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A high-resolution finite-difference method for simulating two-fluid, viscoelastic gel dynamics

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ABSTRACT

An important class of gels are those composed of a polymer network and fluid solvent. The mechanical and rheological properties of these two-fluid gels can change dramatically in response to temperature, stress, and chemical stimulus. Because of their adaptivity, these gels are important in many biological systems, e.g. gels make up the cytoplasm of cells and the mucus in the respiratory and digestive systems, and they are involved in the formation of blood clots. In this study we consider a mathematical model for gels that treats the network phase as a viscoelastic fluid with spatially and temporally varying material parameters and treats the solvent phase as a viscous Newtonian fluid. The dynamics are governed by a coupled system of time-dependent partial differential equations which consist of transport equations for the two phases, constitutive equations for the viscoelastic stresses, two coupled momentum equations for the velocity fields of the two fluids, and a volume-averaged incompressibility constraint. We present a numerical method based on a staggered grid, second order finite-difference discretization of the momentum equations and a high-resolution unsplit Godunov method for the transport equations. The momentum and incompressibility equations are solved in a coupled manner with the Generalized Minimum Residual (GMRES) method using a multigrid preconditioner based on box-relaxation. We present results on the accuracy and robustness of the method together with an illustration of the interesting behavior of this gel model for the four-roll mill problem.

1. Introduction

An important class of gels are those composed of a polymer network immersed in a solvent. Because of their multiphase and multiscale nature, such gels exhibit a number of unique behaviors. In addition to stress due to deformations, these gels may exhibit osmotic and active stresses. Osmotic stress, or swelling stress, results from interactions between the solvent and polymer molecules. Active stresses arise in some biological gels, such as actomyosin, which are crosslinked with molecular motors that convert chemical energy into mechanical work. Additionally, when the polymer network is undergoing polymerization and depolymerization, the rheology of the mixture can be highly variable. In many biological gels such as biofilms, blood clots, mucus, and cytoplasm, polymerization/depolymerization and active/osmotic stresses are regulated as part of their biological function. An essential component in the study of these complex processes is good numerical methods to solve the equations that describe their mechanics.

In many instances, a gel is not adequately described as a single continuous medium. For example, during gel swelling the network moves outward while the solvent moves inward. Modeling the mechanics of gels requires a description beyond a single velocity field and single stress tensor. The two-fluid model is a widely used approach to describe gel mechanics [1,2]. In this model, both network and solvent coexist at each point of space, and each phase (network and solvent) is modeled as a continuum with its own velocity field and constitutive law. The coupled system of partial differential equations that describe the gel presents significant challenges both for analysis and for numerical simulation, and is therefore not well studied. Among the challenges posed by a gel model of this type are the need to determine two velocity fields and a pressure coupled through the two momentum equations and the incompressibility constraint. Another arises if the gel is not homogeneous in which case gel properties, including its elastic modulus, may vary spatially and temporally.

The appropriate rheological description of the network phase depends on the type of gel as well as the time scale of the problem. Gels with permanent crosslinks are usually described as elastic solids. If the crosslinks form and break dynamically, then the network is better described as a viscoelastic fluid or even as a viscous fluid,

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depending on the relative time scales of the deformation and the crosslinking. A model which captures all of these behaviors is the transient network model [3,4], which in its simplest form is like rubber elasticity with formation and rupture of crosslinks. In the limit that the rupture rate goes to zero, the material becomes a neo-Hookean elastic solid, and in the limit of very fast formation and breaking, the material becomes a viscous fluid. Because of its ability to describe such diverse materials behaviors, this is the type of model we consider in this paper. For other types of models of the dynamics of viscoelastic gels see, for example, [5–7] and the references therein.

When the polymer concentration is uniform, and the formation and rupture of crosslinks is in equilibrium, the equation for the stress tensor is equivalent to the upper convected Maxwell equation. We include an additional viscosity within the network, which makes the network an Oldroyd-B fluid. In this paper, we use a version of the model in which polymer concentration is variable, and the kinetics of link formation are not taken to be in equilibrium. This adds an extra equation for the link density. The elastic modulus of the network is proportional to the link density and so it too evolves in time [8].

