Journal of Computational Mathematics, Vol.22, No.2, 2004, 319–330.

A THEORETICAL AND NUMERICAL STUDY FOR THE ROD-LIKE MODEL OF A POLYMERIC FLUID *1)

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Dedicated to Professor Zhong-ci Shi on the occasion of his 70th birthday

Abstract

The first part of this paper is concerned with the well-posedness for the rigid rod-like model in shear flow of a polymeric fluid. The constitutive relations considered in this work are motivated by the kinetic theory. The stress tensor is given by an integral which involves the solution of the Fokker-Planck equation. A novel numerical scheme for the Fokker-Planck equation is proposed, which preserves the positivity of the distribution function. Another part of this work establishes the convergence theory of the fully discretized schemes for a simple micro-macro simulation of a polymeric flow.

Mathematics subject classification: 76B03, 65M12, 35Q35
Key words: Polymeric fluid, Rod-like model, Kinetic theory, Convergence.

1. Introduction

The study of polymeric flow is motivated by the interest of understanding how large molecules interact with each other and with the flow, as well as by the desire of obtaining the continuum constitutive relation in the modeling of the process flow systems. The most well studied continuum constitutive equation for modeling rigid rod polymer comes from the Leslie-Ericksen theory in Chapter 7 of [3]. However, it is only valid for low deformation rates, and is not appropriate for describing the rheological properties such as shear thinning. Other continuum theories for the rigid rod and liquid crystalline solutions have been developed in Chapter 11-13 of [2], which can handle liquid crystalline polymers, as they allow the inclusion of an intermolecular potential. If we denote by $\mathbf{u}$ and p the velocity and pressure of the fluid, ψ the joint position-configuration distribution function, then the rigid rod-like model can be expressed as

$$\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \frac{\gamma}{Re}\triangle\mathbf{u} + \frac{1-\gamma}{ReDe}\nabla\cdot\tau \tag{1.1}$$

$$\nabla\cdot\mathbf{u} = 0 \tag{1.2}$$

$$\frac{\partial\psi}{\partial t} = \frac{1}{De}\mathcal{R}\cdot[\mathcal{R}\psi + \psi\mathcal{R}U] - \mathcal{R}\cdot(\mathbf{m}\times\kappa\cdot\mathbf{m}\psi) \tag{1.3}$$

$$U = U_0\int_{|\mathbf{m}'|=1}|\mathbf{m}\times\mathbf{m}'|^2\psi(\mathbf{x},\mathbf{m}',t)d\mathbf{m}' \tag{1.4}$$

$$\tau_{ij} = 3S_{ij} - \langle(\mathbf{m}\times\mathcal{R}U)_i m_j\rangle + \frac{De}{2}\kappa_{kl}\langle m_i m_j m_k m_l\rangle \tag{1.5}$$

where (1.1) is the governing equation of the macroscopic isothermal flow of an incompressible fluid by the momentum balance, (1.2) the continuity equation, De, Re are Deborah and

* Received January 31, 2004.

1) Hui Zhang acknowledges the financial assistance of the National Post-Doctoral Science Foundation of China. Pingwen Zhang is partially supported by the special funds for Major State Research Projects G1999032804 and National Science Foundation of China for Distinguished Young Scholars 10225103.

Reynolds constants, respectively; $0 < \gamma < 1$ is a given constant; $\mathbf{m}$ is the configuration of the rod-like particle, $\mathcal{R} = \mathbf{m} \times \frac{\partial}{\partial \mathbf{m}}$ is the rotational operator, $\kappa = (\nabla \mathbf{u})^T$, U represents the excluded-volume potential of the Maier-Sauper form [2]; S is the order tensor

$$S_{ij} = \langle m_i m_j - \frac{1}{3}\delta_{ij} \rangle$$

and $\langle \cdot \rangle$ denotes the average operator

$$\langle g \rangle = \int_{|\mathbf{m}|=1} g\psi d\mathbf{m}.$$

In contrast to traditional models of complex fluids which express polymer stress τ using empirical constitutive relations, (1.5) expresses the polymer stress in terms of the microscopic conformations of the polymers.

The Doi theory (1.1)-(1.5) takes into account the effects of flow, Brownian motion and intermolecular forces on the molecular orientation distribution. Thus it gives a good representation of the molecular viscoelasticity. Numerical results in [1, 4, 10, 11, 12, 14] have shown that the rigid rod-like model is indeed capable of predicting most of the rheological response of polymers in the nematic phase, including the existence of ranges of shear rates with negative values of the first normal stress difference, and dynamics such as tumbling, wagging, log rolling and kayaking etc.

The present work aims at giving a global existence theory and a numerical analysis for the system (1.1)-(1.5) in a simple case, which may be useful for analyzing more complicated models. To this end, we will consider the "1+1"-dimensional case and the pressure driven channel flow. More precisely, we assume that the rod-like particles rotate in shear plane, and

$$\mathbf{u} = (u, 0)^T, \;\; \nabla = (0, \partial y)^T, \;\; \nabla p = (c, 0)^T$$

where c is a positive constant. Under these assumptions, (1.1)-(1.5) becomes

$$\begin{cases} u_t + c = \dfrac{\gamma}{Re} u_{yy} + \dfrac{1-\gamma}{De\, Re} \tau_y, & y \in (0,1), \\ \psi_t = \dfrac{1}{De}\psi_{\theta\theta} + \dfrac{1}{De}(\psi U_\theta)_\theta + u_y(\psi \sin^2\theta)_\theta, & \theta \in S^1, \\ U = U_0 \displaystyle\int_0^{2\pi} \sin^2(\theta - \theta')\psi(y, \theta', t) d\theta' \\ \tau = 2\langle \sin\theta\cos\theta \rangle + \langle U_\theta \cos^2\theta \rangle + \dfrac{De}{2} u_y \cdot \langle \sin^2\theta \cos^2\theta \rangle, \end{cases} \tag{1.6}$$

where S^1 is the unit circle. This is a coupled non-linear parabolic system. Despite the simplicity of the underlying model, our work is a first step towards the better understanding for more sophisticated models that are commonly used in the context of the so called micro-macro approach in computational rheology [1, 4, 10, 11, 12, 14].

