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ADVANCES IN THE COMPUTER MODELING OF THE FLOW OF POLYMERIC LIQUIDS[1]

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Abstract

We review recent developments in the field of computational rheology applied to the prediction of the flow of polymeric liquids in complex geometries. After a brief discussion of the challenging rheological behaviour of polymers, we outline the hierarchy of available modeling approaches and point to important recent progress there. The two current avenues towards complex flow simulation are then visited, namely the macroscopic and micro-macro approaches. Throughout the paper, we refer to review and research publications that are representative of current trends in the field.

1 Introduction

To most researchers engaged in Computational Fluid Dynamics, the low-Reynolds number flow of a highly viscous Newtonian fluid would not be considered as a challenging research topic. But add even a minute amount of macromolecules into the fluid, thus producing a *polymer solution*, and the situation is altered drastically: the rheological (i.e. flow) behaviour of the material becomes highly non-Newtonian, resulting in intricate flow phenomena whose prediction requires sophisticated modeling approaches and numerical tools. In this paper, we give a very brief overview of the field of *computational rheology* applied to polymeric liquids. What we mean by computational rheology is the development and use of numerical simulation methods for the analysis of the flow of rheologically-complex fluids in geometries that are relevant to either laboratory or processing work.

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What makes computational rheology such a fascinating research field is its important coupling with experimental and modeling work. Indeed, history shows that progress in one area of rheology has often been supported by the insight provided by the other two [1]. In this short paper, we wish to guide the newcomer to the vast rheology literature. This we do by pointing to introductory textbooks, research monographs, and review publications. We also cite recent research papers that are representative of current progress in rheology. Needless to say, many more references to important work can be found there.

2 Rheological behaviour of polymeric liquids

Polymeric fluids exhibit a variety of non-Newtonian rheological properties [2, 3]. The shear viscosity of these materials is often a non-linear function of the rate of shear. This property alone can easily be taken into account in a phenomenological way, yielding equations of motion that have the form of generalized Navier-Stokes equations and which can be solved numerically by means of methods very similar to those developed for Newtonian liquids [4]. The situation is of course drastically different with the other facets of non-Newtonian behaviour, such as the presence of normal stresses in shear flows, a significant resistance to elongational deformation, and memory effects which manifest themselves in many ways (e.g. stress relaxation and recoil). Indeed, polymeric liquids are *viscoelastic* materials in the sense that the stress experienced by a fluid particle depends upon the *history* of the deformation experienced by that particle. The elastic character of a given flow is measured by the dimensionless Weissenberg number $We = \lambda\dot{\gamma}$, where λ is a characteristic relaxation time of the fluid, and $\dot{\gamma}$ is a characteristic shear rate of the flow. While $We = 0$ for Newtonian fluids, it is of order 1 or 10 in many applications involving polymeric liquids.

Non-Newtonian rheological properties are responsible for a variety of flow phenomena that are unseen with Newtonian liquids and which cannot at all be predicted by the Navier-Stokes equations [5]. For example, large elongational stresses [6-8] have a dramatic impact on vortex structures and pressure drops in creeping flows through abrupt contractions/expansions [9, 10], as well as in industrially important processes such as atomisation [11, 12]. Hydrodynamic instabilities of a purely elastic nature :q are also observed in a variety of flow situations; these occur at very low Reynolds numbers (of-

ten zero for all practical purposes), where the corresponding Newtonian flow would be stable [13-15]. Of particular importance to the polymer processing industry is the issue of extrusion instabilities [16]. Indeed, a polymer melt extruded at low speed will show a smooth extrudate free surface. At progressively higher speeds, though, a series of surface instability modes sets in, leading eventually to gross distortions of the extrudate (melt fracture). The nature of the interactions between the flowing polymer and the die wall appears critical here [17, 18]. All the above flow phenomena (as well as many others) are observed at very low Reynolds numbers. Viscoelastic effects can be important in the turbulent regime as well, as revealed by the drag-reduction phenomenon in dilute polymer solutions [19].

