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ON SOME PDF BASED MOMENT CLOSURE APPROXIMATIONS OF MICRO-MACRO MODELS FOR VISCOELASTIC POLYMERIC FLUIDS *

YUNKYONG HYON †, QIANG DU ‡, AND CHUN LIU§

Abstract. In this paper we will discuss several issues related to the moment-closure approximation of multiscale models for viscoelastic polymeric fluids. These moment-closure approaches are based on special ansatz for the probability density function (PDF) in the finite extensible nonlinear elastic (FENE) dumbbell micro-macro models which consists of the coupled incompressible Navier-Stokes equations and the Fokker-Planck equations. We present the exact energy law of the resulting closure systems and introduce a post-modification scheme to preserve the positivity of PDF. The scheme not only reduces the region of negative PDF values but also preserves the structure of the induced stress tensor resulting from the molecular behaviors such as stretching and rotation. Numerical verifications are provided for the moment-closure system with some standard external flows. We also explore the relation of the maximum entropy principle (MEP) and the moment-closure approach.

Key words. Multiscale modeling, Micro-macro dynamics, Polymeric fluid, Non-Newtonian fluid, FENE model, Moment closure, Fokker-Planck, Numerical simulations

AMS subject classifications. 76A05, 76M99, 65C30

1. Introduction. In this paper, we consider the hydrodynamical systems of dilute polymeric fluids. The viscoelastic flow of rheological complex fluids can be described by a multiscale (micro-macro) model. The multiscale-multiphysics model includes the coupling between the continuum mechanic theory [5] in macroscopic level and the kinetic theory in microscopic level. This micro-macro model also reflects the interaction between two different scales as the macroscopic flow/deformation will affect the microscopic structure through kinematic transport/deformation relation; while the averaging (coarsening) effects of the microscopic molecular configurations such as stretching and orientation will affect the macroscopic flow field through the induced elastic stresses.

In many applications, we are more interested in the macroscopic quantity, such as the induced elastic stresses, rather than the detail behavior of molecular/microscopic variables. These stresses, resulting from the average of molecular behaviors, can be described in many situations by the moments of distribution function of molecular configurations. Notice that the PDF of the molecular configurations carries all the microscopic information of the system. Among different molecular models, the two most used well-known models are the Hookean dumbbell model, which is related to the Oldroyd-B viscoelasticity [1, 12], and the finite-extensible-nonlinear-elastic (FENE) dumbbell model [1, 2].

While the Hookean models are the best understood one and form the basis for most analytic studies, in this paper we focus on the FENE spring dumbbell model

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for which the issues related to the nonlinearities and the singularities in the spring potential must be properly addressed. The usual moment closure methods were in fact motivated by the Hookean model, where the equilibrium distribution is Gaussian and the second moments carry all the information of the original system [1, 2].

In our previous works [15, 16, 17, 18], we introduced a probability density function (PDF) ansatz in the moment closure approximation of the FENE model. The PDF is modeled from the special equilibrium solution to the Fokker-Planck equation without the flow field. The approximated PDF resolves the difficulties caused by the nonlinearity of FENE spring force, and leads us to obtain the analytical expression of the moment-closure system. The moment-closure subspace was solely based on this PDF ansatz. The resulting system in [15], which is referred as FENE-S closure in this paper, was shown to inherit the energy dissipation law from the original system. We will give a detailed derivation of the energy dissipation law associated with FENE-S. This is an enhanced version of the earlier ones shown in [15, 16] and was also motivated by a more recent work in [20]. The numerical simulations indicated that the FENE-S model has an excellent agreement to the solutions in case of moderate flow rates. Moreover, this closure procedure allows the natural incorporation of more (higher) modes in order to increase the range of validation and accuracy [16].

While a closure approximation procedure such as the FENE-S has many advantages, it lacks the positivity-preserving property for the reconstruted PDF. This can contribute to errors in some molecular configuration regions. To resolve this issue we introduce a modification scheme which is applied to the recovered PDF by the moments, and enhances the positivity of PDF in shear flow situations. This modified scheme of the original FENE-S [15, 16] is referred as FENE-SM. The moment-closure system with the modification as a post-processing scheme still satisfies the energy dissipation law. In a number of numerical experiments, we will demonstrate that this modification can provide more accurate results than that of the previous methods, including the FENE-S model [15] and the FENE-P [22] under various shear flow environments.

Another issue we will discuss here is on the application of the maximum entropy principle (MEP) to the moment closure approximations [18, 21]. As in our recent work, we can see that MEP provides an natural PDF ansatz related to the total energy of the micro-macro systems. If we focus on the near equilibrium situations, this approach will yield very similar results as the ad-hoc approaches in [15, 16, 18]. In [21], a positive preserving scheme, FENE-QE, has been introduced using the idea of MEP but it does not provide the analytical corresponding between the moments and the PDF function. The implicit PDF are solved numerically from some nonlinear integral equations which increase the computation overhead although a piecewise linear approximation scheme has been proposed in [21] to such such simulation costs. In our approach [18], we employed MEP with an approximation of PDF which leads to an explicit form of moment-closure system [18] and is thus more cost effective computationally. The moment-closure system obtained in [18] preserves the energy law analogous to the original coupled system, but the approximation of PDF results in the loss of positivity-preserving property. In this paper, we will combine the method of modification (post-processing) and the MEP to obtain the positivity preserving moment closure systems. Moreover, for extension flow cases, the flow effect can be effectively incorporated into our MEP approach.

An outline of this paper is as follows. In the section 2 we recall the FENE micro-macro model and some related results. In the section 3 we derive the energy equation for the FENE-S model. A modification scheme for PDF is presented in section 4 to preserve the positivity. In the next section 5 first we recall the maximum entropy principle, briefly and discuss about the situation far from the equilibrium with the internal energy. We present various numerical experiments to verify the modification scheme for FENE-S model in the configuration fields in section 6. Finally, we give several additional remarks in section 7.

