method of computing the error estimator on an element-by-element basis. As an illustration of the use of our error estimators we proceed to describe an adaptive spectral element method for flow of UCM and Oldroyd B fluids past a sphere in a tube. Numerical results are presented to show how the approximate error and the ‘exact’ error obtained by calculating the difference between the numerical solution and a reference calculation decrease with mesh refinement. The results are compared with those in the literature.

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Asymptotic Structure of the Stress Field in Flow Past a Cylinder at High Weissenberg Number in Flow Past a Cylinder

Michael Renardy

We study the flow of an upper convected Maxwell fluid past a cylinder in the limit of high

Weissenberg number. We make the simplifying assumption that the velocity field is given and similar to the Newtonian case (as will be discussed, this assumption is likely to be wrong) and consider the integration of the stress equations. The asymptotic behavior at high Weissenberg number leads to boundary layers along the edge of the cylinder as well as stress concentration in the wake. The stresses in the boundary layer are of order W while the width of the boundary layer is of order W^{-1} . The stresses in the wake are of order W^3 , and the width of the wake is of order W^{-2} . Just outside the boundary layer near the cylinder and wake, there is a region where the stresses are much larger (order W^3 near the cylinder and W^5 near the wake). The origin of these stresses is in the stretching flow near the upstream stagnation point.

Dynamic strong flows: Liapunov exponents and polymer stretch in flows with complex kinematics

Michael D. Graham, Philip A. Stone and John J. Kasab

An issue of longstanding interest in polymer fluid dynamics is the behavior of polymer molecules in flows with complex kinematics, as arise in porous media or turbulence. We address this issue using some general geometric considerations developed in dynamical systems theory. Given a point moving on a trajectory in phase space, the time-averaged rates of stretching and contraction of an infinitesimal volume centered on that point are given by a set of numbers called Liapunov exponents (LE). For a fluid element in incompressible steady flow the sum of these must be zero and except in special cases, one of them must be zero individually. A positive LE indicates that averaged over time, the fluid element stretches without bound exponentially fast. Thus, we can define a “dynamic strong flow” as one in which trajectories have a positive LE. Furthermore, a general criterion for large extension of Hookean dumbbells with relaxation time λ in a flow with maximum LE $\sigma_{\max}$ can be derived: $\lambda\sigma_{\max} > 1/2$. It then follows that steady two-dimensional flow in a porous medium cannot generate unbounded polymer stretch; both LEs are zero, irrespective of the spatial complexity of the flow field.

The “ABC” flow is a spatially periodic steady 3D velocity field that exactly solves the Euler equations. It generates chaotic fluid trajectories and correspondingly has a positive LE. Computations with (passive) FENE-P dumbbells illustrate the large stretch and energy dissipation of dumbbells that follow the chaotic trajectories. This result allows us to sharpen the notion of Shaqfeh, Koch and coworkers that only stochastic velocity fields can generate strong stretching – here the “stochastic” nature of the flow is only revealed in a Lagrangian point of view: the Eulerian velocity field is steady and spatially periodic. Analogous results are found for another steady 3D periodic flow field, put forward by Waleffe (1995) as a model for the streaky structure of transitional and turbulent shear flow.

Finally, we present a stochastic toy model of the Lagrangian evolution of fluid elements in a steady flow. This model captures the required absence of exponential stretch in 2D, although large transient extensions may arise. Preliminary results imply that in 3D, exponential stretch is universal. In light of these results, it appears that the large stretching observed in polymer flows through porous media is a generic consequence of the chaotic kinematics of three-dimensional incompressible velocity fields.

Rheology and Morphology of Concentrated Rubber Suspensions in Polymer Melts

S-Y. Kang and K. Jayaraman

The relative shear viscosity of concentrated suspensions of elastic rubber particles in both Newtonian and non-Newtonian suspending fluids has been evaluated with different representative microstructure obtained from the morphology observed with different suspending fluids. The rheology of these suspensions with negligible Brownian forces as well as negligible electrostatic charge effects, have been described in terms of lubrication forces. The predicted trends in relative viscosity are compared to observed trends in relative viscosity for these suspensions.