The first part of this study is to establish the global existence theory for the system (1.6), which is done by utilizing the result for the linear parabolic equations. A linearization technique will be used for this nonlinear system. The second part of this study is to analyze some numerical schemes for (1.6). Large scale computer simulations have been proven very valuable in the field of polymeric flow modeling. With continuum models, predictions for the stress and velocity in complicated flow geometries have been achieved mainly by computational simulations. However, the interesting aspects of the polymer flow behavior are inherently due to their molecular structure. The task of solving the continuum model equations involves either computing the all of the molecule configurations or computing the pointwise probability distribution function. In the past, it had been unpractical to attempt such molecular level simulations. However, with the great leaps in the computational capability over the last two decades, this can now be done with very simple molecular models. The success of research in this area is dependent on the numerical methods available and on the validity of the physical models employed. In this work, we take the approach of computing the probability distribution of molecules pointwise in space. We will design a simple implicit finite difference scheme to solve the distribution function, with particular attention to guarantee its non-negativity property. The non-negativity of the probability distribution, second order rate of convergence and the discrete inverse inequality are three crucial elements for the establishment of the convergence theory for the fully discretized scheme.

This paper is organized as follows. We prove the global existence of the solution in Section 2. Section 3 is devoted to the numerical analysis to the model (1.6).

2. Exsistence

In this section, we consider the existence of the (1.6). To this end, we first rewrite (1.6) in the following equivalent form:

$$u_t - a(y,t)u_{yy} + b(y,t)u_y = g(y,t) \tag{2.1}$$

$$\psi_t - \frac{1}{De}\psi_{\theta\theta} + A(y,\theta,t)\psi_\theta + B(y,\theta,t)\psi = 0, \tag{2.2}$$

where

$$b(y,t) = \frac{1-\gamma}{2Re}\int_0^{2\pi} \sin^2\theta\cos^2\theta\psi_y(y,\theta,t)d\theta \tag{2.3}$$

$$a(y,t) = \frac{1-\gamma}{2Re}\int_0^{2\pi} \sin^2\theta\cos^2\theta\psi(y,\theta,t)d\theta + \frac{\gamma}{Re}, \tag{2.4}$$

$$\begin{aligned} g(y,t) = {} & \frac{2(1-\gamma)}{DeRe}\int_0^{2\pi} \sin\theta\cos\theta\psi_y(y,\theta,t)d\theta - c \\ & -\frac{\alpha(1-\gamma)}{DeRe}\int_0^{2\pi}\int_0^{2\pi} \cos^2\theta\sin 2(\theta-\theta')[\psi_y(y,\theta',t)\psi(y,\theta,t) \\ & +\psi_y(y,\theta,t)\psi(y,\theta',t)]d\theta' d\theta, \end{aligned} \tag{2.5}$$

$$A(y,\theta,t) = -\frac{1}{De}\int_0^{2\pi} \sin 2(\theta-\theta')\psi(y,\theta',t)d\theta' - u_y\sin^2\theta, \tag{2.6}$$

$$B(y,\theta,t) = -\frac{1}{De}\int_0^{2\pi} 2\cos 2(\theta-\theta')\psi(y,\theta',t)d\theta' - u_y\sin 2\theta. \tag{2.7}$$

Now we consider the initial-boundary problem (2.1)-(2.2) with the initial data

$$u(y,0) = u_0(y), \qquad \psi(y,\theta,0) = \psi_0(y,\theta) \geq 0, \tag{2.8}$$

and the boundary conditions

$$u(0,t) = u(1,t) = 0. \tag{2.9}$$

Since $\psi(y,\theta,t)$ is the distribution function, it satisfies

$$\int_0^{2\pi} \psi(y,\theta,t)d\theta = 1 \qquad \forall y \in [0,1] \text{ and } t \geq 0 \tag{2.10}$$

and is periodic in space variable θ, i.e.

$$\psi(y,\theta,t) = \psi(y,2\pi+\theta,t), \qquad \forall y,t. \tag{2.11}$$

The restriction to the initial data

$$\int_0^{2\pi} \psi_0(y,\theta,t)d\theta = 1, \text{ and } \psi_0(y,\theta) = \psi_0(y, 2\pi+\theta), \qquad \forall y \tag{2.12}$$

implies that (2.10)-(2.11) are true from the second equation of (1.6). Meanwhile we can see that $\psi \equiv 0$ is one of its sub-solutions. So $\psi \geq 0$ as $\psi_0 \geq 0$ for all $t \geq 0$.