2. The Micro-Macro Models and Moment-Closure System. Let $\vec{Q}$ be the microscopic configuration field which indicates the relative position of two beads of dumbbell model and $\Psi(|\vec{Q}|)$ be a spring potential, which only depends on $Q = |\vec{Q}|$. Throughout this paper, we consider 2-dimensional spaces for macroscopic and microscopic levels. One can easily extend the arguments to 3-dimensional spaces. $f(\vec{Q}, t)$ is the PDF of the configuration field $\vec{Q}$ and time t. The micro-force balance law with the spring potential is demonstrated through the following equation:

$$m\vec{Q}_{tt} + \frac{1}{\eta}\vec{Q}_t = -\nabla_{\vec{Q}}\Psi, \tag{2.1}$$

where η is a damping coefficient and m is the mass of the molecule. If we consider the separation of the scales in time, that is, the time-scale of the small molecular behavior is much faster than that in macroscopic level, then the damping term will dominant the relevant dynamics. In other words, we can neglect the inertial term and results in an gradient flow $\frac{1}{\eta}\vec{Q}_t = -\nabla_{\vec{Q}}\Psi$. Moreover, if we take into account the thermo-fluctuation, an infinitesimal quasi-static Brownian motion effect σdB where σ is ratio coefficient [6], then we can obtain the following Fokker-Planck equation of $f(\vec{Q}, t)$:

$$f_t + \nabla \cdot (-\eta \nabla_{\vec{Q}}\Psi f) = \frac{\sigma^2}{2}\Delta_{\vec{Q}} f. \tag{2.2}$$

Equation (2.2) is only about the microscopic behavior, there is no communication between microscopic and macroscopic effects. The connection between these two levels is made via the deformation of the configuration field $\vec{Q}$ in the flow field through the Cauchy-Born type of kinematic transport assumptions that pass information from macroscopic scale to microscopic scale [12, 15]. The final hydrodynamic system includes a incompressible momentum equations for macroscopic flow field $\vec{u} = \vec{u}(x, t)$ and the Fokker-Planck equation for microscopic molecular PDF, $f = f(\vec{x}, \vec{Q}, t)$ by [1, 14].

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} + \nabla P = \lambda \nabla \cdot \tau_p + \nu \Delta \vec{u}, \tag{2.3}$$

$$\nabla \cdot \vec{u} = 0, \tag{2.4}$$

$$\frac{\partial f}{\partial t} + (\vec{u} \cdot \nabla) f + \nabla_{\vec{Q}} \cdot (\nabla \vec{u} \vec{Q} f) = \frac{2}{\zeta}\nabla_{\vec{Q}} \cdot (\nabla_{\vec{Q}}\Psi f) + \frac{2kT}{\zeta}\Delta_{\vec{Q}} f. \tag{2.5}$$

Here P is the hydrostatic pressure, ν is the fluid viscosity, ζ is the elastic relaxation time of the spring and τ_p is a tensor representing the polymer contribution to the macroscopic stress, $\nabla_{\vec{Q}}\Psi(Q)$ is the elastic spring force, and λ is the polymer density constant. The induced stress from the microscopic configurations is given by

$$\tau_p = \begin{pmatrix} \tau_p^{11} & \tau_p^{12} \\ \tau_p^{21} & \tau_p^{22} \end{pmatrix} = \int (\nabla_{\vec{Q}}\Psi \otimes \vec{Q}) f(\vec{x}, \vec{Q}, t) d\vec{Q}. \tag{2.6}$$

Finally, the micro-macro system (2.3)–(2.5) is established with suitable initial and boundary conditions. For the sake of brevity, we do not delve in depth of these conditions in this paper [19].

The FENE spring potential is given by $\Psi(Q) = -(HQ_0^2/2)\log(1-(Q/Q_0)^2)$ and the FENE spring force law reads

$$\nabla_{\vec{Q}}\Psi = \frac{H\vec{Q}}{1-(Q/Q_0)^2}, \tag{2.7}$$

where Q_0 is the maximum dumbbell extension and H is elasticity constant. The difficulty in using FENE spring potential is that there is no exact macroscopic constitutive equation for the polymeric stress τ_p because of the nonlinearity of the FENE spring potential. In the applications of FENE model, solving the coupled micro-macro system (2.3)–(2.5) numerically becomes a daunting however indispensable job. There have been many numerical methods developed in the literature, like the fast solver for the Fokker-Planck equation, CONNFFESSIT for the Monte-Carlo simulation of the Fokker-Planck equation. As an extension of the CONNFFESSIT approach, the Brownian configuration fields (BCF) method, which is one of various variance reduction techniques based on control variate, have been introduced [9, 13]. Here we are interested in developing various moment-closure approximation procedures and approximations to the stress tensor τ_p.

We may first proceed to derive the moment equations from the Fokker-Planck equation (2.5) in the same way of [15] under a given flow field. By multiplying the equation by Q^2, $Q_1^2 - Q_2^2$, Q_1Q_2 and integrating by parts, using the incompressibility of flow $\nabla\cdot\vec{u} = 0$ and the bracket notation $\langle\cdot\rangle = \int_\Omega f\cdot d\vec{Q}$ for the assemble with respect to the PDF in the configuration field, we have the following equations:

$$\begin{aligned}\frac{\partial}{\partial t}\langle Q^2\rangle + \vec{u}\cdot\nabla\langle Q^2\rangle - 2\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\langle Q_1Q_2\rangle&\\ -\left(\frac{\partial u}{\partial x}-\frac{\partial v}{\partial y}\right)\langle Q_1^2-Q_2^2\rangle = \frac{8kT}{\zeta} - \frac{2}{\zeta}\int(\nabla_{\vec{Q}}\Psi\cdot\nabla_{\vec{Q}}Q^2)f\,d\vec{Q},&\end{aligned} \tag{2.8}$$

$$\begin{aligned}\frac{\partial}{\partial t}\langle Q_1^2-Q_2^2\rangle + \vec{u}\cdot\nabla\langle Q_1^2-Q_2^2\rangle - 2\left(\frac{\partial u}{\partial y}-\frac{\partial v}{\partial x}\right)\langle Q_1Q_2\rangle&\\ -\left(\frac{\partial u}{\partial x}-\frac{\partial v}{\partial y}\right)\langle Q^2\rangle = -\frac{2}{\zeta}\int\left\{\nabla_{\vec{Q}}\Psi\cdot\nabla_{\vec{Q}}(Q_1^2-Q_2^2)\right\}f\,d\vec{Q},&\end{aligned} \tag{2.9}$$

$$\begin{aligned}\frac{\partial}{\partial t}\langle Q_1Q_2\rangle + \vec{u}\cdot\nabla\langle Q_1Q_2\rangle - \frac{1}{2}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\langle Q^2\rangle&\\ +\frac{1}{2}\left(\frac{\partial u}{\partial y}-\frac{\partial v}{\partial x}\right)\langle Q_1^2-Q_2^2\rangle = -\frac{2}{\zeta}\int\left\{\nabla_{\vec{Q}}\Psi\cdot\nabla_{\vec{Q}}(Q_1Q_2)\right\}f\,d\vec{Q}.&\end{aligned} \tag{2.10}$$

The issue of moment-closure is then the determination of the polymeric stress in terms of second order moments and other computable macroscopic quantities. If the spring potential satisfies the Hookean law, $\Psi(\vec{Q}) = HQ^2/2$ then we can derive a macroscopic differential constitutive equation for the stress τ_p. The integrals with $\nabla_{\vec{Q}}\Psi$ in (2.8)–(2.10) can also be expressed analytically by some formulae in terms of the moments, leading to the well known Oldroyd-B model. However, this is not the case for FENE potential due to the nonlinearity of the spring potential.