It should be pointed out that polymeric solutions and melts are only a particular class of materials showing non-Newtonian flow behaviour. Among others we can cite fiber suspensions, emulsions, colloids, liquid crystal polymers, and biological fluids. Generic to non-Newtonian fluids is the role of their internal *microstructure* in governing the macroscopic rheological properties [20]. In a flowing polymeric liquid, the relevant microstructure is the *conformation* of the macromolecules, namely their orientation and degree of stretch. Within each macroscopic material point, there is a large number of polymers with a *distribution* of conformations. The macroscopic flow alters the polymer conformations along the fluid trajectories. On the other hand, the macroscopic stress field is governed by the distribution of polymer conformations within each fluid element. Clearly, there is a strong *nonlinear coupling* between rheological behaviour, flow-induced evolution of the microstructure, and flow parameters (such as geometry and boundary conditions). Furthermore, practioners of processing applications (e.g. injection moulding of plastic parts), are primarily interested in the physical properties of the final product. These are intimately linked to the frozen-in microstructure. To understand and possibly control the above non-linear coupling is the goal (Holly Grail?) of rheology.

3 A hierarchy of modeling approaches

The challenge for the theoretician is to build a proper mathematical model that will *describe*, with a minimum number of state variables and parameters, the rheological behaviour of polymers observed in well-controlled, *rheometrical* experiments developed by the experimentalist (such as simple shear and

uniaxial elongation flows). Then, the hope is that the model can be used, by means of appropriate numerical methods proposed by the computational rheologist, to *predict* flow phenomena in more complex situations.

With polymers, the task is made very difficult indeed by the huge number of microstructural degrees of freedom and the broad range of time and length scales separating the relevant atomistic and macroscopic processes (typically 10^{-15}s $\rightarrow$ 10^{2}s and 10^{-10}m $\rightarrow$ 1m). Clearly, this rules out a modeling approach based on *quantum mechanics* and related *ab initio* computational methods.

Atomistic modeling is the most detailed approach that could realistically be thought of. Since the mid-eighties, researchers have developed a variety of atomistic models and related molecular dynamics methods for the analysis of *equilibrium* polymer structures and properties [21, 22]. Application of atomistic modeling to polymer rheology is an active field of research [23-25]. Flow simulations using non-equilibrium molecular dynamics have also been attempted recently [26-28] to study the behaviour of polymers near walls and geometrical singularities (e.g re-entrant corners). In view of the very significant computer resources involved in such calculations, the atomistic models used in the latter studies are by necessity very coarse. Their potential is great, however, in helping us resolve important issues such as wall slip.

The next level of description of a polymeric liquid is that of *kinetic theory*. Here, one ignores atomistic processes altogether and focuses rather on the evolution of a more or less coarse-grained model of the polymer conformations [29-31]. Kinetic theory models can be exploited by means of *stochastic simulation* or *Brownian dynamics* methods [32].

Within the framework of kinetic theory, there also exists a hierarchy of possible levels of description of a particular fluid. Consider a dilute solution of linear polymers in a Newtonian solvent, for example. In kinetic theory, a rather detailed description of the polymer is the Kramers freely jointed bead-rod chain, which is made of N_B beads connected linearly by $N_B - 1$ rigid segments; for realistic simulations, N_B is of order 100. The beads are the interaction sites of the polymer with the Newtonian solvent: they experience Stokes' drag and Brownian forces. Important effects like excluded volume and hydrodynamic interactions can also be added in the theory. Clearly, this type of model is not meant to describe the chemical structure of the polymer in any detail. It does, however, have the important features needed to describe the polymer conformations (i.e. a large number of internal degrees of freedom, and the property of being oriented and deformed by the macroscopic flow). A

coarser model of the polymer is the freely jointed bead-spring chain, formed from N_b beads connected linearly by N_b-1 springs; N_b is now of order 10. The spring represents the entropic non-linear force that resists to the deformation of the molecule. An even coarser model is the single dumbbell, namely two beads connected by a spring. Brownian dynamics studies using Kramers chains [33-35], bead-spring chains [36], and dumbbells [37, 38], together with the experimental observation of single polymer conformations [39-41], have recently shed much light on the behaviour of dilute polymer solutions in rheometrical flows.

The most successful kinetic theory for concentrated solutions or melts of linear polymers is the Doi-Edwards reptation model [42]. The basic idea, due to de Gennes, is that entanglements with other polymers impose topological constraints on the motion of an individual polymer chain: it is indeed easier for a chain to move in the direction of its backbone than in the transverse direction. Since the mid-nineties, significant additions have been made to the basic Doi-Edwards theory which correct most of its deficiencies [43-48]. Furthermore, detailed reptation models suited for stochastic simulations are becoming available [49-51]. Significant progress has also been made recently in extending the Doi-Edwards theory to branched polymers [52].