Below we will introduce some notations. Let Ω be a bounded domain in $\mathbb{R}^n$ and S the boundary of Ω. $\bar{\Omega}$ is the closure of Ω, i.e. $\bar{\Omega} = \Omega \cup S$ and Q_T is the cylinder $\Omega \times (0,T)$. Let $C^l(\bar{\Omega})$ denote the Banach space whose element $u(x)$ is continuous in Ω, has continuous derivatives up to order $[l]$ in $\bar{\Omega}$ and also has a finite value for quantity

$$|u|_{\Omega}^{(l)} = \ll u \gg_{\Omega}^{(l)} + \sum_{j=0}^{[l]} \ll u \gg_{\Omega}^{(j)}, \tag{2.13}$$

where

$$\begin{aligned}
&|u|_{\Omega}^{(0)} \equiv |u|_{\Omega}^{(0)} = \max_{\Omega} |u|,\\
&\ll u \gg_{\Omega}^{(j)} = \sum_{(j)} |D_x^j u|_{\Omega}^{(0)},\\
&\ll u \gg_{\Omega}^{(l)} = \sum_{([l])} \ll D_x^{[l]} u \gg_{\Omega}^{(l-[l])},\\
&\ll u \gg_{\Omega}^{(\alpha)} = \sum_{x,x'\in\Omega, |x-x'|\leq\rho_0} \frac{|u(x)-u(x')|}{|x-x'|^{\alpha}}, \quad \rho_0 \text{ is a constant.}
\end{aligned}$$

Equality (2.13) defines the norm $|u|_{\Omega}^{(l)}$ in $C^l(\bar{\Omega})$. Furthermore, let $C^{l,l/2}(\bar{Q}_T)$ be the Banach space of functions $u(x,t)$ that are continuous in $\bar{Q}_T$, which has derivatives of the form $D_t^r D_x^s$ for $2r+s<l$, and has a finite norm

$$|u|_{Q_T}^{(l)} = \ll u \gg_{Q_T}^{(l)} + \sum_{j=0}^{[l]} \ll u \gg_{Q_T}^{(j)},$$

where

$$\begin{aligned}
&|u|_{Q_T}^{(0)} \equiv |u|_{Q_T}^{(0)} = \max_{Q_T} |u|,\\
&\ll u \gg_{Q_T}^{(j)} = \sum_{(2r+s=j)} |D_t^r D_x^s u|_{Q_T}^{(0)},\\
&\ll u \gg_{Q_T}^{(l)} = \ll u \gg_{x,Q_T}^{(l)} + \ll u \gg_{t,Q_T}^{(l/2)},\\
&\ll u \gg_{x,Q_T}^{(l)} = \sum_{(2r+s=[l])} \ll D_t^r D_x^s u \gg_{x,Q_T}^{(l-[l])},\\
&\ll u \gg_{t,Q_T}^{(l/2)} = \sum_{0<l-2r-s<2} \ll D_t^r D_x^s u \gg_{t,Q_T}^{(\frac{l-2r-s}{2})};\\
&\ll u \gg_{x,Q_T}^{(\alpha)} = \sup_{(x,t),(x',t)\in\bar{Q}_T; |x-x'|\leq\rho_0} \frac{|u(x,t)-u(x',t)|}{|x-x'|^{\alpha}}, \ 0<\alpha<1,\\
&\ll u \gg_{t,Q_T}^{(\alpha)} = \sup_{(x,t),(x,t')\in\bar{Q}_T; |t-t'|\leq\rho_0} \frac{|u(x,t)-u(x',t)|}{|t-t'|^{\alpha}}, \ 0<\alpha<1.
\end{aligned}$$

We denote by $\mathcal{L}(x,t,\partial/\partial x,\partial/\partial t)$ the linear uniformly parabolic differential operator with real coefficients:

$$\begin{aligned}\mathcal{L}\left(x,t,\frac{\partial}{\partial x},\frac{\partial}{\partial t}\right)u &= \frac{\partial u}{\partial t}-\sum_{i,j=1}^{n}a_{ij}(x,t)\frac{\partial^2 u}{\partial x_i\partial x_j}\\ &\quad +\sum_{i=1}^{n}a_i(x,t)\frac{\partial u}{\partial x_i}+a(x,t)u. \end{aligned} \tag{2.14}$$

A crucial lemma useful for establishing the existence theory for (2.1)-(2.9) is the one given in Section 5 of Chapter IV in [6]. For completeness, it is stated below.

Lemma 2.1. *Let $l>0$ be a non-integral number. Assume that the coefficients of the operator $\mathcal{L}$ defined in (2.14) belongs to $C^{l,l/2}(\bar{Q}_T)$, and that the boundary S belongs to C^{l+2}. Then for any $g\in C^{l,l/2}(\bar{Q}_T), \phi\in C^{l+2}(\bar{\Omega}), \Phi\in C^{l+2,l/2+1}(\bar{S}_T)$ satisfying the compatibility condition of order $[l/2]+1$, the initial boundary problem*

$$\mathcal{L}\left(x,t,\frac{\partial}{\partial x},\frac{\partial}{\partial t}\right)u(x,t)=g(x,t), \tag{2.15}$$

$$u|_{t=0}=\phi(x),\quad u|_{S_T}=\Phi(x,t), \tag{2.16}$$

has a unique solution in $C^{l+2,l/2+1}(\bar{Q}_T)$. Moreover, the solution of the above system satisfies the following estimate:

$$|u|_Q^{(l+2)}\le C(|g|_Q^{(l)}+|\phi|_\Omega^{(l+2)}+|\Phi|_{S_T}^{(l+2)}). \tag{2.17}$$

