REVIEW

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Recent and Traditional Approaches to Numerical Flow Analysis of Complex Fluids

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Abstract

This article reviewed both traditional continuum-mechanics-based and recent micro-macro approaches to the flow analysis of complex fluids. The flow of viscoelastic fluids such as polymeric liquids was mainly treated. As for the continuum-mechanics-based approach, the development in numerical techniques for stabilizing the numerical scheme was introduced. As for the micro-macro approach, numerical simulations using the CONNFFESSIT approach and those based on the Fokker-Planck equation were reviewed. In addition, studies of micro-macro flow analyses of other complex fluids were briefly introduced.

Key Words: Complex fluid, Viscoelastic fluid, Fluid micro structure, Micro-macro simulation, Numerical simulation

1. Introduction

Complex fluid is an art of term that indicates a fluid having micro structures larger than the scale of molecules. For example, complex fluids include polymers, suspensions, surfactant solutions, liquid crystals, and so on [1, 2, 3]. Complex fluids are sometimes referred as *soft matter*. According to de Gennes [4], the 1991 Nobel Prize winner in physics, Americans prefer to call it complex fluids. The author is not sure that it is true or not, but thinks that complex fluids are preferably used in the field of fluid mechanics. In this review, we will use the term of complex fluids.

Complex fluids often show anomalous rheological properties and hence their flow behavior remarkably differs from that of Newtonian fluid [2, 5, 6]. In flow analyses of complex fluids, the relation between rheological properties of fluids and their flow behavior has been investigated to analyze their flow mechanism. Constitutive equations play a significant role in the numerical analysis based on continuum mechanics because characteristics of a model fluid are described by a constitutive equation. Various constitutive equations have been proposed for various kinds of complex fluids. Even for polymeric liquids (viscoelastic fluids), a large number of equations exist and have been employed for the numerical simulation [7, 8]. In flow analyses based on continuum mechanics, governing equations derived from conservation laws and a constitutive equation are simultaneously solved. Because this traditional approach requires low computational cost as compared to so-called micro-macro simulations that are introduced later, it has been widely employed in the flow analysis of complex fluids in relatively complex flow geometries.

On the other hand, the continuum-mechanics-based approach has a weak side. Considering the fact that characteristic rheological properties and flow behavior of complex fluids originates from changes in fluid micro structures induced by flow, it is natural to analyze the structural change in fluids for the clarification of flow mechanics of complex fluids. However, a constitutive equation sometimes loses the information of fluid micro structures during its derivation process owing to approximations or averaging operations even though it is based on the kinetic theory of fluid micro structures. Micro simulations such as molecular dynamics (MD) simulation and Brownian dynamics (BD) simulation are possible methods for the analysis of structural change induced by flows. However, these simulations usually require high computational resources and hence it is not possible for them to treat all flow problems that can be simulated by continuum-mechanics-based computations. However, attempts to numerically simulate the flow of complex fluids considering the fluid micro structure begin to appear as the computational performance progresses. In a micro-macro approach, a micro simulation of fluid micro structures is coupled with macroscopic flow computation. This approach

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is coming into a trend in the numerical flow analysis of complex fluids in these days.

In the present review, both traditional and recent approaches in numerical analysis of complex fluid flows are introduced with focusing the numerical flow analysis of polymeric fluids (viscoelastic fluids). In addition, applications to other complex fluids are also briefly reviewed. This review is structured as follows: In Sec. 2, traditional approaches, *i.e.* continuum-mechanics-based methods, are treated. In Sec. 3, recent approaches of micro-macro simulations are reviewed. In Sec. 4, micro-macro approaches for other complex fluids are briefly introduced. Finally in Sec. 5, we will conclude this review.