The key observation made in [15, 16] is to notice that the Fokker-Planck equation possesses the following equilibrium solution in the absence of the flow field:

$$f_{eq} = \frac{1}{J_{eq}} e^{-\frac{\Psi}{kT}} = \frac{1}{J_{eq}} \left[1 - \left(\frac{Q}{Q_0} \right)^2 \right]^{HQ_0^2/2kT} \tag{2.11}$$

where J_{eq} is the normalizing factor, T is the temperature, k is the Planck constant. Based on the special solution (2.11) the PDF f is approximated in the second order terms of $\vec{Q}$, by the following ansatz:

$$f(\vec{Q}) = \frac{1}{J_b} \left[1 - \left(\frac{Q}{Q_0} \right)^2 \right]^{b/2} (1 + \beta Q_1 Q_2 + \gamma (Q_1^2 - Q_2^2)), \tag{2.12}$$

where J_b is the normalizing factor and b, β, γ are unknowns which can be related/ determined by the second order moments.

Let $M_1 = \langle Q^2 \rangle$, $M_2 = \langle Q_1^2 - Q_2^2 \rangle$, and $M_3 = \langle Q_1 Q_2 \rangle$ be the second order moments of the PDF (2.12). Then the derivation of the second order moments to that in [15] gives the explicit analytic representation between the second moments M_i's and constants, b, β, γ.

$$\left\{ \begin{array}{lcl} M_1 & = & < Q^2 >= \frac{2Q_0^2}{(b+4)}, \\ M_2 & = & < Q_1^2 - Q_2^2 >= \frac{4\gamma Q_0^4}{(b+4)(b+6)}, \\ M_3 & = & < Q_1 Q_2 >= \frac{\beta Q_0^4}{(b+4)(b+6)} \end{array} \right. \tag{2.13}$$

The calculations involve the following well-known, however, very useful identity in our derivation of the closure system:

$$\int_0^{R_0} \left[1 - \left(\frac{R}{R_0} \right)^2 \right]^{b/2} R^n dR = \frac{1}{2} R_0^{n+1} B\left(\frac{n+1}{2}, \frac{b+2}{2} \right) \tag{2.14}$$

where $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x + y)$ and $\Gamma(x)$ is the gamma function.

Conversely, with simple direct calculation, we can determine the parameters b, β, γ by the second order moments (2.13):

$$b = \frac{2Q_0^2}{M_1} - 4 \tag{2.15}$$

$$\beta = \frac{M_3(b+4)(b+6)}{Q_0^4} = \frac{4M_3(Q_0^2 + M_1)}{Q_0^2 M_1^2} \tag{2.16}$$

$$\gamma = \frac{M_2(b+4)(b+6)}{4Q_0^4} = \frac{M_2(Q_0^2 + M_1)}{Q_0^2 M_1^2}. \tag{2.17}$$

Thus, in light of (2.8)-(2.10), we obtain the closure-system for the original multiscale system (2.3)–(2.5) as follows:

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} + \nabla p = \lambda \nabla \cdot \tau_p + \nu \triangle \vec{u}, \tag{2.18}$$

$$\nabla \cdot \vec{u} = 0, \tag{2.19}$$

$$\frac{\partial}{\partial t} M_1 + \vec{u} \cdot \nabla M_1 - 2\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) M_3 - \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) M_2 \tag{2.20}$$

$$= \frac{8kT}{\zeta} - \frac{4H}{\zeta}\left(\frac{Q_0^2}{Q_0^2 - 2M_1}\right) M_1,$$

$$\frac{\partial}{\partial t} M_2 + \vec{u} \cdot \nabla M_2 - 2\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right) M_3 - \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) M_1 \tag{2.21}$$

$$= -\frac{4H}{\zeta}\left(\frac{Q_0^2 + M_1}{Q_0^2 - 2M_1}\right) M_2,$$

$$\frac{\partial}{\partial t} M_3 + \vec{u} \cdot \nabla M_3 - \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) M_1 + \frac{1}{2}\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right) M_2 \tag{2.22}$$

$$= -\frac{2H}{\zeta}\left(\frac{Q_0^2 + M_1}{Q_0^2 - 2M_1}\right) M_3.$$

Here, the tensor τ_p as given in (2.6) is calculated using the ansatz (2.12) for the PDF with the coefficients b, γ and β determined by (2.15)–(2.16) [17].

In the following section we derive the new exact energy law that including the entropic term which is $kTf \ln f$ for the above moment-closure system (2.18)–(2.22) of FENE-S.

3. Exact Energy Law for FENE-S System. We now derive the exact energy law corresponding to the closure system, FENE-S, (2.18)–(2.22). To see this we recall that the original multiscale system (2.3)–(2.5) has the following energy estimate under the boundary condition $\vec{u} = 0$ on $\partial\Omega$:

$$\begin{aligned} &\frac{d}{dt}\int \left\{\frac{1}{2}|\vec{u}|^2 + \lambda \int (kTf \ln f + \Psi f)\, d\vec{Q}\right\} dx \\ &\quad = -\int \left(\nu |\nabla \vec{u}|^2 + \frac{2\lambda}{\zeta}\int f |\nabla_{\vec{Q}}(kT \ln f + \Psi)|^2\, d\vec{Q}\right) dx. \end{aligned} \tag{3.1}$$

In [15] an energy law for FENE-S which is analogous to the above energy equation (3.1) was obtained as

$$\begin{aligned} &\frac{d}{dt}\int \left\{\frac{1}{2}|\vec{u}|^2 + \lambda G(M_1)\right\} dx \\ &= -\int \left\{\mu |\nabla \vec{u}|^2 + \frac{2H^2 Q_0^2 M_1 (Q_0^2 + M_1)}{\zeta (Q_0^2 - 2M_1)^2} - \frac{4kTH(Q_0^2 + M_1)}{\zeta (Q_0^2 - 2M_1)}\right\} dx \end{aligned} \tag{3.2}$$

where $G(M_1) = -\frac{HM_1}{4} - \frac{3HQ_0^2}{8} \ln\left(1 - \frac{2M_1}{Q_0^2}\right)$. This energy equation only considered the potential part in the internal energy without the "entropic" term, $kTf \ln f$.