Finally, besides atomistic modeling and kinetic theory lies the macroscopic approach of *continuum mechanics*. Here, details of the fluid microstructure are not taken into account explicitly. Rather, the stress experienced by the macroscopic fluid elements is related to the deformation history through a suitable *constitutive equation*. Added to the conservation laws for mass, energy, and linear momentum, the constitutive model yields a closed set of partial differential (or integro-differential) equations that can be solved by means of a suitable grid-based numerical method, such as the finite element technique [53]. A very large majority of publications in computational rheology has been based on the macroscopic approach, which is briefly reviewed in the next section.

It should be noted that macroscopic constitutive equations can in principle be *derived* from kinetic theory. In fact, almost all constitutive equations used today in computational rheology [54] have been inspired in one way or another by a kinetic theory model (a recent significant addition to the list is the pom-pom constitutive equation for branched polymers [55, 56]). These molecular-based constitutive equations yield quantitative information on the distribution of polymer conformations within a macroscopic fluid element in the form of *averaged* quantities such as the second moment of the

distribution. The latter can be related to birefringence [54]. Unfortunately, mathematical closure approximations are usually needed in the derivation of a constitutive model from kinetic theory. For example, in the context of dilute solutions, only the linear dumbbell model yields a mathematically equivalent constitutive equation (the Oldroyd-B model [30]). A closure approximation is needed for more sophisticated (and realistic) dumbbell models, which can have a significant qualitative impact [57]. In particular, it changes the meaning of some molecular parameters of the underlying kinetic theory. Thus, in view of the closure issue, it is not always easy to connect the results obtained with molecular-based constitutive equations to the actual distribution of polymer conformations.

Finally, we wish to close this section on modeling by pointing to important recent developments in non-equilibrium thermodynamics of complex fluids [58-62]. These should provide guidance in linking the various levels of description of polymeric liquids that we have briefly discussed. They should also help in the development of improved theories [63, 64].

Since its pioneering days (circa 1975), computational rheology has followed the purely macroscopic approach. The amazing increase in computer processing capacity has made feasible a complementary *micro-macro* approach, which involves the coupled solution of the macroscopic conservation laws and a microscopic kinetic theory model. Issues and progress in these two lines of research are reviewed in the next two sections. Finally, we wish to point out that alternative approaches to computer modeling of polymeric liquids have been advanced very recently, most notably Dissipative Particle Dynamics [65] and Lattice Boltzmann Models [66, 67].

4 Macroscopic simulations

Let us consider for the sake of illustration the particular problem of incompressible, isothermal creeping flow in a confined geometry. The conservation laws read

$$\boldsymbol{\nabla} \cdot \{-p\,\boldsymbol{\delta} + 2\eta_s\,\boldsymbol{D} + \boldsymbol{\tau}_p\} = \boldsymbol{0}, \qquad \boldsymbol{\nabla} \cdot \boldsymbol{v} = 0, \tag{1}$$

where p is the pressure, $\boldsymbol{v}$ is the velocity, $\boldsymbol{\tau}_p$ is the polymer contribution to the stress tensor, and $2\eta_s\,\boldsymbol{D}$ is a purely viscous component of the stress. The latter represents the contribution of the solvent in dilute solutions, or of fast

relaxation modes in more concentrated systems; it involves the rate of strain tensor $\boldsymbol{D}$ and a solvent viscosity η_s.

In macroscopic simulations, one closes the governing equations with a suitable constitutive equation of either the *differential* type

$$\frac{D\boldsymbol{\tau}_p}{Dt} = \boldsymbol{f}(\boldsymbol{\tau}_p, \boldsymbol{\nabla v}), \tag{2}$$

or of the *integral* type

$$\boldsymbol{\tau}_p = \int_{-\infty}^{t} m(t-t')\boldsymbol{S}_t(t')dt'. \tag{3}$$

Here, $D\boldsymbol{\tau}_p/Dt$ denotes the material derivative of the polymer stress, $\boldsymbol{f}$ is a model-dependent tensor function, $m(t-t')$ is the memory function of linear viscoelasticity, and $\boldsymbol{S}_t(t')$ is a model-dependent non-linear strain measure relative to the present time t. Note that the integral in (3) is computed along fluid trajectories that are *a priori* unknown. The above generic constitutive equations express the memory of polymeric liquids, namely the polymer stress carried by a fluid particle at present time t is a function of the deformation history experienced at past times t' by the particle flowing along its trajectory. Note that constitutive equations derived recently from kinetic theory [55, 68, 69] give the stress as an algebraic function of a number of microstructural tensor variables, which themselves follow an evolution equation similar to (2).