Modeling of Viscoelastic Material Behavior for Process Simulation

A. Pomp and S. Zelenka

In modern VLSI technology thermal grown SiO₂ is used as a high-value insulator between electronic devices. While at low process temperatures this oxide behaves nearly like an elastic solid, it behaves at temperatures above about 1000 degC like a purely viscous fluid. For intermediate temperatures a viscoelastic behavior can be observed. Experiments have shown that shear stresses relax to zero (as faster as higher the temperature) and that the oxide is compressible. The simplest (and widely accepted) possibility for the simulation is to take Maxwell's model of viscoelasticity for the deviatoric part and a linear elastic model for the dilatational part. Experiments also have shown that the viscosity depends on the actual shear stress in the material, which leads to a nonlinear model. We have adopted this model in our process simulator

The driving force for the motion of the oxide during the oxidation process is the volume production at the silicon/oxide interface. Oxidants, normally H₂O or O₂, diffuse through the existing oxide and react at the interface with the silicon to new oxide. Dependent on the concentration of these oxidants at the interface, a certain amount of silicon per time is converted into oxide. This conversion process is accompanied by a volume production of 125layer system. The diffusion of the oxidants and the reaction at the interface are affected on there part by the mechanical stresses, i.e the diffusivity is decreased by by increasing pressure and the reaction rate depends on the normal stresses at the interface. That means, to simulate an oxidation process in an accurate way one has to take this coupling between diffusion and mechanical problem into account.

The problem is solved within our 2D process simulator as follows: For one time step the oxidant diffusion is solved in the existing oxide region with present stress distribution. From this solution one obtains the concentration of the oxidants at the silicon/oxide interface. From the concentration and the normal stresses one can calculate via the reaction rate the velocities of the oxide into the oxide region at the interface. These velocities serve as boundary condition for the mechanical problem. The non-linear constitutive equation is solved elementwise on triangular

elements with linear shape functions. As global equilibrium condition, vanishing divergence of the stress tensor is required. The divergence is transformed into a surface integral which is solved via finite box method on a Delaunay grid. Once the mechanical problem is solved, the new stresses serve as input for the next diffusion time step. For other materials used in VLSI technology like Si₃N₄ there is controverse discussion about the mechanical behavior. Within our simulator every material can be treated over the whole range from purely elastic to purely viscous. The 3D version of this simulator is already under development. We like to present simulation results of some typical oxidation processes used in manufacturing of semiconductor devices. Also the underlying theory of the simulation will be discussed.

List of Participants

Dr. Marios Avgousti
Polymers Research and Development
Union Carbide Corporation
Weston Canal Center
P.O. Box 450
Somerset, NJ 08875
USA
email: amxapo1@peabody.sct.ucarb.com

Prof. Frank P.T. Baaijens
Materials Technology, Department of Mechanical
Engineering
Eindhoven University of Technology
P.O. Box 513, 5600 MB Eindhoven
The Netherlands
email: baaijens@wfw.wtb.tue.nl

Dr. Patrick D. Anderson
Materials Technology Department of Mechanical
Engineering
Eindhoven University of Technology
P.O. Box 513, 5600 MB Eindhoven
The Netherlands
email: patricka@wfw.wtb.tue.nl

Prof. Donald G. Baird
Department of Chemical Engineering
Virginia Tech.
Blacksburg, VA 24061-0123
USA
email: baird@vt.edu

Prof. Antony N. Beris
Department of Chemical Engineering
University of Delaware
Newark DE 19716
USA
email: beris@zeus.che.udel.edu

Prof. Barry Bernstein
Department of Mathematics
Illinois Institute of Technology
108 Wishnick Hall, Chicago IL 60616
USA
email: barry@cepssc.che.iit.edu