Next we will consider the well-posedness of the initial boundary value problem (2.1)-(2.9). Let $\{u^{(0)},\psi^{(0)}\}=\{u_0,\psi_0\}$. We define $\{u^{(n)},\psi^{(n)}\}$ recursively by alternately solving the following decoupled linear problem:

$$u_t^{(n+1)}-a(y,t)u_{yy}^{(n+1)}+b(y,t)u_y^{(n+1)}=g(y,t) \tag{2.18}$$

$$u^{(n+1)}(y,0)=u_0(y),\qquad u^{(n+1)}(0,t)=u^{(n+1)}(1,t)=0, \tag{2.19}$$

where

$$b(y,t)=\frac{1-\gamma}{2Re}\int_0^{2\pi}\sin^2\theta\cos^2\theta\psi_y^{(n)}(y,\theta,t)d\theta \tag{2.20}$$

$$a(y,t)=\frac{1-\gamma}{2Re}\int_0^{2\pi}\sin^2\theta\cos^2\theta\psi^{(n)}(y,\theta,t)d\theta+\frac{\gamma}{Re} \tag{2.21}$$

$$\begin{aligned}g(y,t)&=\frac{2(1-\gamma)}{DeRe}\int_0^{2\pi}\sin\theta\cos\theta\psi_y^{(n)}(y,\theta,t)d\theta-c\\ &\quad-\frac{\alpha(1-\gamma)}{DeRe}\int_0^{2\pi}\int_0^{2\pi}\cos^2\theta\sin 2(\theta-\theta')[\psi_y^{(n)}(y,\theta',t)\psi^{(n)}(y,\theta,t)\\ &\quad+\psi_y^{(n)}(y,\theta,t)\psi^{(n)}(y,\theta',t)]d\theta'd\theta;\end{aligned} \tag{2.22}$$

and

$$\psi_t^{(n+1)}-\frac{1}{De}\psi_{\theta\theta}^{(n+1)}+A(y,\theta,t)\psi_\theta^{(n+1)}+B(y,\theta,t)\psi^{(n+1)}=0, \tag{2.23}$$

$$\psi^{(n+1)}(y,\theta,0)=\psi_0(y,\theta)\ge 0, \tag{2.24}$$

where

$$A(y,\theta,t) = -\frac{1}{De}\int_0^{2\pi} \sin 2(\theta-\theta')\psi^{(n)}(y,\theta',t)d\theta' - u_y^{(n)}\sin^2\theta, \tag{2.25}$$

$$B(y,\theta,t) = -\frac{1}{De}\int_0^{2\pi} 2\cos 2(\theta-\theta')\psi^{(n)}(y,\theta',t)d\theta' - u_y^{(n)}\sin 2\theta. \tag{2.26}$$

It can be verified that for any constant $\gamma > 0$ the function $a(y,t)$ is upper bounded by γ/Re. Hence the equation (2.18) is uniformly parabolic. By Lemma 2.1 we can obtain:

Lemma 2.2. *Let $l > 0$ be a non-integral number. Assume that $\psi_0 \in C^{l+2}(S^1) \cap C^{l+1}([0,1] \times S^1)$, $u_0 \in C^{l+2}([0,1])$, $u_0(y)$ satisfies the compatibility condition of order $[l/2]+1$. For any given $T > 0$, if $u^{(n)} \in C^{l+2,l/2+1}([0,1]\times[0,T])$ and $\psi^{(n)} \in C^{l+2,l/2+1}(S^1\times[0,T]) \cap C^{l+1,l/2+1/2}(([0,1]\times S^1)\times[0,T])$ are given, then the initial boundary problem (2.18)-(2.19) has a unique solution $u^{(n+1)} \in C^{l+2,l/2+1}([0,1]\times[0,T])$ for any given $\gamma > 0$. Moreover, the solution of (2.18)-(2.19) satisfies the following estimate:*

$$|u^{(n+1)}|^{(l+2)} \le Te^{CT}|u_0|^{(l+2)}_{([0,1])}. \tag{2.27}$$

Proof. Since $\psi^{(n)} \in C^{l+2,l/2+1}(S^1\times[0,T]) \cap C^{l+1,l/2+1/2}(([0,1]\times S^1)\times[0,T])$, it is easy to verify that the coefficients of the equation (2.18) satisfies the conditions stated in Lemma 2.1. A direct application of Lemma 2.1 yields the existence and uniqueness result. The estimate (2.27) can be established following the method of Lemma 1 of Page 229 in [5].

Next we consider the equation for $\psi^{(n+1)}$. The equation (2.23) is a uniformly parabolic equation, in which the derivatives are with respect to θ and t, while y appears only as a parameter.

Lemma 2.3. *Let $l > 0$ be a non-integral number. Assume that $\psi_0 \in C^{l+2}(S^1) \cap C^{l+1}([0,1] \times S^1)$, and is periodic for the variable θ of order $[l]+2$. For any given $T > 0$, if $u^{(n)} \in C^{l+2,l/2+1}([0,1]\times[0,T])$ and $\psi^{(n)} \in C^{l+2,l/2+1}(S^1\times[0,T]) \cap C^{l+1,l/2+1/2}(([0,1]\times S^1)\times[0,T])$ are given, then the problem (2.23)-(2.24) has a unique solution $\psi^{(n+1)} \in C^{l+2,l/2+1}(S^1\times[0,T]) \cap C^{l+1,l/2+1/2}(([0,1]\times S^1)\times[0,T])$ which is periodic for the variable θ of order $[l]+2$. Moreover, the following estimates for $\psi^{(n+1)}$ hold:*

$$|\psi^{(n+1)}|^{(l+2)}_{S^1} \le e^{C'T}|\psi_0|^{(l+2)}_{S^1}, \qquad |\psi^{(n+1)}|^{(l+1)}_{([0,1]\times S^1)} \le e^{C'T}|\psi_0|^{(l+1)}_{([0,1]\times S^1)}. \tag{2.28}$$

