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Three-Phase Model of Visco-Elastic Incompressible Fluid Flow and its Computational Implementation

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Abstract. Energetic Variational Approach is used to derive a novel thermodynamically consistent three-phase model of a mixture of Newtonian and visco-elastic fluids. The model which automatically satisfies the energy dissipation law and is Galilean invariant, consists of coupled Navier-Stokes and Cahn-Hilliard equations. Modified General Navier Boundary Condition with fluid elasticity taken into account is also introduced for using the model to study moving contact line problems. Energy stable numerical scheme is developed to solve system of model equations efficiently. Convergence of the numerical scheme is verified by simulating a droplet sliding on an inclined plane under gravity. The model can be applied for studying various biological or biophysical problems. Predictive abilities of the model are demonstrated by simulating deformation of venous blood clots with different visco-elastic properties and experimentally observed internal structures under different biologically relevant shear blood flow conditions.

AMS subject classifications: 92C05, 92C10, 65M12, 35Q35, 35Q92

Key words: Phase field method, Energetic Variational Approach, multi-phase flow, visco-elasticity, variable density, slip boundary condition, deformation of blood clot, thrombus.

1 Introduction

Phase field models [3, 5, 19, 28, 29, 40, 44, 46, 84, 86, 87] derived using the energy-based variational formulation, are widely used for studying multi-phase fluid flow problems. Labeling function or phase function is used in a phase field model to represent each of the phases. The sharp interface separating different species is replaced by narrow transition layer in which species mix. Free energy density functional of the labeling functions is

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constructed for coupling different phases. (See, among others, [3, 41, 47] for reviews of phase field approach.) A careless design of the free energy density functional may lead to meta stable states [11]. For instance, traditional pairwise combinations of double-well free energy functionals for coupling multiple fluid components may give rise to non-physical results, such as growth of one phase due to the presence of saddle points inside the Gibbs triangle [88].

Additional problems with deriving a phase field model arise when some fluid components are non-Newtonian. Many existing non-Newtonian flow phase field models [2, 7, 10] do not satisfy the energy dissipation law. This implies that numerical schemes designed for solving system of equations of these models likely do not to satisfy the discrete energy dissipation law either, and can result in large numerical errors [50]. These numerical errors significantly undermine accuracy of numerical model solutions over long time periods.

While most of the existing models [1, 3, 5, 17, 18, 37, 47, 52, 86, 89] focus on two-phase or Newtonian fluids, many biological and biophysical applications require multi-phase or non-Newtonian fluid flow models. There are only few existing three (or more)-phase field models [20, 45, 46, 79]. In particular, Wu and Xu [79] established the unisolvent property of coefficient matrix involved in N-phase models based on pairwise surface tensions. By using obtained matrix, authors derived an N-phase inherently invariant Cahn-Hilliard model from the free energy functional. Important properties of Wu and Xu models are that the dynamics of concentrations are independent of the choice of phase variable, and the symmetric positive-definite property of the coefficient matrix can be proved equivalent to some physical condition for pairwise surface tensions. Among other multi-phase models, the model in [45] does not include components representing hydrodynamics, and models in [20, 46, 79] describe only Newtonian fluids. We use the Energy Variational Approach (EnVarA) [21, 83] to derive in this paper a novel thermodynamically consistent phase field model of three-phase incompressible fluid system with visco-elastic fluid components. Main novel modeling and numerical contributions of the paper in comparison with existing models, are as follows.

- A systematic approach is introduced to derive phase field model coupling Newtonian and Non-Newtonian fluids with large variations in densities or viscosities of individual fluid components. The Boussinesq approximation under the assumption that density ratio between two fluids is relatively small [50, 51] is not needed in our model. Components of the fluid mixture are combined in a binary tree manner [12, 73]. The feasibility of this approach is demonstrated by deriving a three-phase fluid flow model, in which two of the fluid components are visco-elastic. The resulting model can be reduced in a physically consistent manner to the two-phase model [51].

- The derived model is Galilean invariant and automatically satisfies the energy dissipation law resulting in straightforward development of an efficient and energy stable numerical scheme. All model equations are described in the Eulerian coordi-