Prof. Richard J. Braun
Department of Mathematical Sciences
University of Delaware
Newark DE 19716
USA
email: braun@math.udel.edu

Prof. Robert A. Brown
Department of Chemical Engineering
M.I.T.
Cambridge, MA 02139
USA
email: rab@mit.edu

Prof. Wesley R. Burghardt
Department of Chemical Engineering
Northwestern University
Evanston, IL
USA
email: w-burghardt@nwu.edu

Dr. Jeffrey A. Byars
Department of Chemical Engineering
University of Melbourne
Parkville Victoria 3052
Australia
email: jeff_byars.chem_eng@muwaye.unimelb.edu.au

Dr. Kostas Christodoulou
Avery-Dennison Research Center
2900 Bradley Street
Pasadena, CA 91107-1599
USA
email:
christodoulouKostas@email.averydennison.com

Prof. A. Russell Davies
Department of Mathematics
University of Wales
Aberystwyth SY23 3BZ
UK
email: ard@aber.ac.uk

Mr. Costas D. Dimitropoulos
Department of Chemical Engineering
University of Delaware
Newark DE 19716
USA
email: costas@zeus.che.udel.edu

Dr. Marc I. Gerritsma
Department of Mathematics
University of Wales
Aberystwyth, Dyfed SY23 3BZ
UK
email: mig@aber.ac.uk

Prof. Michael D. Graham
Department of Chemical Engineering and Rheology Research Center
University of Wisconsin-Madison
Madison, WI 53706-1691
USA
email: graham@coefac.engr.wisc.edu

Mr. Pierre Halin
CESAME (Center for Systems Engineering and Applied Mechanics)
Université catholique de Louvain
Batiment Euler
Av. Georges Lemaitre, 4
B-1348 Louvain-la-Neuve
Belgium

Prof. O.G. Harlen
Department of Applied Mathematical Studies
University of Leeds
Leeds LS2 9JT
UK
email: oliver@amsta.leeds.ac.uk

Dr. A.P.G. van Heel
Laboratory for Aero and Hydrodynamics
Delft University of Technology
Rotterdamseweg 145, 2628 AL Delft
The Netherlands
email: tonh@dutw1500.wbmt.tudelft.nl

Prof. Martien A. Hulsen
Laboratory for Aero and Hydrodynamics
Delft University of Technology
Rotterdamseweg 145, 2628 AL Delft
The Netherlands
email: m.a.hulsen@wbmt.tudelft.nl

Ms. Ingrid Jaumain
CESAME (Center for Systems Engineering and Applied Mechanics)
Université catholique de Louvain
Batiment Euler
Av. Georges Lemaitre, 4
B-1348 Louvain-la-Neuve
Belgium

Prof. K. Jayaraman
Department of Chemical Engineering
Michigan State University
East Lansing MI
USA
email: jayarama@che.udel.edu

Prof. R. Keunings
CESAME (Center for Systems Engineering and
Applied Mechanics)
Université catholique de Louvain
Batiment Euler
Av. Georges Lemaitre, 4
B-1348 Louvain-la-Neuve
Belgium
email: rk@mema.ucl.ac.be

Prof. Bamin Khomami
Department of Chemical Engineering
Washington University
Saint Louis, MO 63130-4899
USA
email: bam@wuche2.wustl.edu

Prof. Bob W. Kolkka
Dept. of Math Sci.
Mich. Tech. Univ.
Houghton, Mich. 49931
USA
email: rwkolkka@mtu.edu

Mr. Jaydeep A. Kulkarni
Department of Chemical Engineering
University of Delaware
Newark DE 19716
USA
email: jaydeep@zeus.che.udel.edu

Dr. Raz Kupferman
Department of Applied Mathematics
Lawrence Berkeley Laboratory
Mail-Stop 50A-2152
1 Cyclotron Road
Berkeley CA 94720
USA
email: raz@mekong.lbl.gov