Previously we developed algorithms for simulating the equations of gel mechanics using the two-fluid model in which the network and solvent were modeled as viscous fluids without inertia [9–11]. In this paper we extend this work to the case when the network is modeled as an Oldroyd-B fluid and inertia has an effect. The inertia of the fluid can play an important role in applications where the gel is in contact with a rapidly moving Newtonian fluid [12]. We use a conservative, high-resolution unsplit Godunov method on a staggered grid for treating the scalar equations describing the transport of the network and solvent volume fractions. We extend this method to handle the tensor equations for the viscoelastic stresses and elastic modulus. There are similarities of this method with previously developed techniques for treating single-phase viscoelastic fluids [8,13,14]. We use a second order finite-difference discretization of the momentum and incompressibility equations and adapt our iterative method from [9] to handle nonzero Reynolds number flows. This iterative method uses a Krylov subspace method together with a multigrid preconditioner for solving this coupled set of equations without splitting. We find that the adapted method is efficient and robust.

We present numerical experiments showing that our computational technique achieves second order accuracy in space and time for smooth solutions and is stable provided an appropriate CFL-type condition is satisfied. The experiments also show that our method can handle sharp material interfaces without problems, and that it is robust over a wide range of parameters, from cases where the gel behaves like a viscoelastic fluid to others in which it behaves like a viscoelastic solid.

The remainder of the paper is organized as follows. In Section 2 we give a brief introduction to the two-fluid, viscoelastic gel model. In Section 3, we describe the computational method for simulating the gel model. In Section 4, we present several numerical examples including refinement studies illustrating the accuracy of the method and results from simulations involving strongly elastic materials and sharp interfaces between material parameters. In these numerical examples the flow is driven by a background force corresponding to the four-roll mill problem. We conclude the paper with some remarks in Section 5 on future enhancements to the model and computational method that will be considered.

2. Gel model

Our intention in this section is to give a brief introduction to the gel model considered in the present study. A more thorough derivation and discussion of this model and more general gel models can be found in the recent reviews [1,2] and the references therein.

We consider a gel composed of two materials, a polymer network and a fluid solvent. Each point in space is assumed to be occupied by a mixture of network and solvent, which is described by the volume fractions of the two different phases. Each material moves with its own velocity and the total amount of gel is assumed to remain constant. For the model considered in this study, the densities of the two materials are equal and set to a constant value, i.e. the networked material is neutrally buoyant. With these assumptions, conservation of mass leads to the following two equations for the volume fractions:

$$(\theta_{\mathrm{s}})_t + \nabla\cdot(\mathbf{u}_{\mathrm{s}}\theta_{\mathrm{s}}) = 0 \tag{1}$$

$$(\theta_{\mathrm{n}})_t + \nabla\cdot(\mathbf{u}_{\mathrm{n}}\theta_{\mathrm{n}}) = 0 \tag{2}$$

where θ_{n}, and $\theta_{\mathrm{s}} = 1-\theta_{\mathrm{n}}$ are the respective volume fractions of the network and solvent, and $\mathbf{u}_{\mathrm{s}}$ and $\mathbf{u}_{\mathrm{n}}$ are the respective transport velocities. Adding Eqs. (1) and (2) and using $\theta_{\mathrm{s}}+\theta_{\mathrm{n}} = 1$ reveals that the volume averaged velocity is incompressible:

$$\nabla\cdot(\theta_{\mathrm{s}}\mathbf{u}_{\mathrm{s}} + \theta_{\mathrm{n}}\mathbf{u}_{\mathrm{n}}) = 0. \tag{3}$$

The transport velocities are determined by Newton's second law, which in this case are described by the solvent and network momentum equations

$$\begin{aligned}\rho\big((\theta_{\mathrm{s}}\mathbf{u}_{\mathrm{s}})_t + \nabla\cdot(\theta_{\mathrm{s}}\mathbf{u}_{\mathrm{s}}\mathbf{u}_{\mathrm{s}})\big) &= -\theta_{\mathrm{s}}\nabla p + \nabla\cdot\left(\theta_{\mathrm{s}}\underline{\underline{\boldsymbol{\sigma}}}^{\mathrm{s,v}}\right)\\ &\quad - \xi\theta_{\mathrm{s}}\theta_{\mathrm{n}}(\mathbf{u}_{\mathrm{s}}-\mathbf{u}_{\mathrm{n}}),\end{aligned} \tag{4}$$