2. Numerical analysis based on continuum mechanics

In flow analyses based on continuum mechanics, balance equations derived from a corresponding conservation law and a constitutive equation form a mathematically-closed set of equations and they are simultaneously solved with appropriate initial and boundary conditions. Most constitutive equations for viscoelastic fluids that express rheological properties of real polymeric liquids relatively well are non-linear differential or integral equations, *e.g.* the Phan-Thien Tanner model [9, 10], the Giesekus model [11], and families of FENE dumbbell model (FENE-P [12, 13], FENE-CR [14], FENE-L [15] etc.). In general, nonlinear constitutive equations cause numerical instability under some computational conditions. Consequently, numerical instability is an inevitable issue in the flow analysis of viscoelastic fluids. For example, the high Weissenberg number problem (HWNP) is a challenging issue in the numerical simulation of viscoelastic fluids. The numerical scheme usually becomes unstable under conditions at high Weissenberg numbers [6, 16, 17], while characteristic and anomalous behaviors of viscoelastic fluids appear in highly elastic flows *i.e.* at high Weissenberg numbers. Consequently, it is important to simulate viscoelastic flows at high Weissenberg numbers. Various numerical techniques have been proposed to overcome HWNPs. It was recognized that the hyperbolic nature of constitutive equations in differential type was an important factor of the numerical instability. Thus stabilization techniques for the solution of differential type constitutive equations with the hyperbolic nature such as upwind differential methods and the streamline upwind Petrov-Galerkin (SUPG) method have been employed. The streamline integral method is also a technique useful for the solution of hyperbolic type differential equations. Although this method has disadvantages that it requires particle tracking procedures and it is not easy to apply to a flow with recirculation, it was applied to the analysis of die swell in extrusion process using an integral type constitutive equation [18–20]. Elastic viscous stress splitting (EVSS) methods are based on the idea to stabilize the numerical scheme by adding a viscous term, which is derived by splitting the extra stress tensor into viscous and elastic parts, to a constitutive equation. Early studies of numerical simulation of viscoelastic flows up to the first half of the 1980s are summarized in Ref [21]. Applications to polymer processing in 1970s and early 80s are introduced in Ref [22]. Although the technique of computational analysis of polymer processing has been progressed remarkably until today, the modeling method of processing introduced in the reference is still useful. Some results of progress in numerical simulations of polymer processing are available in Ref [6]. Keunings [23] has introduced the situation of this research field in late 80s. Baaijens [24] reviewed the development in numerical techniques for the flow analysis of viscoelastic fluids in around one decade from the latter half of 1980s. This review introduces stabilization techniques, in particular, for the FEM-based numerical computation for viscoelastic flows such as the elastic viscous stress splitting (EVSS) method, the streamline-upwind Petrov-Galerkin (SUPG) method, and the discontinuous Galerkin (DG) method. These techniques have been successfully applied to various flow problems. A book by Owens and Phillips [17] is a suitable literature for readers who want to learn relatively recent numerical techniques of viscoelastic flow analyses. In this book, fundamentals of numerical methods such as the finite difference method, the finite volume method, and the finite element method are explained and many numerical techniques for the simulation of viscoelastic flows such as several finite element schemes, EVSS-type stabilization techniques, time integral schemes, and error estimation methods are summarized.

Various numerical stabilization techniques have been applied to the computation of viscoelastic flows to make upper limit Weissenberg numbers increase. For a 4 to 1 axisymmetric contraction flows of the upper-convected Maxwell (UCM) model which have singularity at a re-entrant corner, Baaijens [25] indicated stable and accurate results up to Weissenberg numbers of 4 using the DEVSS/DG method and Susmal [26] obtained the results at the Weissenberg numbers of 5 using EVSS/finite volume method. In specific problems, numerical simulations at higher Weissenberg number have been performed, *e.g.* Iwata and coworkers [27, 28] employed the singular finite element method [29–31] to achieve computations at the Weissenberg number up to 130 for a die swell problem in extrusion process using the Giesekus model as a constitutive equation.

The continuum-mechanics-based approach is a traditional and most commonly used method for numerical simulations of viscoelastic flows especially in relatively complex flow fields, which are seen in polymer processing. Recent numerical studies of flows of complex fluids tend to aim the simulation of more realistic problems such as three-dimensional non-isothermal flows in complicated geometry and more accurate quantitative predictions. For the latter aim, often employed are multi-mode constitutive equations, which express the stress tensor as a superposition of stress tensors computed using different values of model parameters. In addition, the development of constitutive equations is still an important issue. To the author's knowledge, there is no constitutive equation for viscoelastic fluids that can describe their rheological properties perfectly; it may be impossible to obtain such a universal constitutive equation because of the variety of the origin of viscoelasticity. For some kinds of complex fluids, the constitutive equation has not been sufficiently developed. For example, in the case of surfactant solutions (wormlike micellar solutions), constitutive equations such as the diffusive Johnson-Segalman model [32–35] and the Giesekus model [36, 37], and the Bautista-Manero model and its modifications [38–41] have been used as a constitutive equation. However, they can not describe the kinematics of micelles and hence the development of such a constitutive equation for wormlike micellar solutions should be necessary.

3. Micro-macro simulation

As indicated previously in the traditional approach, a constitutive equation is necessary to close the system of governing equations that consist of the balance equations. In addition, some approximations are required to obtain a mathematically closed form of constitutive equation and these procedures diminish the capability of original theory of kinematics of macro structures of complex fluids on which the constitutive equation is based [1, 6–8]. These approximations sometimes result in failure in adequate prediction of rheological properties of real complex fluids. To avoid such a problem, so-called micro-macro simulations have been carried out. In the micro-macro approaches, stochastic simulations or direct simulations of kinematics of polymers are performed and macroscopic quantities such as stress are evaluated using the ensemble average of results of micro simulations.