The macroscopic equations (1-2 or 3), supplemented with suitable boundary and initial conditions, present formidable numerical challenges. The governing equations are of mixed mathematical type (elliptic-hyperbolic), with possible local changes of type [70]. Stress boundary layers develop in many flow fields where the corresponding Newtonian fluid mechanical problem is quite smooth [71-73]. Stress singularities (e.g. at re-entrant corners) are much stronger than in the Newtonian case [74-76]. Finally, the non-linear qualitative behaviour of the solutions is very rich (e.g. multiplicity, of solutions, bifurcations), and can be affected by the discretization process [77-79]. Whether these difficulties reflect the actual physics of polymeric liquids (in which case we have to live with them!) or result from inadequate modeling is an open issue which continuum mechanics alone cannot resolve.

Progress in macroscopic simulations has been steady since the early days (circa 1975), along the path of (i) getting numbers, (ii) assessing their numerical accuracy, and (iii) assessing their physical relevance. For successive

reviews, see [4,80-82]. Step (i) was quickly found to be by no means a trivial matter: obtaining numerical solutions of the discrete, non-linear algebraic equations at significant values of the Weissenberg number We has long been difficult or even impossible (this is known as the High Weissenberg Number Problem or HWNP). It is fair to say that the HWNP is now *partially* resolved, in the sense that high-We numerical solutions have been made available over the years for a variety of flow problems. Step (ii) can only be performed by means of careful mesh-refinement experiments. Indeed, the mathematical analysis of numerical methods for viscoelastic fluids is quite difficult [83, 84]. Step (iii) is a test of the validity of the physical model (constitutive equation, values of the material parameters, and boundary conditions).

Although a wide spectrum of techniques and problems has been investigated, most of the published work deals with *mixed finite element methods* for 2d steady-state flows using a differential constitutive equation [82,85-87]. Recent developments are related to integral constitutive equations [88-90], time-dependent flows [91-97], temporal stability analysis of complex flows [98-100], iterative solvers [101], parallel algorithms [102, 103], 3d flows [104, 105], or various combinations thereof. Methods for high-Reynolds number viscoelastic flows have also been proposed recently, to study in particular the drag-reduction phenomenon [106-109].

In addition to these various extensions in numerical technology, macroscopic simulations have been exploited for two important tasks, namely (i) the evaluation of constitutive equations in benchmark complex flows (usually through a detailed comparison with experimental observations), and (ii) *computational rheometry*, or use of numerical simulation to aid the experimentalist in reducing its data. Representative examples of the former are reported in [110-122], while computational rheometry is illustrated in [123-126].

5 Micro-macro simulations

Although there is still much room for further numerical and algorithmic developments in macroscopic computational rheology, advances made there has revealed that improved modeling of the rheological behaviour is necessary. Further progress will not come from continuum mechanical arguments alone. While the direct molecular dynamics simulation of polymer flows in geometries of macroscopic dimensions is likely to remain out of reach for many

years to come, use of the simpler, coarse grain models of kinetic theory is becoming feasible with the availability of powerful parallel computers.

In the *micro-macro* approach, one solves the macroscopic conservation equations (1) by means of a grid-based numerical method, and uses a kinetic theory model rather than a constitutive equation to evaluate the polymer contribution to the stress. Clearly, this approach is much more demanding in computer resources than macroscopic methods. On the other hand, it allows the direct evaluation of kinetic theory models in complex flows without having to resort to mathematical closure approximations of questionable value.

A possible approach for evaluating the polymer stress in the micro-macro approach is to solve numerically the diffusion or Fokker-Planck equation [32] for the probability density $\psi(\boldsymbol{X},t)$ of the conformation $\boldsymbol{X}$ of the polymer chains within a material point. The diffusion equation has the generic form

$$\frac{\partial\psi(\boldsymbol{X},t)}{\partial t} = -\frac{\partial}{\partial\boldsymbol{X}}\cdot\{\boldsymbol{A}(\boldsymbol{X},t)\,\psi(\boldsymbol{X},t)\} + \frac{1}{2}\,\frac{\partial}{\partial\boldsymbol{X}}\frac{\partial}{\partial\boldsymbol{X}} : \{\boldsymbol{D}(\boldsymbol{X},t)\,\psi(\boldsymbol{X},t)\}\,. \tag{4}$$