Dr. Vincent Legat
CESAME (Center for Systems Engineering and
Applied Mechanics)
Université catholique de Louvain
Batiment Euler
6 Av. Georges Lemaitre
B-1348 Louvain-la-Neuve
Belgium
email: vl@mema.ucl.ac.be

Mr. Gregory Lielens
CESAME (Center for Systems Engineering and
Applied Mechanics)
Université catholique de Louvain
Batiment Euler
Av. Georges Lemaitre, 4
B-1348 Louvain-la-Neuve
Belgium

Prof. Arkady I. Leonov
Department of Polymer Engineering
The University of Akron
Akron, OH 44325-0301
USA
email: leonov@uakron.edu

Prof. Gareth H. McKinley
Division of Engineering and Applied Sciences
Harvard University
Cambridge, MA 02138
USA
email: gareth@stokes.harvard.edu

Prof. Gilmar Mompean
EPFL-DGM
Swiss Federal Institute of Technology
CH1015 Lausanne
Switzerland
email: mompean@imhfh28.epfl.ch

Ms. Radha Nayak
Department of Chemical Engineering
M.I.T.
Cambridge, MA 02139
USA
email: rnayak@mit.edu

Prof. R.G. Owens
Department of Mathematics
Napier University
219 Colinton Road
Edinburgh EH14 1DJ
SCOTLAND, UK
email: rgo@maths.napier.ac.uk

Prof. Timothy N. Phillips
Department of Mathematics
University of Wales
Aberystwyth, Dyfed SY23 3BZ
UK
email: tnp@aber.ac.uk

Dr. Dilip Rajagopalan
E.I. duPont and Company
Central Research and Development
Experimental Station, E304/A230
Wilmington DE 19880
USA
Email: rajagod@rajagod.es.dupont.com

Prof. Michael Renardy
Department of Mathematics
Virginia Tech.
Blacksburg, VA 24061-0123
USA
email: renardym@math.vt.edu

Dr. G.W. Roberts
School of Mathematics
University of Wales
Dean Street
Bangor
Gwynedd LL55 1UT
UK
email: g.w.roberts@bangor.ac.uk

Dr. Todd R. Salamon
Bell Laboratories, Lucent Technologies
Room 7D-212
600 Mountain Avenue
Murray Hill, NJ 07974-0636
USA
email: tsalamon@bell-labs.com

Prof. Jay D. Schieber
Department of Chemical Engineering
Illinois Institute of Technology
Chicago IL 60616
email: cheschieber@iit.edu

Prof. Gilberto Schleinig
Department of Mathematical Sciences
University of Delaware
Newark DE 19716
USA
email: schleini@euler.math.udel.edu

Mr. R. Sizaire
CESAME (Center for Systems Engineering and
Applied Mechanics)
Université catholique de Louvain
Batiment Euler
6 Av. Georges Lemaitre
B-1348 Louvain-la-Neuve
Belgium

Mr. Mark D. Smith
Department of Chemical Engineering
M.I.T.
Cambridge, MA 02139
USA
email: mdsmith@wiggles.mit.edu

Mr. Junsuo Sun
Department of Chemical Engineering
M.I.T.
Cambridge, MA 02139
USA
email: junsuo@mit.edu

Dr. R. Sureshkumar
Department of Chemical Engineering
M.I.T.
Cambridge, MA 02139
USA
email: sureshk@mit.edu

Dr. J. T. Twu
Union Carbide Corporation
1 River Road
P. O. Box 670
Bound Brook, NJ 07920
USA
email: ajttp01@peabody.sct.ucarb.com

Mr. Jose Valenciano
Department of Mathematics
Napier University
219 Colinton Road
Edinburgh EH14 1DJ
SCOTLAND, UK
email: josev@maths.napier.ac.uk

Prof. John M. Wiest
Department of Chemical Engineering
University of Alabama
Tuscaloosa, AL 35487-0203
USA
email: jwiest@coe.eng.ua.edu

Mr. Bin Yang
Department of Chemical Engineering and the Ma-
terials Research Lab.
Washington University
Saint Louis, MO 63130
USA