We briefly introduce the process of derivation of a constitutive equation based on a polymer kinematics theory to remind the readers of procedures in derivation of a closed form of constitutive equation; Detail discussions are

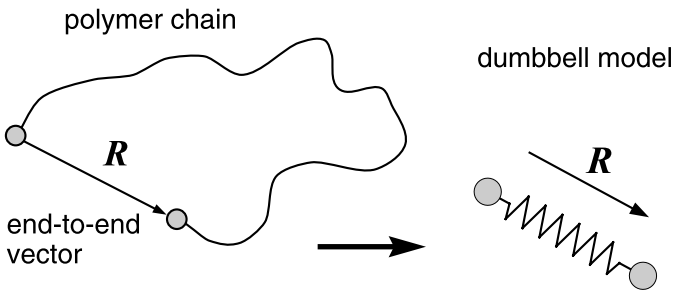

Fig. 1 Schematic diagram of elastic dumbbell model.

available in literatures [1, 6–8]. Here we will take an elastic dumbbell model as an example. A polymer chain is modeled by a pair of beads connected by an elastic spring, which expresses equivalent potential energy between ends of a polymer chain, and the orientation of dumbbell is represented by the end-to-end vector $\boldsymbol{R}$ (Fig. 1). The forces acting on a bead are inertia, viscous drag, the elastic spring force $\boldsymbol{F}$, a random Brownian force $\boldsymbol{F}_B$ except for the external forces such as the gravity force and the electromagnetic force. From the equations of motion of each bead, one obtains the equation of motion of $\boldsymbol{R}$:

$$m\ddot{\boldsymbol{R}} = \zeta(\boldsymbol{L}\cdot\boldsymbol{R} - \dot{\boldsymbol{R}}) - 2\boldsymbol{F} + \boldsymbol{F}_B\,, \tag{1}$$

where ζ is the frictional factor, $\boldsymbol{L}$ is the velocity gradient tensor. Neglecting the acceleration term and substituting $\boldsymbol{F}_B = -\,2k_BT\,(\partial\ln\psi\,/\,\partial\boldsymbol{R})$ to Eq. (1) yield the following equation:

$$\dot{\boldsymbol{R}} = \boldsymbol{L}\cdot\boldsymbol{R} - \frac{2}{\zeta}\boldsymbol{F} - \frac{2}{\zeta}k_BT\frac{\partial\ln\psi}{\partial\boldsymbol{R}}, \tag{2}$$

where k_B is the Boltzmann constant, T is the absolute temperature, and ψ is a probability density function: The probability that a dumbbell having an end-to-end vector in the range $\boldsymbol{R}$ to $\boldsymbol{R} + d\boldsymbol{R}$ at time t is given by $\psi\,(\boldsymbol{R}, t)\,d\boldsymbol{R}$.

This equation can be directly solved with the BD simulation, while the computational cost is very expensive. It can be reduced by introducing a stochastic procedure as follows: Multiplying Eq. (2) by ψ, differentiating with respect to $\boldsymbol{R}$, and using the probability balance equation in the $\boldsymbol{R}$-space

$$\frac{\partial\psi}{\partial t} + \frac{\partial}{\partial\boldsymbol{R}}\cdot(\dot{\boldsymbol{R}}\psi) = 0\,, \tag{3}$$

one obtains a diffusion equation of probability density called as the Fokker-Planck (F-P) equation (4) after some calculations:

$$\frac{\partial\psi}{\partial t} + \boldsymbol{L}\cdot\frac{\partial\psi}{\partial\boldsymbol{R}} - \frac{2}{\zeta}\frac{\partial}{\partial\boldsymbol{R}}(\psi\boldsymbol{F}) - \frac{2k_BT}{\zeta}\frac{\partial^2\psi}{\partial\boldsymbol{R}^2}\boldsymbol{I} = 0, \tag{4}$$

where $\boldsymbol{I}$ is the unite tensor. The time evolution of ψ is predicted by solving this equation. The numerical cost may be lower than that of the BD simulation but is still high. The F-P equation can be transformed into an evolution equation of a second order tensor $<\boldsymbol{RR}>$ by multiplying the both sides of Eq. (4) by $\boldsymbol{RR}$ and integrating over the $\boldsymbol{R}$-space:

$$\frac{D}{Dt}<\boldsymbol{RR}> - \boldsymbol{L}\cdot<\boldsymbol{RR}> - <\boldsymbol{RR}>\cdot\boldsymbol{L}^{\mathrm{T}} = -\frac{2}{\zeta}<\boldsymbol{RF}> + \frac{2k_BT}{\zeta}\boldsymbol{I}\ , \tag{5}$$

where the superscript T means the transposition operator and an ensemble average $<\cdots>$ is defined by

$$<\cdots> = \int_{R^3}\cdots\ \psi\,(R, t)\,d\boldsymbol{R}\ . \tag{6}$$

The stress tensor $\boldsymbol{\tau}$ is expressed with the Kramers expression as follows:

$$\boldsymbol{\tau} = -nk_BT\boldsymbol{I} + 2\eta_s\boldsymbol{D} + n<\boldsymbol{RF}>\ , \tag{7}$$