Here, we derive an energy law different from (3.2) including the "entropic" term. First of all, we define a symmetric tensor A that is defined by $A = \langle \vec{Q} \otimes \vec{Q} \rangle$. In 2-dimension the tensor A has the form,

$$A = \begin{pmatrix} < Q_1^2 > & < Q_1 Q_2 > \\ < Q_1 Q_2 > & < Q_2^2 > \end{pmatrix} = \begin{pmatrix} \frac{M_2}{2} & M_3 \\ M_3 & -\frac{M_2}{2} \end{pmatrix} + \begin{pmatrix} \frac{M_1}{2} & 0 \\ 0 & \frac{M_1}{2} \end{pmatrix}. \tag{3.3}$$

From Fokker-Planck equation (2.5) we can easily obtain the following equation for the tensor A :

$$A_t + \vec{u}\cdot\nabla A = \nabla\vec{u}A + A(\nabla\vec{u})^T - \frac{4H}{\zeta}A - \frac{4HQ_0^2}{\zeta}\left(\frac{M_1^2/2Q_0^2}{1-2M_1/Q_0^2}\right)I + \frac{4kT}{\zeta}I. \quad (3.4)$$

Now we proceed to dynamic for the trace $\mathrm{tr}(A)$ and the determinant $\det A$.

$$\begin{aligned}(\mathrm{tr}(A))_t &= 2\nabla\vec{u}:A - \frac{4H}{\zeta}\left(\frac{1+M_1/Q_0^2}{1-2M_1/Q_0^2}\right)\mathrm{tr}(A)\\ &\quad+\frac{4H}{\zeta}\left(\frac{M_1^2/(2Q_0^2)}{1-2M_1/Q_0^2}\right)d + \frac{4kT}{\zeta}d, && (3.5)\\ (-\ln(\det A))_t &= -\frac{4H}{\zeta}\left(\frac{1+M_1/Q_0^2}{1-2M_1/Q_0^2}\right)d - \frac{4H}{\zeta}\left(\frac{M_1/(2Q_0^2)}{1-2M_1/Q_0^2}\right)\mathrm{tr}(A^{-1})\\ &\quad-\frac{4kT}{\zeta}\mathrm{tr}(A^{-1}) && (3.6)\end{aligned}$$

where d is the dimension of the microscopic configuration space.

Using (3.5), (3.6), and the identity, $\mathrm{tr}((I-A^{-1})^2A) = \mathrm{tr}(A) - 2d + \mathrm{tr}(A^{-1})$, we get the new exact energy law for the closure system (2.18)–(2.22) :

$$\begin{aligned}&\frac{d}{dt}\int\left[\frac{|\vec{u}|^2}{2} - \left\{\frac{kT}{2}\ln(\det A) + \frac{H}{4}\left(\mathrm{tr}(A) + \frac{3Q_0^2}{2}\ln\left(1-\frac{2\mathrm{tr}(A)}{Q_0^2}\right)\right)\right\}\right]dx =\\ &-\int\left[\mu|\nabla\vec{u}|^2 + \frac{2H^2}{\zeta}\left(\frac{1+M_1/Q_0^2}{1-2M_1/Q_0^2}\right)^2\left\{\mathrm{tr}(A) - \left(\frac{M_1^2}{2Q_0^2} + \frac{2kT}{H}\right)\left(\frac{1-2M_1/Q_0^2}{1+M_1/Q_0^2}\right)d\right\}\right]dx.\end{aligned}$$

If H is sufficiently large and the moment term, M_1, satisfies the following inequality:

$$\frac{Q_0}{\sqrt{HkTd}} < M_1 < \frac{Q_0^2}{2},$$

then we can prove the positivity of the following part in the above energy equation:

$$-\frac{kT}{2}\ln(\det A) - \frac{H}{4}\left\{\mathrm{tr}(A) + \frac{3Q_0^2}{2}\ln\left(1-\frac{2\mathrm{tr}(A)}{Q_0^2}\right)\right\}$$

assuming the tensor A is positive definite. Also, the positivity of the following part can be obtained through a careful calculation:

$$\begin{aligned}&\mathrm{tr}(A) - \left(\frac{M_1^2}{2Q_0^2} + \frac{2kT}{H}\right)\left(\frac{1-2M_1/Q_0^2}{1+M_1/Q_0^2}\right)d\\ &= \mathrm{tr}(A) - \left(\frac{M_1^2}{2Q_0^2} + \frac{2kT}{H}\right)\left(\frac{1-2M_1/Q_0^2}{1+2(M_1/Q_0^2)}\right)\left\{\mathrm{tr}(A) - \mathrm{tr}((I-A^{-1})^2A) + \mathrm{tr}(A^{-1})\right\}.\end{aligned}$$

From the above computations, we can observe the close relation between the microscopic entropy term, $f\ln f$, and the macroscopic terms, A, $\mathrm{tr}A$, and $\det A$ involving the second moments.

4. Post-Modifications of PDF. In this section we discuss the issue related to preserving the positivity of PDF in the microscopic level. Although the main interests in the moment-closure approximation procedure are the macroscopic quantities, for instance, the induced stress τ_p, the positivity property of the PDF could be an issue in the attempt to accurately describe the molecular behavior with the moment-closure approximation.

In our studies [15, 16] for moment-closure system, we became aware that for large flow rate, the approximated PDF given by the ansatz (2.12) can have negative values in some region due to the large contributions of Q_1Q_2, $Q_1^2 - Q_2^2$ terms in PDF (2.12). The presence of these negative values leads to a low accuracy in computations of the stress based on the second order moments, which is one of the important factors why the final moment closure system, FENE-S, fails to converge in large flow rate cases. Here, we introduce a modification scheme using the second order term Q^2 to enhance the positivity property of PDF by reducing the negative region of the PDF. This is rather independent of the higher order linear closure model proposed in [16].