Proof. The periodicity of $\psi^{(n+1)}$ with respect to θ can easily be obtained by the second equation of (1.6). So we only prove the existence and regularity for $\theta \in S^1$. Since $u^{(n)} \in C^{l+2,l/2+1}([0,1]\times[0,T])$, we can verify that $A(y,\theta,t)$ and $B(y,\theta,t)$ belong to $C^{l+1,l/2+1/2}(([0,1]\times S^1)\times[0,T])$. If we take the variable y as a parameter, then the equation (2.23) satisfies the conditions stated in Lemma 2.1 with respect to θ and t. Therefore, we have the existence of $\psi^{(n+1)}$ and the regularity of $\psi^{(n+1)}(\theta,t) \in C^{l+2,l/2+1}(S^1\times[0,T])$. Next we prove $\psi^{(n+1)}$ possesses the desired regularity with respect to y. For $y \in (0,1)$ and $y+\Delta y \in [0,1]$, we set

$$\Psi(y,\theta,t) = \delta_{y,\beta}\psi^{(n+1)}(y,\theta,t),$$

where the operator δ is defined by

$$\delta_{y,\beta}w(y,\theta,t) = \frac{w(y+\Delta y,\theta,t) - w(y,\theta,t)}{|\Delta y|^\beta}, \quad 0 < \beta < 1. \tag{2.29}$$

Then $\Psi(y,\theta,t)$ satisfies the equation

$$\Psi_t(y,\theta,t) - \frac{1}{De}\Psi_{\theta\theta}(y,\theta,t) + A(y+\Delta y,\theta,t)\Psi_\theta(y,\theta,t) + B(y+\Delta y,\theta,t)\Psi(y,\theta,t)$$
$$= -\delta_{y,\beta}A(y,\theta,t)\psi_\theta^{(n+1)}(y,\theta,t) - \delta_{y,\beta}B(y,\theta,t)\psi^{(n+1)}(y,\theta,t), \tag{2.30}$$
$$\Psi(y,\theta,0) = \delta_{y,\beta}\psi_0(y,\theta). \tag{2.31}$$

Since $u_y^{(n)}(y,t) \in C^{1+l,l/2+1}([0,1]\times[0,T])$, $\psi^{(n)} \in C^{l+1,l/2+1/2}(([0,1]\times S^1)\times[0,T])$ and $\psi^{(n+1)}(\theta,t) \in C^{l+2,l/2+1}(S^1\times[0,T])$, it can be verified that the coefficients of (2.30) also satisfy the conditions of Lemma 2.1 for the variables θ and t. Therefore, it follows that $|\Psi(y,\theta,t)|$ is bounded for the parameter $y \in (0,1)$, which implies that $\psi^{(n+1)}$ is hölder continuous with respect to β. Similarly, we set

$$\phi(y,\theta,t) = \psi_y^{(n+1)}(y,\theta,t), \qquad \Phi(y,\theta,t) = \delta_{y,\beta}\phi^{(n+1)}(y,\theta,t),$$

where the operator $\delta_{y,\beta}$ is defined by (2.29). By differentiating the equation (2.23) with respect to y, we can obtain the equations for ϕ and Φ:

$$\phi_t - \frac{1}{De}\phi_{\theta\theta} + A\phi_\theta + B\phi = -A_y(y,\theta,t)\psi_\theta^{(n+1)} - B_y(y,\theta,t)\psi^{(n+1)} \tag{2.32}$$

$$\begin{aligned}&\Phi_t - \frac{1}{De}\Phi_{\theta\theta} + A(y+\Delta y,\theta,t)\Phi_\theta + B(y+\Delta y,\theta,t)\Phi\\ = \;& -\delta_{y,\beta}A(y,\theta,t) - \delta_{y,\beta}B\cdot\phi(y,\theta,t) - A_y(y+\Delta y,\theta,t)\Psi(y,\theta,t)\\ & -\delta_{y,\beta}A_y\cdot\psi_\theta^{(n+1)}(y,\theta,t) - B_y(y+\Delta y,\theta,t)\Psi(y,\theta,t) - \delta_{y,\beta}B_y\cdot\psi^{(n+1)}.\end{aligned} \tag{2.33}$$

The repeated utilization of the above method concludes that $\phi(y,\theta,t)$ and $\Phi(y,\theta,t)$ are bounded for the parameter $y\in(0,1)$. Higher order derivatives with respect to θ and y can be estimated similarly. Thus we obtain

$$\psi^{(n+1)} \in C^{l+2,l/2+1}(S^1\times[0,T]) \cap C^{l+1,l/2+1/2}(([0,1]\times S^1)\times[0,T]).$$

This completes the proof of this lemma.

It follows from the above two lemmas that there exist two sequences $\{u^{(n)}\}$ and $\{\psi^{(n)}\}$ possessing certain regularity for the variables y,θ and t. Arzelà Lemma implies that there exists a pair of convergent sub-sequences $\{u^{(n)},\psi^{(n)}\}$ (still denoted by the same notation) which are the solution of the problem (2.1)-(2.9). More precisely, we end up with the following result.