where n is the number density of the dumbbells and $\boldsymbol{D}$ is the rate-of-deformation tensor ($\boldsymbol{D} = (\boldsymbol{L} + \boldsymbol{L}^{\mathrm{T}})/2$). The spring force $\boldsymbol{F}$ depends on characteristics of spring: The Hookean elastic spring ($\boldsymbol{F} = H\boldsymbol{R}$: H is the spring constant) is a simple model and the UCM model is derived from Eqs. (5) and (7) with the Hookean elastic spring. The UCM model can not express shear-rate-dependent viscosity and predict unbounded stretch-thickening in elongational viscosity at a critical elongation rate. These unrealistic properties are due to an inadequate modeling of spring force. The FENE (Finitely Extensible Nonlinear Elastic) spring is a more realistic model for polymer molecules. The relation between $\boldsymbol{F}$ and $\boldsymbol{R}$ for the FENE spring is expressed by

$$\boldsymbol{F} = \frac{H\boldsymbol{R}}{1 - R^2/R_0^2}\ , \tag{8}$$

where R_0 is the maximum length of a spring. The FENE spring model and its modifications have been widely applied to numerical simulations of polymer dynamics. Recent studies of modeling and micro simulations of complex fluids using the FENE dumbbell model have been reviewed in detail by Kröger [42]. When the FENE spring is employed, a mathematically closed form of constitutive equation is not obtained from Eqs. (7) and (8). Thus some closure approximations have been proposed, *e.g.* [12–15]. One of familiar closure approximations is the Peterlin approximation in which the spring force (8) is approximated by

$$\boldsymbol{F} = \frac{H\boldsymbol{R}}{1 - <R^2/R_0^2>}\ . \tag{9}$$

Substituting Eq. (9) to Eqs. (5) and (7) yields the FENE-P model [12, 13]:

$$Z\boldsymbol{\tau} + \lambda\frac{\delta\boldsymbol{\tau}}{\delta t} - \lambda\frac{D\ln Z}{Dt}(\boldsymbol{\tau} + nk_BT\boldsymbol{I}) = 2nk_BT\lambda\boldsymbol{D}\ , \tag{10}$$

where $Z(\boldsymbol{\tau}) = 1 + (3/b)(1 + \mathrm{tr}\boldsymbol{\tau}/(3nk_BT))$, $b = HR_0^2/(k_BT)$, $\lambda = \zeta/(4H)$, and $\delta/\delta t$ means the upper-convected derivative. This model predicts the shear-thinning in shear viscosity and bounded stretch-thickening in elongation viscosity. Other closure approximations have been proposed to derive other FENE-dumbbell-based constitutive equations such as FENE-CR [14] and FENE-L [15] models.

Although the computational cost remarkably decreases, it can be known from Eq. (10) that information of fluid micro structures is not obtained from this equation. Theoretically speaking, we can simulate the dynamics of polymer molecules at several stages during the process of derivation of a constitutive equation. If Eq. (2) is directly computed for a large number of dumbbells and $<\boldsymbol{RR}>$ (or $<\boldsymbol{RF}>$) is obtained as the ensemble average of results for each dumbbell, the stress tensor can be evaluated without any closure approximation. This direct computation corresponds to the BD simulation, which generally requires huge computational resources. The numerical simulation based on the F-P equation (4) needs low computational costs as compared to the BD simulation, while it still requires heavy computation.

A relatively recent approach that does not require closed form constitutive models are the so-called micro-macro formulations based on kinetic theories. The CONNFFESSITT approach [43] is a familiar micro-macro approach, which was first proposed by Laso and Öttinger [44] and Feigl et al. [45]: CONNFFESSIT is an abbreviation of Calculation Of Non-Newtonian Flow: Finite Element and Stochastic SImulation Techniques. As one can recognized from this denomination, macroscopic flow computation with a finite element method is combined with micro simulation based on stochastic calculations in CONNFFESSIT. For a dilute polymer solution, the kinematics of polymers is simulated by solving a stochastic differential equation equivalent to Eq. (2) and stress is evaluated using the ensemble average of results of the stochastic simulation. Laso and Öttinger [44] simulated a startup of plane Couette flow of elastic dumbbell models by computing the kinematic equation of $\boldsymbol{R}$ with stochastic simulation and found a significant deviation between the behavior of the FENE-P and FENE models. Feigl et al. [45] have computed abrupt contraction flows for the Hookean dumbbells with the CONNFFESSIT approach and compared the results with the counterparts for the Oldroyd-B fluids and indicated the potential of the CONNFFESSIT approach. Laso et al. [46] have computed journal bearing flows of

FENE fluids.