Here, the symbol $\boldsymbol{X}$ is the set of variables defining the coarse-grained microstructure. For example, it reduces to the vector connecting the two beads in the simple dumbbell model of a polymer solution. The factors $\boldsymbol{A}$ and $\boldsymbol{D}$ define the deterministic and stochastic components of the model, respectively. In particular, the macroscopic velocity gradient $\boldsymbol{\nabla v}$ enters in the formulation of $\boldsymbol{A}$, while diffusion phenomena are described in $\boldsymbol{D}$. Equation (4) allows the computation of the probability density ψ. Relevant macroscopic variables (such as the polymer contribution to the stress tensor) are then computed as statistical averages of some function of the polymer conformation $\boldsymbol{X}$. In a complex flow, the time derivative of ψ in (4) is replaced by the material derivative and one must solve (4) at each material point of the flow domain.

An early micro-macro method [127] was based on the solution of the Fokker-Planck equation (4). This approach, however, is limited to kinetic theory models with a conformation space of small dimension. Brownian dynamics or *stochastic simulation* techniques provide a powerful alternative [32]. They draw on the mathematical equivalence between the Fokker-Planck equation (4) and the following Itô stochastic differential equation

$$d\boldsymbol{X} = \boldsymbol{A}(\boldsymbol{X},t)\,dt + \boldsymbol{B}(\boldsymbol{X},t)\cdot d\boldsymbol{W}, \tag{5}$$

where $\boldsymbol{D} = \boldsymbol{B} \cdot \boldsymbol{B}^T$ and $\boldsymbol{W}$ is a multi-dimensional Wiener process. Thus, instead of solving the deterministic diffusion equation (4) for ψ, one solves the associated stochastic differential equation (5) by means of suitable numerical techniques, which can be a considerably simpler task. Macroscopic fields of interest are then obtained by averaging over a large ensemble of realizations of the stochastic process $\boldsymbol{X}$. In a complex flow, the stochastic differential equation (5) applies along the macroscopic flow trajectories.

The idea of combining a stochastic simulation of a kinetic theory model with the numerical solution of the conservation equations has been pioneered in [128, 129], and further developed in [130-133]. Second-generation micro-macro methods, with much improved numerical properties, have been proposed recently for computing 2d transient flows. They are referred to as Brownian Configuration Field [134, 135] and Lagrangian Particle [96, 97] methods. Although their implementation is currently limited to elementary kinetic theory models, their potential range of applications is quite wide indeed.

6 Conclusions and perspectives

Research in computational rheology has been steadily producing over the last two decades a variety of complementary tools which will help us better understand the dynamics of polymeric liquids. It has indeed gone a long way since the first successful attempts [136, 137] to predict the flow of a memory fluid in a complex geometry.

Macroscopic methods, which rely on a constitutive equation to describe the polymer dynamics, have reached a state of relative maturity. Techniques are indeed available that allow, at least in principle, the computation of 3d time-dependent flows with either differential or integral models. They are used increasingly to validate constitutive theories in complex flows, and to aid the data reduction process in rheometrical experiments. Computing numerically accurate solutions at high Weissenberg numbers remains, however, a challenge which should not be overlooked. That the task is made considerably easier with more realistic constitutive equation is a fact that has long been known [138] and which has often been witnessed since. While certainly very comforting, it should not hide the need for careful numerical validation of present and future methods. The role of benchmark flow problems is crucial in that regard, especially for 3d and time-dependent flows where our

experience is rather meager.

Over the last few years, the scope of computational rheology has expanded considerably with the development of micro-macro techniques. These allow in principle the direct use of a hierarchy of kinetic theory models in complex flow simulations, without the dubious closure approximations that are invariably needed to derive a constitutive equation from kinetic theory. It thus becomes possible to assess the validity of coarse-grain molecular theories that are being developed by theoretical rheologists. Collaborative work with experimentalists, in particular those who develop methods for probing the microstructure of polymers undergoing flow [20], should ease the identification of the most important physical mechanisms to blend into a model. Also, the knowledge accumulated with the more detailed levels of description of kinetic theory should provide guidance for the development of improved constitutive equations. Finally, even more detailed molecular dynamics simulations are becoming feasible to study important phenomena such as wall rheology. These should provide useful information on the relevant boundary conditions to specify in macroscopic or micro-macro simulations. The need for careful numerical validation of these micro-macro and atomistic approaches is undeniable as well.

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