The most naive way to prevent the negativity is to add some new terms that is positive, such as Q^2 term. However if we simply put this term as a correction term into the PDF ansatz, then this modification will bring in one extra unknown coefficient of Q^2 which would need the fourth order moments in the moment-closure equations. To avoid this drawback, we first assume that b, β, γ are known coefficients after solving the moment-closure system, and then we will treat the second order term Q^2 as a post-processing factor against negativity region of distribution function to get a better approximation with known three coefficients,

Now we describe the detail derivation of the modification scheme with simple calculations starting from considering the PDF model (2.12). Its numerical simulation results will be shown in the next section. To illustrate the method, we first try to obtain the minimum value in negative of (2.12) for the to-be-defined coefficient ω for Q^2. We consider the case when $1 + \beta Q_1Q_2 + \gamma(Q_1^2 - Q_2^2) < 0$,. Then this is rewritten as follows:

$$Q^2 \sin(2\theta + \phi)\sqrt{\left(\frac{\beta}{2}\right)^2 + \gamma^2} < -1, \tag{4.1}$$

where $\phi = \cos^{-1}(\beta/\sqrt{\beta^2 + 4\gamma^2})$ and (Q, θ) is the polar coordinate of $\vec{Q}$. Hence, if there exists a negative value, then the minimum value of (4.1) is on the line, $\hat{\theta} = \frac{3\pi}{4} \pm \frac{\phi}{2}$ with fixed Q. Thus, we only need to calculate the radial component $\hat{Q}$ of the minimum point $(\hat{Q}(\hat{\theta}), \hat{\theta})$. For fixed θ, the explicit form of $\hat{Q}$ is given by one of the following extreme points:

$$\hat{Q}(\theta) = Q_0\sqrt{\frac{\beta\sin\theta + 2\gamma\cos\theta - b\cos\theta/Q_0^2}{b\beta\cos^2\theta\sin\theta + b\gamma(\cos^3\theta - \cos\theta\sin^2\theta) + (\beta\sin\theta + 2\gamma\cos\theta)}}$$

or

$$\hat{Q}(\theta) = Q_0\sqrt{\frac{\beta\cos\theta - 2\gamma\sin\theta - b\sin\theta/Q_0^2}{b\beta\cos\theta\sin^2\theta + b\gamma(\cos^2\theta\sin\theta - \sin^3\theta) + (\beta\cos\theta - 2\gamma\sin\theta)}}.$$

Hence, the minimum value of f_a is one of its values at the extreme points $(\hat{Q}(\hat{\theta}), \hat{\theta})$ where $\hat{\theta} = \frac{3\pi}{4} - \frac{\phi}{2}$. Since f is symmetric to the origin, we only need to inspect the values at two extreme points.

Next, let $\tilde{f}$ be the modified PDF with an unknown coefficient $\omega(>0)$ for the second order term Q^2, which is given by

$$\tilde{f}(\vec{Q}) = \frac{1}{\tilde{J}_b}\left[1-\left(\frac{Q}{Q_0}\right)^2\right]^{b/2}(1+\beta Q_1Q_2+\gamma(Q_1^2-Q_2^2)+\omega Q^2) \tag{4.2}$$

under the assumption which is b, β, γ are known. Using the obtained minimum value, the ω is easily determined by

$$\omega = \left|\frac{1+\beta\hat{Q}^2\cos\hat{\theta}\sin\hat{\theta}+\gamma\hat{Q}^2(\cos^2\hat{\theta}-\sin^2\hat{\theta})}{\hat{Q}^2}\right|. \tag{4.3}$$

Consequently, the original moments, M_1, M_2, M_3, and normalizing factor J_b are changed to $\tilde{M}_1$, $\tilde{M}_2$, $\tilde{M}_3$ and $\tilde{J}_b$ respectively. The explicit forms of changed moments and normalizing factor are given by

$$\tilde{M}_1 = \frac{\left(1+\frac{4\omega Q_0^2}{b+6}\right)}{\left(1+\frac{2\omega Q_0^2}{b+4}\right)}M_1, \quad \tilde{M}_2 = \frac{J_b}{\tilde{J}_b}M_2, \quad \tilde{M}_3 = \frac{J_b}{\tilde{J}_b}M_3, \tag{4.4}$$

where $\tilde{J}_b = \frac{2\pi Q_0^2}{b+2}\left(1+\frac{2\omega Q_0^2}{b+4}\right)$, and the modified stress $\tilde{\tau}_p$ is

$$\tilde{\tau}_p = \lambda\frac{H(Q_0^2+\tilde{M}_1)}{Q_0^2-2\tilde{M}_1}\begin{pmatrix} \frac{1}{2}\tilde{M}_2 & \tilde{M}_3 \\ \tilde{M}_3 & -\frac{1}{2}\tilde{M}_2 \end{pmatrix}.$$

The modification affects the stress τ_p and the energy directly. When the parameter ω is sufficiently small, the moments $\tilde{M}_1$, $\tilde{M}_2$, $\tilde{M}_3$ will be close to the original moments M_1, M_2, M_3, respectively. On the other hand if ω is large, then the rate of change, $J_b/\tilde{J}_b$, for $\tilde{M}_2$, $\tilde{M}_3$ in (4.4) is more susceptible to the macroscopic stress on the flow than that for $\tilde{M}_1$. This implies that the modification ωQ^2 effectively moderates the response of the PDF to the change of flow rates. Moreover, the energy law with the modification is also changed as the energy law is a function that depends on the M_1. This means that the scheme almost preserves the previous energy approximation in certain range of flow rate. We also see that the rate of change $J_b/\tilde{J}_b \leq 1$, to M_2, M_3 is the same as in (4.4). This means that the ratio of stresses caused by stretching and rotation is preserved, hence the modification is not biased to the stresses. For convenience, we call the modified closure scheme described above the FENE-SM model.

It is known that the negative portion of PDF in the moment-closure system may significantly affect the errors of the approximate macroscopic moments from the coarse-graining point of view [2, 4]. Yet, when a shear flow rate is a quite large, such as 7 (non-dimensionalized value as in [15]), even though the approximate PDF has a negative region, the results for normal and shear stress are still accurate. Thus, if the an over-adjustment with ω may lead to worse results. Currently we lack an carefully designed analytical methodology to choose an optimal ω. In the next section, We present numerical result to verify the effect of this modification remedy for the case of a shear flow.

Let us note that for large extensional flow rates, the FENE dumbbell model displays some drastic behavior with the PDF behaving like two $\delta-$function (two spikes).