The CONNFFESSIT approach has been adapted also to concentrated polymer solutions and polymer melts by using the Doi-Edwards (DE) or the Curtiss-Bird (CB) models [43]. The DE model [47–49] is based on the concept of reputation theory [50] and the CB model [51, 52] was derived using an anisotropic friction tensor to describe the restriction of sideway motion of polymers in concentrated systems. Although these models were derived from different concepts, the final expressions of these models are basically the same. Hence, the stochastic differential equation of these model can be also expressed in the same form of a diffusion equation of $\psi(\boldsymbol{u}, s, t)$ which is a probability density of the polymer chain whose direction is $\boldsymbol{u}$ at the position $s \in [0, 1]$ in a chain at time t [47–49, 51]. The diffusion equation can be translated into stochastic differential equations of two processes: one relates $\boldsymbol{u}$ and the other s [43]. For example, computation of the DE and the CB models with the CONNFFESSIT approach have been carried out for the startup of Couette flow for polymer solutions, polymer melts, and liquid crystals [53]; the startup of two dimensional flow past a cylinder [54]; the startup flow between parallel plates [55]; and fiber spinning flows [56].

In principle, the CONNFFESSIT approach requires the stochastic simulation for a large number of "polymers" for the evaluation of macroscopic quantities. Temporal and spatial fluctuations occur if the number of simulation runs is not enough large. The spatial fluctuation causes numerical error in polymer stress and derives fatal error in the calculation of divergence of stress tensor ($\nabla \cdot \boldsymbol{\tau}$) in the momentum equation (the equation of motion): This error may cause numerical instability in the numerical scheme of a macroscopic flow computation.

To reduce the statistical error and improve the numerical scheme, variance reduction techniques have been proposed by Melchior and Öttinger [57, 58]. Their strategy is based on importance sampling and the idea of control variables. Moreover, other strategies for the variance reduction have been developed: In the Brownian configuration field (BCF) method proposed by Hulsen et al. [59, 60], the evolution of a large number of continuous configuration fields $\boldsymbol{R}(\boldsymbol{x}, t)$ are computed instead of the computation of the end-to-end vector $\boldsymbol{R}(t)$ of each polymer. The evolution of $\boldsymbol{R}(\boldsymbol{x}, t)$ is solved in an Eulerian sense without particle tracking procedures. Consequently the stochastic differential equation of BCF method includes a term describing the convection of fields, which provides the variant reduction effect. On the other hand, Lagrangian techniques such as the Lagrangian particle method (LPM) [61] and the backward Lagrangian particle tracking method (BLPM) [62] have been proposed and were applied to micro-macro simulations. Halin et al. [61] applied LPM to the numerical simulation of journal bearing flows of the FENE model. Warappom et al. [62] simulated journal bearing flows and abrupt contraction flows of the FENE model by using the DEVSS/DG method combining the BLPM.

In recent studies, the improvement of the CONNFFESSIT scheme has been studied: Jourdain et al. [63] analyzed a variance reduction method, Ellero and Kröger [64] proposed a hybrid Brownian and distribution function storing strategy as a memory saving method for the CONNFFESSIT approach, and Laso et al. [65] showed an implicit time integral scheme for micro-macro simulations. In recent studies, the CONNFFESSIT approach has been applied to relatively complex flows, *e.g*. flows through fibrous media [66], die exit flows [67], free surface flows such as jets and mold filling [68] and transient flows in a planer contraction channel and flows around a confined cylinder [69].

Next, we will review numerical simulations of viscoelastic fluids based on the F-P equation. In this approach, one can obtain the information of the distribution of molecular orientation, which is useful for the analysis of flow induced structure of complex fluids. It is relatively recent that the results of F-P equation based simulation have appeared in research journals and this research field is under development [70]. Chauvière and Lozinski [71] have proposed a fast solver of the F-P equation of FENE dumbbells and simulated a flow past a cylinder. They also computed planer homogeneous flows and a flow through a cylinder for two-dimensional FENE dumbbell model [72] and three-dimensional flows through a confined cylinder using the FENE model [73]. Lozinski et al. [74] proposed a mixed finite-difference/spectral method based on a F-P equation to numerically simulate inhomogeneous flows of FENE fluids.

4. Brief introduction of micro-macro approach for other complex fluids

We can see similar situation in the derivation process of a closed type constitutive equation for other complex fluids. Here we will briefly introduce a case of particulate suspensions. For relatively dilute suspensions of hard spheres, the suspensions can be treated as Newtonian fluids with a volume-fraction-dependent shear viscosity η expressed by [75]

$$\eta = \eta_s (1 + 2.5\phi + 6.2\phi^2), \tag{11}$$

where η_s is the solvent viscosity and ϕ is the volume fraction of particles. At very low ϕ, η can be well described by the first two terms in the right hand side of Eq. (11): This model is called as Einstein's formula. For suspensions of spheres,