Theorem 2.1. *Let $l > 0$ be a non-integral number. Assume that $u_0 \in C^{l+2}([0,1]), \psi_0 \in C^{l+2}(S^1)\cap C^{l+1}([0,1]\times S^1)$, $u_0(y)$ satisfies the compatibility condition of order $[l/2]+1$, and ψ_0 satisfies the restriction* (2.12). *For any give $T > 0$ and $\gamma > 0$, the problem* (2.1)-(2.9) *possesses a unique pair of solutions $\{u,\psi\} \in C^{[l]+2,[l]/2+1}_{([0,1]\times[0,T])} \times \left(C^{[l+2],[l]/2+1}_{(S^1\times[0,T])} \cap C^{[l+1],[l+1]/2}_{(([0,1]\times S^1)\times[0,T])}\right)$.*

3. Numerical Analysis

Several landmarks studies of Brownian dynamics for polymers have been performed in past to assess the effect of including hydrodynamic interaction in the governing equations. Öttinger and Laso [8] were the first to combine finite element techniques with Brownian dynamics simulation to compute particle orientation averages at every node in the solution domain. Their method is known as CONNFFESSIT (Calculation Of Non-Newtonian Flow: Finite Elements and Stochastic SImulation Techniques). Brownian Configuration Fields (BCF) introduced by van den Brule et al. [7] abandons the CONNFFESSIT idea of computing stress by averaging over large collections of independently acting molecules, in analogy with real physical systems.

Instead, it introduces a large ensemble of configuration fields. The Langevin equations for the motion of collection of polymer molecules are stochastic equivalent, both physically and mathematically, of the Fokker-Planck equations for evolution of the probability distribution of configurations. Spherical harmonic [4, 10] were chosen because an expansion in this basis not only can describe the equilibrium spherical distribution function exactly, but also can describe very accurately the small deviations from the equilibrium distribution that are produced by lower shear rate flow. The wavelet basis is known to provide efficient representation of peaked and localized functions. Nayak [13] uses the wavelets as basis functions in solution of the equation for the orientation probability distribution. The finite element method on sphere [9] is developed based on spherical geodesic grid to solve the Fokker-Planck equation.

In this section, we want to show the convergence of a fully discretized scheme for the problem (1.6). We will use finite difference and backward Euler method in spatial and temporal directions, respectively. The discrete velocity is defined on a uniform mesh $\mathcal{T}_h$, where $h = 1/N$ is the space discretization step. The time interval $(0, T)$ is discretized with a uniform step size Δt. We will define the discrete functions $\bar{u}^n_{j+1/2}$ and $\bar{\psi}^n_{j,k}$ at $((j+1/2)h, n\triangle t)$ and $(jh, k\sigma, n\triangle t)$, respectively. We also let $y_j = jh, \theta_k = k\sigma$, where $\sigma = 2\pi/M$ is the discretization configuration space step.

The problem (1.6) can be discretized in the following form:

$$\frac{\bar{u}^{n+1}_{j+1/2} - \bar{u}^n_{j+1/2}}{\Delta t} = \frac{\gamma}{Re}\frac{(D_h\bar{u})^{n+1}_{j+1} - (D_h\bar{u})^{n+1}_j}{h} + \frac{1-\gamma}{ReDe}\frac{(\bar{\tau}_\alpha)^n_{j+1} - (\bar{\tau}_\alpha)^n_j}{h}$$
$$+\frac{1-\gamma}{2Re}\frac{(D_h\bar{u})^{n+1}_{j+1}(\bar{\tau}_\beta)^n_{j+1} - (D_h\bar{u})^{n+1}_j(\bar{\tau}_\beta)^n_j}{h} - c \tag{3.1}$$

$$\frac{\bar{\psi}^{n+1}_{j,k} - \bar{\psi}^n_{j,k}}{\Delta t} = \frac{1}{De}\frac{(D_\sigma\bar{\psi})^{n+1}_{j,k+1/2} - (D_\sigma\bar{\psi})^{n+1}_{j,k-1/2}}{\sigma} + \frac{1}{De}\frac{(\bar{\psi}\bar{U}_\theta)^{n+1}_{j,k+1/2} - (\bar{\psi}\bar{U}_\theta)^{n+1}_{j,k-1/2}}{\sigma}$$
$$+(D_h\bar{u})^n_j\frac{(\bar{\psi}\sin^2\theta)^{n+1}_{j,k+1/2} - (\bar{\psi}\sin^2\theta)^{n+1}_{j,k-1/2}}{\sigma} \tag{3.2}$$

with initial and boundary conditions:

$$\bar{u}^0_{j+1/2} = u_0((j+1/2)h), \qquad j = 0, \cdots, N-1; \tag{3.3}$$

$$\bar{\psi}^0_{j,k} = \frac{1}{\sigma}\int_{(k-1/2)\sigma}^{(k+1/2)\sigma}\psi_0(jh,\theta)d\theta, \qquad j = 0, \cdots, N; k = 0, \cdots, M-1, \tag{3.4}$$

$$\bar{u}^n_{-1/2} = -\bar{u}^n_{1/2}, \qquad \bar{u}^n_{N+1/2} = -\bar{u}^n_{N-1/2}, \qquad n = 1, 2, \cdots, \tag{3.5}$$

where

$$(\bar{\tau}_\alpha)^n_j = \sum_{k=0}^{M-1}(\sin(2\theta_k) + (\bar{U}_\theta)^n_{j,k}\cos^2\theta_k)\bar{\psi}^n_{j,k}\sigma \tag{3.6}$$

$$(\bar{\tau}_\beta)^n_j = \sum_{k=0}^{M-1}\sin^2\theta_k\cos^2\theta_k\bar{\psi}^n_{j,k}\sigma \tag{3.7}$$

$$(\bar{U}_\theta)^n_{j,k} = U_0[\sin 2\theta_k\sum_{l=0}^{M-1}\cos 2\theta_l\bar{\psi}^{n-1}_{j,l}\sigma - \cos 2\theta_k\sum_{l=0}^{M-1}\sin 2\theta_l\bar{\psi}^{n-1}_{j,l}\sigma] \tag{3.8}$$

$$(D_h\bar{u})^n_j = \frac{\bar{u}^n_{j+1/2} - \bar{u}^n_{j-1/2}}{h}, \qquad (D_\sigma\bar{\psi})^n_{j,k+1/2} = \frac{\bar{\psi}^n_{j,k+1} - \bar{\psi}^n_{j,k}}{\sigma} \tag{3.9}$$

$$(\bar{\psi}\sin^2\theta)^n_{j,k+1/2} = \frac{(\bar{\psi}\sin^2\theta)^n_{j,k+1} + (\bar{\psi}\sin^2\theta)^n_{j,k}}{2}. \tag{3.10}$$