One can find a simple proof in [17], asymptotically. Resolving this behavior is one of important thing for FENE model. We introduced a FENE model denoted by FENE-D to catch its drastic behavior with employing a new variable for the spike positions [17]. The PDF for FENE-D closure system is in the form of

$$f_{\alpha,p}(\vec{Q}) = \frac{1}{2} f\left((\vec{Q}-\vec{\alpha})p\right) + \frac{1}{2} f\left((\vec{Q}+\vec{\alpha})p\right) . \tag{4.5}$$

and the additional equations for the spike positions are

$$\frac{\partial}{\partial t}\alpha_1 + \vec{u}\cdot\nabla\alpha_1 - \frac{\partial u}{\partial x}\alpha_1 - \frac{\partial u}{\partial y}\alpha_2 = -\frac{4}{\zeta}\int_{U_H}\left(\nabla\Psi\cdot\nabla_{\vec{Q}}Q_1\right) f\, d\vec{Q}, \tag{4.6}$$

$$\frac{\partial}{\partial t}\alpha_2 + \vec{u}\cdot\nabla\alpha_2 - \frac{\partial v}{\partial x}\alpha_1 - \frac{\partial v}{\partial y}\alpha_2 = -\frac{4}{\zeta}\int_{U_H}\left(\nabla\Psi\cdot\nabla_{\vec{Q}}Q_2\right) f\, d\vec{Q} \tag{4.7}$$

where U_H is a half domain of the microscopic domain U.

FENE-D model showed excellent agreement for the spike position in numerical simulations. On the other hand, because of approximation procedure of PDF it has some negative values of its PDF. Thus, the above modification scheme could be employed for FENE-D.

5. Maximum Entropy Principle with Macroscopic Flow Field. In this section we discuss the MEP for FENE model in the presence of external flow field. Let use recall the application of MEP for FENE model [21] in the stationary situation. To employ MEP, we consider the internal energy in the energy law (3.1). The internal energy form denoted by s, including entropy term is given by

$$s = -\int kTf\ln f + \Psi f\, d\vec{Q} \tag{5.1}$$

where Ψ is the FENE spring potential. Since we already assumed the stationary situation of macroscopic flow field, the internal energy form (5.1) does not have any macroscopic flow field relation.

The maximum entropy principle leads us to the following PDF

$$f_M = Ce^{-\Psi/kT}e^{\sum_a \lambda_a w_a} \tag{5.2}$$

where $C > 0$ is the normalizing constant, w_a denotes one of terms like 1, Q_1, Q_2, Q_1Q_2, Q_1^2, Q_2^2, $\cdots$, and λ_a is the Lagrange multiplier for the constraint which is the relation with moment given by

$$M_a = \int w_a f\, d\vec{Q}. \tag{5.3}$$

Using the FENE spring potential Ψ, the explicit form of PDF (5.2) is given by

$$f_M(\vec{Q}) = \frac{1}{J_M}\left[1-\frac{Q^2}{Q_0^2}\right]^{HQ_0^2/(2kT)} e^{\sum_a \lambda_a w_a} \tag{5.4}$$

where J_M is the normalizing factor.

In the moment-closure procedure based on the MEP, the PDF (5.4) leads to highly nonlinear integral equations. It requires much computational overhead costs [21]. To avoid the difficulty we introduced an approximation of (5.4) [18] of the form

$$f_M(\vec{Q}) \approx C\left[1-\frac{Q^2}{Q_0^2}\right]^{b/2}\left\{1+\eta Q^2+\beta Q_1Q_2+\gamma(Q_1^2-Q_2^2)\right\} \tag{5.5}$$

with unknown variables, β, γ, η which are related to the Lagrange multiplier where J is the normalizing factor for PDF, and here, b is a constant, $b = HQ_0^2/(kT)$. Then one can easily obtain the corresponding closure system [18] analytically.

The approximated PDF (5.5) is similar to that of FENE-S model. It has many advantages in deriving the corresponding energy law and in numerical simulations [18]. Yet, the PDF (5.5) suffers the same loss of positivity issue due to the approximation. The post-modification scheme given in the Section 4 can also be employed here to enhance the positivity of PDF (5.5). The form of PDF after modification is given by

$$f_{M,\omega}(\vec{Q}) = \frac{1}{J_{M,\omega}} \left[1 - \frac{Q^2}{Q_0^2}\right]^{b/2} \left\{1 + (\eta + \omega)Q^2 + \beta Q_1 Q_2 + \gamma(Q_1^2 - Q_2^2)\right\} \tag{5.6}$$

where ω is the post-modification factor and $J_{M,\omega}$ is the normalizing factor.

We now consider non-stationary situations with macroscopic flow field which is a simple extensional flow, $\vec{u} = (rx, -ry)$ where r is constant. The internal energy has an additional term caused by the flow field interaction.

Consider the energy functional, $\tilde{s}(\vec{u}, f)$,

$$\tilde{s}(\vec{u}, f) = -\int \left\{ kTf \ln f + \left(\Psi - \frac{\zeta}{4}\vec{Q}^T \kappa \vec{Q}\right) f \right\} d\vec{Q} \tag{5.7}$$

where $\kappa = \nabla \vec{u} = \mathrm{diag}(r, -r)$.

Applying MEP for (5.7), we easily get the following PDF maximizing the energy (5.7) under the constraint (5.3), M_a:

$$\tilde{f}_M(\vec{Q}) = \tilde{C} e^{-\Psi/(kT)} e^{\zeta \vec{Q}^T \kappa \vec{Q}/(4kT)} e^{\sum_a \lambda_a w_a}. \tag{5.8}$$

For the FENE model we have

$$\tilde{f}_M = \frac{1}{\tilde{J}_M} \left[1 - \frac{Q^2}{Q_0^2}\right]^{HQ_0^2/(2kT)} e^{\zeta r(Q_1^2 - Q_2^2)/(4kT)} e^{\sum_a \lambda_a w_a} \tag{5.9}$$

where $\tilde{J}_M$ is the normalizing factor.

As mentioned in Section 2, the second order terms play crucial roles in the moment-closure approximation procedure. Thus, $\sum_a \lambda_a w_a$ should include all the second order terms for microscopic level. For this reason, we see that the term, $\zeta r(Q_1^2 - Q_2^2)/(4kT)$, obtained from the simple extensional flow interaction, can be absorbed into $\sum_a \lambda_a w_a$ in (5.9).

Therefore, the PDF (5.9) has the same resulting form as the PDF (5.4) after absorbing $\zeta r(Q_1^2 - Q_2^2)/(4kT)$. This shows the fact that MEP for the internal energy (5.1) intrinsically includes the special case of flow field effects such as those in a simple extensional flow. Yet it remains unclear how to apply MEP in general cases of flow fields.