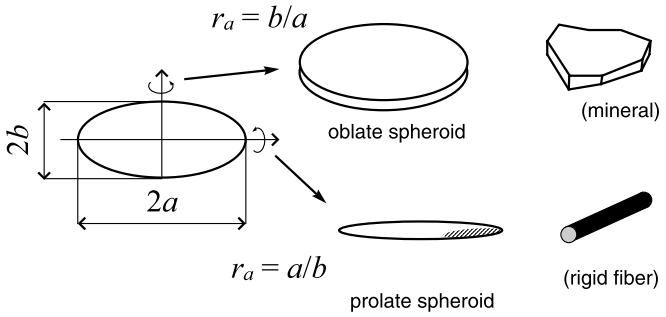

Fig. 2 Schematic diagram of spheroidal particles.

the orientation of particles does not affect their rheological properties because the particle shape is isotropic. On the other hand, for suspended particles having anisotropic shapes such as fibers and clay minerals, the orientation of particles dominates the flow behavior of suspensions. Consequently, it is necessary to consider the particle orientation in a constitutive equation of a suspension of anisotropic particles. A spheroidal particle is a simple model of a particle with an anisotropic shape: When the aspect ratio of a spheroid r_a defined as shown in Fig. 2 is much larger than unity, it is a model of rod-like particles such as short fibers; when r_a is much smaller than unity it is a model of disc-like particles such as clay minerals. The kinematics of spheroidal particles is described by an evolution equation of a director $\boldsymbol{p}$, which is a unit vector directed along the major axis of spheroid. For dilute spheroidal suspensions, the evolution equation is described by Jeffery's equation [76]:

$$\dot{\boldsymbol{p}} = \boldsymbol{W}\cdot\boldsymbol{p} - \frac{r_a^2-1}{r_a^2+1}(\boldsymbol{D}\cdot\boldsymbol{p} - \boldsymbol{D}:\boldsymbol{ppp}), \tag{12}$$

where $\boldsymbol{W}$ is the vorticity tensor, and the extra stress tensor σ is expressed as follows:

$$\sigma = 2\eta_s\phi\{A\boldsymbol{D}:\langle\boldsymbol{pppp}\rangle + B[\boldsymbol{D}\cdot\langle\boldsymbol{pp}\rangle + \langle\boldsymbol{pp}\rangle\cdot\boldsymbol{D}] + C\boldsymbol{D}\}, \tag{13}$$

where A, B, and C are coefficients depending on r_a [77, 78].

A Fokker-Planck equation can be derived from Eq. (12) [1, 79] and be applied to the micro simulation of suspensions. Similarly to the case of the FENE dumbbell model, closure approximations [80–83] are required to obtain a closed type constitutive equation. At the limit of $r_a \to \infty$, this model describes the motion of rod-like particles and hence it is applicable as a model of short fibers. Recent studies of numerical simulation of kinematics of fiber suspensions and particle suspensions have been reviewed by Chiba [84].

The CONNFFESSIT approach has been employed also in micro-macro simulations of fiber suspensions. Fan et al. [85] used the BCF method and analyzed flows past a cylinder in a tube and Phan-Thien and Fan [86] computed flows past a sphere settling in a tube. Chinesta et al. [87] have performed numerical simulations of steady recirculating flows based on the F-P equation. Similarly to the case of viscoelastic fluids, the numerical simulation based on the F-P equation is a developing issue at present.

5. Conclusion

In the present article, we reviewed both traditional and recent approaches to the flow analysis of complex fluids by taking polymeric liquids as an example. The traditional continuum-mechanics-based simulation is still commonly-used approach in the flow analysis of complex fluids, in especial, for flows in complex geometries encountered in engineering applications such as polymer processing. On the other hand, the recent micro-macro approaches provide essential information of fluid micro structures. They are expensive numerical methods that require large amount of computational power and memory. However, the micro-macro simulation are recent trends in research field because one can avoid the closure approximation, and moreover one can analyze the flow-induced change in fluid micro structures, which is an origin of typical flow behavior of complex fluids. Applications of the traditional approach to practical engineering problems, *i.e.* numerical simulations under more realistic flow conditions, and micro-macro approaches considering the flow-induced change in fluid micro structures will be two trends in future studies of the flow of viscoelastic fluids or complex fluids.

Although the micro-macro simulation has important advantages that no closure approximation is need and that the information of change in micro structures in flows is available, results of micro simulation such as the motion of individual polymer and the probability density function are not enough utilized for the flow analysis of complex fluids; in many cases, only the ensemble average of the results of micro simulation is used to avoid a closure approximation for the evaluation of macroscopic quantities, *e.g.* stress, that is necessary for the computation of macroscopic flows. In future study, the flow analysis of complex fluids should consider multi-scale problems in which analyses of both the microscopic behavior of fluid micro structures and the macroscopic flow behavior should be performed in the flow analysis of complex fluids.

