Non-Newtonian Fluid Mechanics Using Molecular Theory

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Many natural and synthetic fluids are viscoelastic materials, in the sense that the stress endured by a macroscopic fluid element depends upon the history of the deformation experienced by that element. Notable examples include polymer solutions and melts, liquid crystalline polymers, and fibre suspensions. The remarkable rheological properties of viscoelastic liquids cannot be described by the Navier-Stokes equations, but rather are governed by the flow-induced evolution of molecular configurations [1].

Models of kinetic theory provide a coarse-grained description of molecular configurations wherein atomistic processes are ignored altogether [2]. They are meant to display in a more or less accurate fashion the important features that govern the flow-induced evolution of configurations. In recent years, kinetic theory of entangled systems, such as concentrated polymer solutions and polymer melts, has known major developments that go well beyond the classical reptation tube model developed by Edwards, de Gennes, and Doi [3]. In addition to reptation, other physical mechanisms such as convective constraint release, contour length fluctuations, and tube stretch, have been shown to play an important role. The most recent tube models take account of these effects and correct many of the deficiencies of the basic theory (for a review, see [4]).

Kinetic theory models can be very complicated mathematical objects. It is usually not easy to compute their rheological response in rheometrical flows (although these flows have simple, specified kinematics), and their use in numerical simulations of complex flows has long been thought impossible. The traditional approach has been to derive from a particular kinetic theory model a macroscopic constitutive equation that relates the viscoelastic stress to the deformation history. One then solves the constitutive model together with the conservation laws using a suitable numerical method, to predict velocity and stress fields in complex flows. The majority of constitutive equations used in continuum numerical simulations are indeed derived (or at least very much inspired) from kinetic theory. Their use in numerical simulations of complex flows is reviewed in [5-6]. Clearly, the continuum approach remains an essential component of theoretical and computational rheology. There is however a basic issue in the above scheme which motivates the development of the complementary micro-macro approach.

Indeed, derivation of a constitutive equation from a model of kinetic theory usually involves closure approximations of a purely mathematical nature, such as decoupling or pre-averaging. It is now widely accepted that closure approximations can have a significant impact. Thus, micro-macro methods of computational rheology that couple the coarse-grained molecular scale of kinetic theory to the macroscopic scale of continuum mechanics have an important role to play. In a micro-macro simulation, the conservation equations are solved together with a model of kinetic theory. This approach is much more demanding in computer resources than more conventional continuum simulations that integrate a constitutive equation to evaluate the viscoelastic contribution to the stress tensor. On the other hand, micro-macro techniques allow the direct use of kinetic theory models and thus avoid potentially harmful closure approximations. Micro-macro methods have been reviewed recently in [7].

In the present lecture, I survey the field of multiscale simulation of viscoelastic flow using molecular models, and present recent results based on tube theory of linear entangled polymers [8-11]. The talk will be of a general nature so that it is (hopefully) both understandable and useful for colleagues and students working on other topics in theoretical and applied mechanics.

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