6. Numerical Simulations. In this section we perform several numerical experiments to validate/verify the positivity preserving scheme with FENE model. The closure equations on the microscopic configuration field are first considered with fixed flow field which is steady shear flows. Since the Fokker-Planck equation has no analytic solution except with symmetric velocity gradients, we compare the results with that from the direct computing the Chapman-Kolmogorov (Fokker-Planck) equations. For numerical experiments, we consider the spatially homogeneous situations, where the configuration field is independent of the microscopic spatial variables. We will focus on the following Fokker-Planck equation which is derived from (2.5) by using a standard scaling:

$$\frac{\partial f}{\partial t} + \nabla_{\vec{Q}} \cdot (\kappa \vec{Q} f) = \frac{1}{2}\left(\nabla_{\vec{Q}} \cdot (\nabla_{\vec{Q}} \Psi f) + \Delta_{\vec{Q}} f\right), \tag{6.1}$$

in the open domain $\Omega = \{\vec{Q} \in \mathbb{R}^2 \,|\, |\vec{Q}| < Q_0,\ Q_0 > 0\}$. To simplify the numerical simulations we use the following FENE spring force $\nabla_{\vec{Q}} \Psi$:

$$\nabla_{\vec{Q}} \Psi = \frac{\vec{Q}}{1 - Q^2/Q_0^2}.$$

When κ is symmetric, for instance a simple extensional flow with $\vec{u} = (rx, -ry)$, the steady-state solution to the Fokker-Planck equation (6.1) is given by

$$f(\vec{Q}) = \frac{1}{J_{eq}}\left[1 - \frac{Q^2}{Q_0^2}\right]^{Q_0^2/2} \exp(\vec{Q}^T \kappa \vec{Q}), \tag{6.2}$$

where J_{eq} is the normalizing constant.

If the velocity gradient has the exact form of $\nabla_{ij}\vec{u} = (\kappa_{ij})$, $i, j = 1, 2$ in $\mathbb{R}^2$, for arbitrary fluid flow, then from the reduced equation (6.1) the FENE-P model can be written as

$$\frac{\partial A}{\partial t} - \kappa A - A\kappa^T = 1 - \frac{A}{1 - \mathrm{tr}A/Q_0^2} \tag{6.3}$$

where A is the conformation tensor $\langle \vec{Q} \otimes \vec{Q} \rangle$ and $\mathrm{tr}A$ is the trace of A. The equation (6.3) can be rewritten again as the following system :

$$\frac{\partial M_1}{\partial t} - (\kappa_{11} - \kappa_{22})M_2 - (\kappa_{12} + \kappa_{21})M_3 = 2 + \frac{Q_0^2}{Q_0^2 - M_1}M_1, \tag{6.4}$$

$$\frac{\partial M_2}{\partial t} - (\kappa_{11} - \kappa_{22})M_1 - (\kappa_{12} - \kappa_{21})M_3 = -\frac{Q_0^2}{Q_0^2 - M_1}M_2, \tag{6.5}$$

$$\frac{\partial M_3}{\partial t} - (\kappa_{11} + \kappa_{22})M_1 + (\kappa_{12} - \kappa_{21})M_2 = -\frac{Q_0^2}{Q_0^2 - M_1}M_3, \tag{6.6}$$

and the corresponding explicit form of the moment-closure equations (2.20)–(2.22) for general κ case are as follows:

$$\frac{\partial M_1}{\partial t} - 2(\kappa_{12} + \kappa_{21})M_3 - (\kappa_{11} - \kappa_{22})M_2 = 2 - \frac{Q_0^2}{Q_0^2 - 2M_1}M_1, \tag{6.7}$$

$$\frac{\partial M_2}{\partial t} - 2(\kappa_{12} - \kappa_{21})M_3 - (\kappa_{11} - \kappa_{22})M_1 = -\frac{Q_0^2 + M_1}{Q_0^2 - 2M_1}M_2, \tag{6.8}$$

$$\frac{\partial M_3}{\partial t} - \frac{1}{2}(\kappa_{12} + \kappa_{21})M_1 + \frac{1}{2}(\kappa_{12} - \kappa_{21})M_2 = -\frac{Q_0^2 + M_1}{Q_0^2 - 2M_1}M_3. \tag{6.9}$$

The above system can then be solved by the 4th-order Runge-Kutta method in various cases.

Here, we consider the simple steady state shear flow situations, i.e., $\vec{u} = (ry, 0)$ where r is a constant shear rate. Then the homogeneous velocity gradient tensor κ