It follows from (3.2) that

$$\sigma\sum_{l=0}^{M-1}\psi^n_{j,l} = 1, \qquad \text{for all } n \in \mathbb{N} \tag{3.11}$$

provided that $\sigma\sum_{l=0}^{M-1}\psi^0_{j,l} = 1$.

We define $u^n_{j+1/2} = u((j+1/2)h, n\Delta t), \psi^n_{j,k} = \psi(jh, k\sigma, n\Delta t)$ and define $(\tau_\alpha)^n_j, (\tau_\beta)^n_j, (U_\theta)^n_{j,k}$ similarly. It is easy to verify that $u^n_{j+1/2}, \psi^n_{j,k}$ satisfy the difference equations (3.1) and (3.2)with the truncation errors $\mathcal{O}(\Delta t + h^2 + \sigma^2)$. The numerical boundary condition (3.5) is also of second order accuracy in space.

Throughout this paper, the generic constant C is assumed to be independent of the mesh size h, σ and Δt. Suppose $\|u_y\|_\infty \le C_1$ and define

$$T^* = \sup\Big\{t_1 \in [0,T]; \|D_h\bar{u}^n\|_{l^\infty} \le C_1 + 1, n\Delta t \in [0,t_1]\Big\}.$$

Then there exists an σ_0 such that

$$\bar{\psi}^n_{j,k} \ge 0, \quad \sigma < \sigma_0, \qquad n\Delta t < T^*, \tag{3.12}$$

by using the property of the M-matrix. The non-negativity property of the probability distribution and (3.11) yield

$$(\bar{\tau}_\beta)^n_j \ge 0, \tag{3.13}$$

$$\|\bar{\tau}^n_\alpha\|_{l^\infty} \le C, \quad \|\tau^n_\alpha\|_{l^\infty} \le C, \tag{3.14}$$

$$\|\bar{U}^n_\theta\|_{l^\infty} \le C. \tag{3.15}$$

We define

$$e^n_{j+1/2} = \bar{u}^n_{j+1/2} - u^n_{j+1/2}, \tag{3.16}$$

$$E^n_{j,k} = \bar{\psi}^n_{j,k} - \psi^n_{j,k}. \tag{3.17}$$

We then have

$$\begin{aligned}\frac{e^{n+1}_{j+1/2} - e^n_{j+1/2}}{\Delta t} = {} & \frac{\gamma}{Re}\frac{(D_he)^{n+1}_{j+1} - (D_he)^{n+1}_j}{h} + \frac{1-\gamma}{ReDe}\frac{(\bar{\tau}_\alpha - \tau_\alpha)^n_{j+1} - (\bar{\tau}_\alpha - \tau_\alpha)^n_j}{h} \\ & + \frac{1-\gamma}{2Re}\frac{(D_he)^{n+1}_{j+1}(\bar{\tau}_\beta)^n_{j+1} - (D_he)^{n+1}_j(\bar{\tau}_\beta)^n_j}{h} \\ & + \frac{1-\gamma}{2Re}\frac{(D_hu)^{n+1}_{j+1}(\bar{\tau}_\beta - \tau_\beta)^n_{j+1} - (D_hu)^{n+1}_j(\bar{\tau}_\beta - \tau_\beta)^n_j}{h} \\ & + C(\Delta t + h^2 + \sigma^2),\end{aligned} \tag{3.18}$$

and

$$
\begin{aligned}
\frac{E_{j,k}^{n+1}-E_{j,k}^{n}}{\Delta t} &= \frac{1}{De}\frac{(D_\sigma E)_{j,k+1/2}^{n+1}-(D_\sigma E)_{j,k-1/2}^{n+1}}{\sigma} \\
&+\frac{1}{De}\frac{(E\bar{U}_\theta)_{j,k+1/2}^{n+1}-(E\bar{U}_\theta)_{j,k-1/2}^{n+1}}{\sigma} \\
&+\frac{1}{De}\frac{(\psi(\bar{U}_\theta-U_\theta))_{j,k+1/2}^{n+1}-(\psi(\bar{U}_\theta-U_\theta))_{j,k-1/2}^{n+1}}{\sigma} \\
&+(D_h e)_j^{n+1}\frac{(\psi\sin^2\theta)_{j,k+1/2}^{n+1}-(\psi\sin^2\theta)_{j,k-1/2}^{n+1}}{\sigma} \\
&+(D_h \bar{u})_j^{n+1}\frac{(E\sin^2\theta)_{j,k+1/2}^{n+1}-(E\sin^2\theta)_{j,k-1/2}^{n+1}}{\sigma} \\
&+C(\Delta t+h^2+\sigma^2). \qquad (3.19)
\end{aligned}
$$