$$\begin{aligned}\rho\big((\theta_{\mathrm{n}}\mathbf{u}_{\mathrm{n}})_t + \nabla\cdot(\theta_{\mathrm{n}}\mathbf{u}_{\mathrm{n}}\mathbf{u}_{\mathrm{n}})\big) &= -\theta_{\mathrm{n}}\nabla p + \nabla\cdot\left(\theta_{\mathrm{n}}\underline{\underline{\boldsymbol{\sigma}}}^{\mathrm{n,v}}\right)\\ &\quad - \xi\theta_{\mathrm{s}}\theta_{\mathrm{n}}(\mathbf{u}_{\mathrm{n}}-\mathbf{u}_{\mathrm{s}}) + \nabla\cdot\left(\theta_{\mathrm{n}}\underline{\underline{\boldsymbol{\tau}}}\right) - \nabla\Psi.\end{aligned} \tag{5}$$

The solvent momentum equation reflects our assumption that the solvent behaves as a Newtonian fluid subject to a viscous force $\nabla\cdot\left(\theta_{\mathrm{s}}\underline{\underline{\boldsymbol{\sigma}}}^{\mathrm{s,v}}\right)$ and a pressure force $\theta_{\mathrm{s}}\nabla p$, and that it is also acted upon by a drag force $\xi\theta_{\mathrm{s}}\theta_{\mathrm{n}}(\mathbf{u}_{\mathrm{n}}-\mathbf{u}_{\mathrm{s}})$ when the solvent and polymer velocities differ. Similarly, the network is subject to viscous, pressure, and drag forces given, respectively, by $\nabla\cdot\left(\theta_{\mathrm{n}}\underline{\underline{\boldsymbol{\sigma}}}^{\mathrm{n,v}}\right)$, $\theta_{\mathrm{n}}\nabla p$, and $\xi\theta_{\mathrm{s}}\theta_{\mathrm{n}}(\mathbf{u}_{\mathrm{s}}-\mathbf{u}_{\mathrm{n}})$, as well as to two additional forces. One is a viscoelastic force $\nabla\cdot\left(\theta_{\mathrm{n}}\underline{\underline{\boldsymbol{\tau}}}\right)$ due to deformation and restructuring of the network, and the other is a chemical pressure (or osmotic pressure) force $\nabla\Psi$ arising from chemical interactions due to the presence of the network. In these equations, ρ is the density of the two fluids and ξ is the drag coefficient.

The viscous stresses for both materials are the standard ones for a Newtonian fluid

$$\underline{\underline{\boldsymbol{\sigma}}}^{\mathrm{s,v}} = \mu_{\mathrm{s}}\big(\nabla\mathbf{u}_{\mathrm{s}} + \nabla\mathbf{u}_{\mathrm{s}}^{\mathrm{T}}\big) + (\lambda_{\mathrm{s}}\nabla\cdot\mathbf{u}_{\mathrm{s}})\underline{\underline{\boldsymbol{\delta}}} \tag{6}$$

$$\underline{\underline{\boldsymbol{\sigma}}}^{\mathrm{n,v}} = \mu_{\mathrm{n}}\big(\nabla\mathbf{u}_{\mathrm{n}} + \nabla\mathbf{u}_{\mathrm{n}}^{\mathrm{T}}\big) + (\lambda_{\mathrm{n}}\nabla\cdot\mathbf{u}_{\mathrm{n}})\underline{\underline{\boldsymbol{\delta}}} \tag{7}$$

where $\mu_{\mathrm{s,n}}$ are the shear viscosities and $\lambda_{\mathrm{s,n}} + 2\mu_{\mathrm{s,n}}/d$ are the bulk viscosities of the solvent and network (d is the spatial dimension). For this paper we assume that the chemical pressure is that used in Flory–Huggins polymer theory [15, p. 143]

$$\Psi(\theta_{\mathrm{n}}) = \psi_0(n_1\log(\theta_{\mathrm{n}}) - n_2\log(1-\theta_{\mathrm{n}}) + \chi(1-2\theta_{\mathrm{n}})), \tag{8}$$

where $\psi_0 > 0$, n_1, n_2, and χ are constants. The constant χ affects the amount of mixing of polymer and solvent. In this study, we set $n_1 = n_2 = 1$ and $\chi = 2$. With this choice of parameters, the chemical pressure favors some mixing and penalizes full phase separation of the gel.