References

[1] Larson RG (1999) "The Structure and Rheology of Complex Fluids", Oxford University Press, New York

[2] Hamley IW (2000) "Introduction to Soft Matter", Wiley, Chichester, New York, Weinheim, Brisbane, Singapore, Toronto

[3] Barrat J-L, Hansen J-P (2003) "Basic Concepts for Simple and Complex Liquids", Cambridge University Press, Cambridge
[4] de Gennes PG (1992) Rev Mod Phys, **64**, 645–648
[5] Bird RB, Armstrong RC, Hassager O (1987) "Dynamics of Polymeric Liquids", 2nd Ed, Vol.1 Fluid Mechanics, Wiley, New York
[6] Tanner RI (2000) "Engineering Rheology", 2nd Ed, Oxford Univ Press, New York
[7] Bird RB, Curtiss CF, Armstrong RC, Hassager O (1987) "Dynamics of Polymeric Liquids", 2nd Ed, Vol.2 Kinetic Theory, Wiley, New York
[8] Larson RG (1988) "Constitutive Equations for Polymer Melts and Solutions", Butterworth, Boston, London, Singapore, Sydney, Toronto, Wellington
[9] Phan-Thien N, Tanner RI (1977) J Non-Newtonian Fluid Mech, **2**, 353–365
[10] Phan-Thien N, Tanner RI (1978) J Rheol, **22**, 259–283
[11] Giesekus (1985) J Non-Newtonian Fluid Mech, **17**, 349–372
[12] Warner HR (1972) Ind Eng Chem Fundam, **11**, 379–387
[13] Fan X-J (1985) J Non-Newtonian Fluid Mech, **17**, 125–144
[14] Chilcott MD, Rallison JM (1988) J Non-Newtonian Fluid Mech, **29**, 381–432
[15] Lielens G, Halin P, Jaumain I, Keunings R, Legat V (1998) J Non-Newtonian Fluid Mech, **76**, 249–279
[16] Keunings R (1986) J Non-Newtonian Fluid Mech, **20**, 209–226
[17] Owens RG, Phillips TN (2002) "Computational Rheology", Imperial College Press, Singapore
[18] Dupont S, Marchal JM, Crochet MJ (1985) J Non-Newtonian Fluid Mech, **17**, 157–183
[19] Luo X-L, Tanner RI (1986) J Non-Newtonian Fluid Mech, **21**, 179–199
[20] Wapperon P, Hulsen MA, van der Zanden JPPM (1998) Rheol Acta, **37**, 73–88
[21] Crochet MJ, Davies AR, Walters K (1984) "Numerical Simulation of Non-Newtonian Flow", Elsevier, Amsterdam, Oxford, New York, Tokyo
[22] Pearson JRA, Richardson SM (1983) "Computational Analysis of Polymer Processing", Applied Science, London
[23] Keunings R (1990) Rheol Acta, **29**, 556–570
[24] Baaijens FPT (1998) J Non-Newtonian Fluid Mech, **79**, 361–385
[25] Baaijens FPT (1998) J Non-Newtonian Fluid Mech, **75**, 119–138
[26] Susmal GP (1995) J Non-Newtonian Fluid Mech, **56**, 15–47
[27] Iwata S, Aragaki T, Mori H, Hattori M, Waki H (2002) J Chem Eng Japan, **35**, 660–669
[28] Iwata S, Mori H, Aragaki T, Takahashi Y, Hattori M Goto I (2004) J Chem Eng Japan, **37**, 1140–1149
[29] Georgiou GC, Olson LG, Schultz WW, Sagan S (1989) Int J Numer Methods Fluids, **9**, 1357–1367
[30] Georgiou GC, Schultz WW, Olson LG (1990) Int J Numer Methods Fluids, **10**, 357–372
[31] Georgiou GC, Boudouvis AG (1999) Int J Numer Methods Fluids, **29**, 363–371
[32] Johnson M, Segalman D (1977) J Non-Newtonian Fluid Mech, **2**, 255–270
[33] Lu C-YD, Olmsted PD, Ball RC (1999) Phys Rev Lett, **84**, 642–645
[34] Olmsted PD, Radulescu O, Lu C-YD (2000) J Rheol, **44**, 257–275
[35] Radulescu O, Olmsted PD (2000) J Non-Newtonian Fluid Mech, **91**, 143–164
[36] Fischer P, Rehage H (1997) Rheol Acta, **36**, 13–27
[37] Holtz T, Fischer P, Rehage H (1999) J Non-Newtonian Fluid Mech, **88**, 133–148
[38] Bautista F, de Santos JM, Puig JE, Manero O (1999) J Non-Newtonian Fluid Mech, **93**, 93–113
[39] Bautista F, Soltero JFA, Pétrez-López JH, Puig JE, Manero O (2000) J Non-Newtonian Fluid Mech, **94**, 57–66
[40] Manero O, Bautista F, Soltero JFA, Puig JE (2002) J Non-Newtonian Fluid Mech, **106**, 1–15
[41] Boek ES, Paddinga JT, Anderson VJ, Tardy PMJ, Crawshaw JP, Pearson JRA (2005) J Non-Newtonian Fluid Mech, **126**, 39–46
[42] Kröger M (2004) Phys Rep, **390**, 453–551
[43] Öttinger HC (1996) "Stochastic Processes in Polymeric Fluids", Springer, Berlin
[44] Laso M, Öttinger HC (1993) J Non-Newtonian Fluid Mech, **47**, 1–20
[45] Feigl K, Laso M, Öttinger HC (1995) Macromolecules, **28**, 3261–3274
[46] Laso M, Picasso M, Öttinger HC (1997) AIChE J, **43**, 877–892
[47] Doi M, Edwards SF (1978) J Chem Soc Faraday Trans II, **74**, 1789–1801
[48] Doi M, Edwards SF (1978) J Chem Soc Faraday Trans II, **74**, 1801–1817
[49] Doi M, Edwards SF (1978) J Chem Soc Faraday Trans II, **74**, 1818–1832
[50] de Gennes PG (1971) J Chem Phys, **55**, 572–579
[51] Curtiss CF, Bird RB (1981) J Chem Phys, **74**, 2016–2025
[52] Curtiss CF, Bird RB (1981) J Chem Phys, **74**, 2026–2033
[53] Hua CC, Schieber JD (1996) Chem Eng Sci, **51**, 1473–1485
[54] van Heel APG, MA Hulsen, BHAA van den Brule (1999) J Rheol, **43** 1239–1260
[55] Yamamoto T, Mori N (2004) JSME Int J, Ser B, **47**, 1–8
[56] Yamamoto T (2007) J Text Eng, **53**, 123–130
[57] Melchior M, Öttinger HC (1995) J Chem Phys, **103**, 9506–9509
[58] Melchior M, Öttinger HC (1996) J Chem Phys, **105**, 3316–3331