Multiplying (3.19) with $e_{j+1/2}^{n+1}$ and summing the resulting equation with respect to j give

$$
\begin{aligned}
&\frac{h}{2\Delta t}\sum_{j=0}^{N-1}|e_{j+1/2}^{n+1}|^2+\frac{\gamma h}{2Re}\sum_{j=0}^{N-1}|D_h e_j^{n+1}|^2 \\
\leq\ &\frac{h}{2\Delta t}\sum_{j=0}^{N-1}|e_{j+1/2}^{n}|^2+C\|\bar{\tau}_\alpha^n-\tau_\alpha^n\|_{l^2([0,1])}^2 \\
&+C\|\bar{\tau}_\beta^n-\tau_\beta^n\|_{l^2([0,1])}^2+C(\Delta t+h^2+\sigma^2)^2. \qquad (3.20)
\end{aligned}
$$

Similarly, we obtain by using (3.19) that

$$
\begin{aligned}
&\frac{h\sigma}{2\Delta t}\sum_{j,k}|E_{j,k}^{n+1}|^2+\frac{h\sigma}{2De}\sum_{j,k}|D_\sigma E_{j,k+1/2}^{n+1}|^2 \\
\leq\ &\frac{h\sigma}{2\Delta t}\sum_{j,k}|E_{j,k}^{n}|^2+Ch\sum_{j=0}^{N-1}|D_h e_j^{n+1}|^2+Ch\sigma\sum_{j,k}|E_{j,k}^{n+1}|^2 \\
&+C\|\bar{U}_\theta^{n+1}-U_\theta^{n+1}\|_{l^2([0,1]\times[0,2\pi])}^2+C(\Delta t+h^2+\sigma^2)^2. \qquad (3.21)
\end{aligned}
$$

It is easy to verify that

$$
\|\bar{\tau}_\alpha^n-\tau_\alpha^n\|_{l^2([0,1])}^2 \leq Ch\sigma\sum_{j,k}|E_{j,k}^n|^2 \qquad (3.22)
$$

$$
\|\bar{\tau}_\beta^n-\tau_\beta^n\|_{l^2([0,1])}^2 \leq Ch\sigma\sum_{j,k}|E_{j,k}^n|^2 \qquad (3.23)
$$

$$
\|\bar{U}_\theta^{n+1}-U_\theta^{n+1}\|_{l^2([0,1]\times[0,2\pi])}^2 \leq Ch\sigma\sum_{j,k}|E_{j,k}^{n+1}|^2 . \qquad (3.24)
$$

Combining (3.19)-(3.24) gives

$$\begin{aligned} & h\sum_{j=0}^{N-1}|e_{j+1/2}^{n+1}|^2+h\sigma\sum_{j,k}|E_{j,k}^{n+1}|^2 \\ \leq\ & (1+C\Delta t)\left(h\sum_{j=0}^{N-1}|e_{j+1/2}^{n}|^2+h\sigma\sum_{j,k}|E_{j,k}^{n}|^2\right)+C(\Delta t+h^2+\sigma^2)^2. \qquad (3.25)\end{aligned}$$

The above Gronwall-type inequality leads to

$$h\sum_{j=0}^{N-1}|e_{j+1/2}^{n}|^2+h\sigma\sum_{j,k}|E_{j,k}^{n}|^2 \ \leq\ C(\Delta t+h^2+\sigma^2)^2. \qquad (3.26)$$

Theorem 3.1. *Let $0<l<1$, (u^n,ψ^n) be the solutions of the problem* (2.1)-(2.9) *and $(\bar{u}^n,\bar{\psi}^n)$ be the solutions of the corresponding discrete problem* (3.1)-(3.5). *If $\psi_0\in C^{l+2}(S^1)\cap C^{l+1}([0,1]\times S^1), u_0\in C^{l+2}([0,1])$, $\Delta t\leq Ch^2,\sigma\leq Ch$, then the following error estimate holds:*

$$\|\bar{u}^n-u^n\|_{l^2([0,1])}+\|\bar{\psi}^n-\psi^n\|_{l^2([0,1]\times[0,2\pi])} \ \leq\ C(\Delta t+h^2+\sigma^2). \qquad (3.27)$$

Proof. It follows from Theorem 2.1 and the regularity assumption for u_0 and ψ_0 that

$$\psi\in C^{2,1}(S^1\times[0,T])\cap C^{1,0}(([0,1]\times S^1)\times[0,T]), \quad u\in C^{2,1}([0,1]\times[0,T]).$$

The estimate (3.26) implies

$$\|\bar{u}^n-u^n\|_{l^2([0,1])}+\|\bar{\psi}^n-\psi^n\|_{l^2([0,1]\times[0,2\pi])}\leq C(\Delta t+h^2+\sigma^2), \qquad (3.28)$$

which holds on some interval $[0,T^*]$. Using the discrete inverse inequality, we have

$$\begin{aligned}\|D_h\bar{u}^n\|_{l^\infty} &\leq \|D_hu^n\|_{l^\infty}+\|D_h\bar{u}^n-D_hu^n\|_{l^\infty}\\ &\leq C_1+Ch+h^{-3/2}\|\bar{u}^n-u^n\|_{l^2}\\ &\leq C_1+Ch^{1/2}, \qquad (3.29)\end{aligned}$$

provided that $\Delta t<Ch^2$ and $\sigma<Ch$. Let us verify $T^*=T$. If this does not hold, then (3.29) gives

$$\|D_h\bar{u}^n\|_{l^\infty}\leq C_1+Ch_0^{1/2}<C_1+1,$$

for $n\Delta t\in[0,T^*]$, where h_0 is sufficiently small. Thus we can enlarge T^* by continuity and thus deduce a contradiction. This completes the proof of the theorem.

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