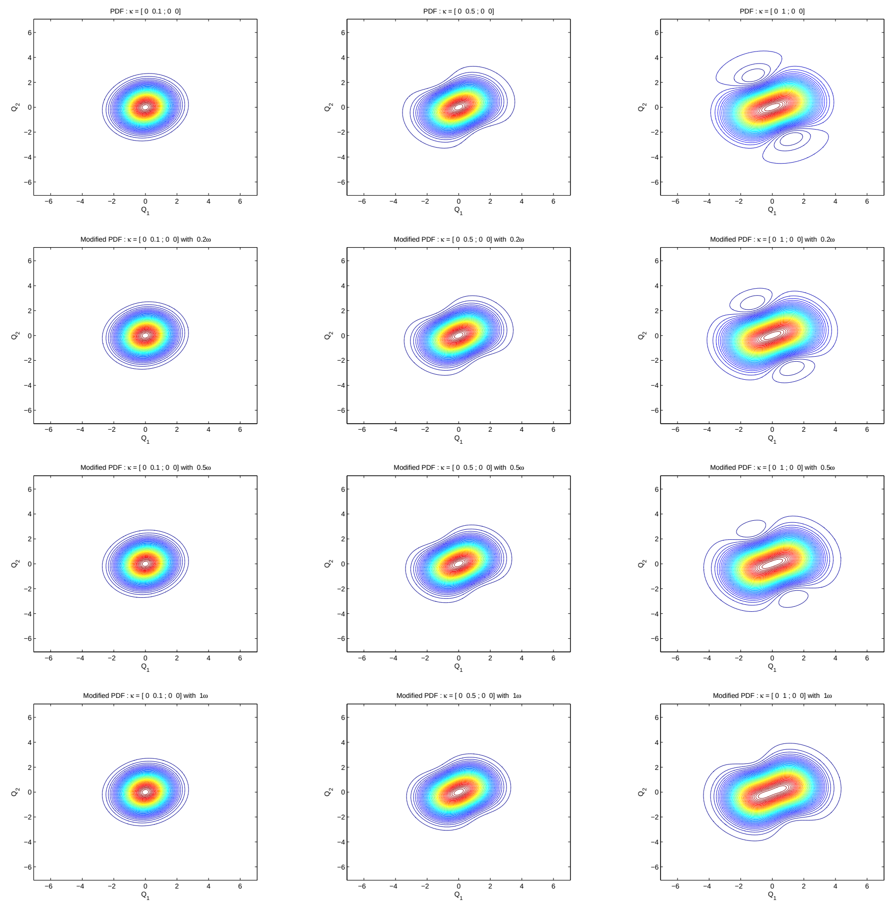

FIG. 6.1. *Comparison of the contour plots of the probability distribution functions solved from the FENE-S (first row), the FENE-SM(second, third, forth rows with* $0.2\omega Q^2$*,* $0.5\omega Q^2$*,* $1.0\omega Q^2$*, respectively) for* $r = 0.1,\ 0.5,\ 1.0$*, column-wise.*

is given by $\kappa_{11} = \kappa_{21} = \kappa_{22} = 0$ and $\kappa_{12} = r$. In this experiment we also consider the modification scheme which is described in section 4 for the PDF (2.12), which is referred as the FENE-SM model. In Figure 6.1, we show the contour plot of PDF for which the flow rate in units of $\zeta/4H$ are $r = 0.1,\ 0.5,\ 1.0$, for each column. The pictures in the first row are obtained by the moment-closure system FENE-S with the PDF (2.12). We can see that the first and second column pictures are almost identical for each columns in certain moderate flow rate because the PDF (2.12) has a minimum value which is negative and its absolute value is very small. On the other hand, in the third column the pictures for $r = 1.0$ graphically show that the positivity preserving scheme is effective to adjust the negative value of the PDF (2.12) though it also reduces the concentration of PDF value around the origin.

In Figure 6.2, we show a comparison of the normal stress, $\tau_{11} - \tau_{22}$, and the shear stress, τ_{12}, or τ_{21}, with modification via FENE-SM using 0.2ω, 0.5ω, 1.0ω. We have much better results of the stresses when the factor is 0.2, especially, on the normal stress. In shear stress case the modification enhances results except for flow rate $r > 1.7$. Thus, this post-processing can be an efficient remedy scheme for certain large flow rate without requiring much extra computational efforts.

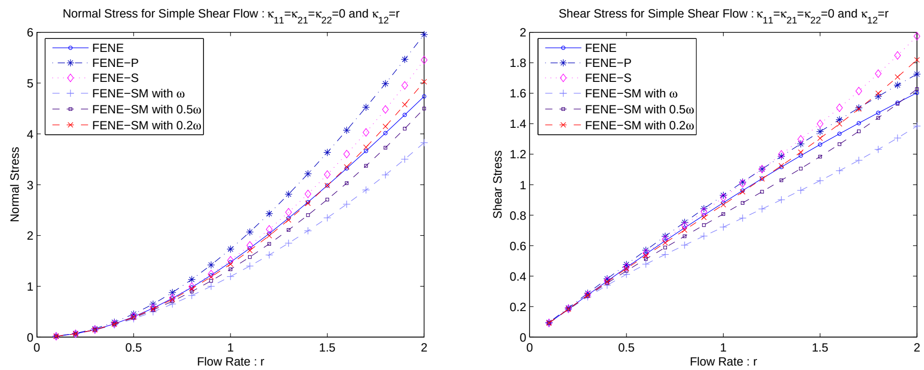

FIG. 6.2. *Comparison of the elastic energy for the shear flow by solving Fokker-Planck and that from FENE-SM with* 0.2ω, 0.5ω, 1.0ω *for the PDF (2.12).*

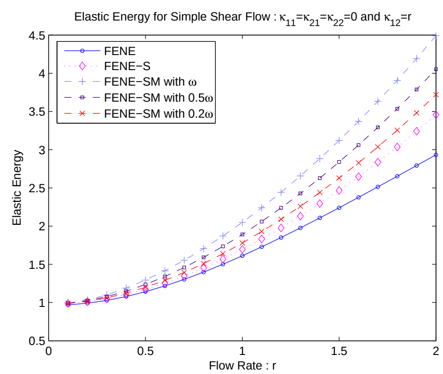

FIG. 6.3. *Comparison of the normal stress (left) and the shear stress (right) for the shear flow by solving Fokker-Planck and that from FENE-SM with* 0.2ω, 0.5ω, 1.0ω *for the PDF (2.12).*

We show that normal and shear stresses for FENE-SM are better than that of FENE-P in moderate simple shear flow cases, and in normal stress case the modified PDF has better results than FENE-P for quite large flow rates. Additionally, we also get better approximation of the macroscopic stress and PDF using the modification scheme.

In Figure 6.3 we show a comparison of the elastic energy, $\int \Psi f \, d\vec{Q}$ for FENE, $E(M_1) = -\frac{1}{4}M_1 - \frac{3}{8}Q_0^2 \log\left(1 - \frac{2M_1}{Q_0^2}\right)$ derived in [15], for FENE-S, and $E(\tilde{M}_1)$ for FENE-SM with various ratio of ω. Since the energy equation $E(M_1)$ only depends on the moment M_1 and more sensitive on changing of the logarithm part, the positivity preserving scheme shows that the energy obtained by the modified moment, $\tilde{M}_1$, is similar to that for FENE-S in certain range of flow rate, $r \leq 1$, with small ratio of ω in Figure 6.3. In other cases of the ratio of ω or large flow rates, the positivity preserving scheme increases the elastic energy.

7. Conclusions. In this study, we discussed the issue of preserving positivity of the PDF for FENE-S. We introduced a modification scheme as an effective post-processing scheme. The exact energy law for FENE-S was also presented. The numerical experiments showed significant improvement for representing the PDF as well as for evaluating the induced stresses, especially, with $0.2\omega Q^2$. We should mention the fact that the modification scheme reduces some negative region but not the whole negative region. The scheme can be interpreted as providing an adjustment to obtain better PDF and the induced stress. Another important factor in the modification scheme is to obtain the optimal value for ω. In this paper the ratio of ω is obtained in a empirical way. Thus, to find the optimal ratio for ω in analytic from is an important project in our ongoing work. In this study, we also discussed the application of MEP with macroscopic flow field. We made the first attempt to include the simple extensional flow. To extend the method to more general flow is still open at the current stage.

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