[59] Hulsen MA, van Heel APG, van den Brule BHAA (1997) J Non-Newtonian Fluid Mech, **70**, 79–101
[60] Öttinger HC, van den Brule BHAA, Hulsen MA (1997) J Non-Newtonian Fluid Mech, **70**, 255–261
[61] Halin P, Lielens G, Keunings R, Legat V (1998) J Non-Newtonian Fluid Mech, **79**, 387–403
[62] Wapperom P, Keunings R, Legat V (2000) J Non-Newtonian Fluid Mech, **91**, 273–295
[63] Jourdain B, le Bris C, Lelièvre T (2004) J Non-Newtonian Fluid Mech, **122**, 91–106
[64] Ellero M, Kröger M (2004) J Non-Newtonian Fluid Mech, **122**, 147–158
[65] Laso M, Ramírez J, Picasso M (2004) J Non-Newtonian Fluid Mech, **122**, 215–226
[66] Hua CC, Schieber J (1998) J Rheol, **42**, 477–491
[67] Cormenzana J, Ledda A, Laso M, Debbaut B (2001) J Rheol, **45**, 237–258
[68] Grande E, Laso M, Picasso M (2003) J. Non-Newtonian Fluid Mech, **113**, 127–145
[69] Hu X, Ding Z, Lee LJ (2005) J Non-Newtonian Fluid Mech, **127**, 107–122
[70] Chinesta F, Cueto E (2007) "Advances in Material Forming", Springer, Paris
[71] Chauvière C , Lozinski A (2003) J Comput Phys, **189**, 607–625
[72] Chauvière C , Lozinski A (2004) Computers & Fluids, **33**, 687–696
[73] Chauvière C, Lozinski A (2004) J Non-Newtonian Fluid Mech, **122**, 201–214
[74] Lozinski A, Owens RG, Fang J (2004) J Non-Newtonian Fluid Mech, **122**, 273–286
[75] Batchelor BK (1970) J Fluid Mech, **41**, 545–570
[76] Jeffery GB (1922) Proc Roy Soc Lond, **A102**, 161–179
[77] Hinch EJ, Leal LG (1972) J Fluid Mech, **52**, 683–712
[78] Leal LG, Hinch EJ (1973) Rheol Acta, **12**, 127–132
[79] Huilgol RR, Phan-Thien N (1997) "Fluid Mechanics of Viscoelasticity", Chap 4, Elsevier, Amsterdam
[80] Hinch EJ, Leal LG (1976) J Fluid Mech, **76**, 187–208
[81] Advani SG, Tucker III CL (1987) J Rheol, **31**, 754–784
[82] Advani SG, Tucker III CL (1990) J Rheol, **34**, 367–386
[83] Szeri AJ, Leal LG (1992) J Fluid Mech, **242**, 549–576
[84] Chiba K (2006) J Text Eng, **52**, 227–236
[85] Fan X-J, Phan-Thien N, Zheng R (1999) J Non-Newtonian Fluid Mech, **84**, 257–274
[86] Phan-Thien N, Fan X-J (1999) J Rheol, **43**, 1–8
[87] Chinesta F, Chaidron G, Poitou A (2003) J Non-Newtonian Fluid Mech, **113**, 97–125