8 Dilute polymer models

The model introduced in this part of the notes is not solely based on continuum mechanical principles. We look at a solution of "big" molecules in a Newtonian fluid. These molecules have an elastic structure which interacts with the overall flow. The "density" of interactions of the single molecules with the surrounding fluid introduces an additional stress into the Navier-Stokes equations for the solvent. In the following, we look at the basic ideas and assumptions for modelling this extra stress. In the last section of this chapter, we show that in some special cases, the stress from molecular theory reduces to the non-linear Maxwellian stress model. The modelling and mathematics in this chapter is taken mainly from [10, Section 2.4] and from the lecture and lecture notes "Kinetic Models of Dilute Polymers: Analysis, Approximation and Computation" by Endre Süli.[1]

8.1 The dumbbell model

In the following, we assume that the fluid which contains the big molecules is a Newtonian solvent and that it has velocity u. Every single macromolecule is modelled as an "elastic dumbbell", i.e. it consists of two beads or rigid balls, whose center of gravity is in their geometric centers r_1, r_2 and which have the same radius, connected by a spring. In the more complicated chain models, several beads are each connected by a spring, but we do not consider this case here.

At least the following three basic assumptions are made.

- the polymer molecules do not interact, i.e. the polymer solution is "dilute"
- the solvent fluid is Newtonian
- the beads have no (relevant) mass

In the Newtonian solvent, the forces which act on the two beads are collected as follows,

$$F_i = F_i^d + B_i + F_i^s, \qquad i \in \{1, 2\}, \tag{8.1}$$

where F_i^d are drag forces exerted by the solvent on the beads, B_i is the force due to Brownian Motion of solvent and polymer molecules and F_i^s is the force exerted by the spring. The dumbbell molecule interacts with the flow through its stretching and through its orientation. To fit this picture, in the following, we sometimes consider the coordinates $x = \frac{1}{2}(r_1 + r_2), q = r_2 - r_1$, i.e. the center of gravity of the complete dumbbell and its

[1] held at the *Eleventh School on Mathematical Theory in Fluid Mechanics* which took place in Kacov, May 22-29, 2009

configuration vector, instead of r_1, r_2 . By Newton's second law, $F_i = m_i a_i$. Here, the limit $m_i \to 0$ is taken to obtain $F_i = 0$.

The first question is which kind of spring force law to use. In general, it is given by

$$F^s(q) = HU'(\frac{1}{2}|q|^2)q,$$

where $U : \mathbb{R}_+ \to \mathbb{R}$ is a given potential and $H > 0$ the spring constant. The simplest is the linear Hookean model, where $U(s) = s$, i.e. $F^s(q) = Hq$. This model implies in particular that the polymer may be infinitely stretched. This is unrealistic, but it is also a mathematical problem if the fluid flow is considered on a domain with a boundary. In Section 1.3 however, it is shown that this model reduces to the Oldroyd-B model under additional assumptions.

A second model which is widely used is the *FENE (Finitely Extensible Nonlinear Elastic) model*, where the spring force is given by

$$U(\frac{1}{2}|q|^2) = -\frac{l^2}{2}\ln(1 - \frac{|q|^2}{l^2}), \qquad F^s(q) = \frac{Hq}{1 - \frac{|q|^2}{l^2}},$$

so that $U \to \infty$ as $|q| \to l$ and an infinite force would have to be used to stretch the polymer beyond the critical length l. In particular, the *configuration space*

$$D := \{q \in \mathbb{R}^3 : q = r_2 - r_1, r_1 \text{ and } r_2 \text{ belong to one dumbbell}\}$$

of all admissable q is given by $\mathbb{R}^3$ in the Hookean case and by $D = B(0, l)$ for FENE dumbbells.

For the drag force F^d, the *Stokes drag*

$$F_i^d = -\zeta(\frac{dr_i}{dt}(t) - u(r_i, t))$$

is assumed, where the constant $\zeta > 0$ is called the *drag coefficient*, given by $6\pi\eta a$, where η is the solvent's viscosity and a the radius of the bead. The formula only says that the difference in velocity of bead and solvent is linearly related to some force, here, this is the force resulting from Brownian motion and the spring.

The Brownian force B is assumed to be given by a Wiener process $W(t)$, i.e. $B_i(t)\,\mathrm{d}t = C\,\mathrm{d}W_i(t)$, where $C = \sqrt{2k_BT\zeta}$ is the constant or diffusion coefficient for this Brownian motion, k_B the Boltzmann constant, T the absolute temperature.

8.2 The Fokker-Planck Navier-Stokes equations

Using the above assumptions on the forces involved, equation (8.1) can be rewritten as a stochastic differential equation, in the form

$$\mathrm{d}X(t) = b(X(t)) + C\zeta^{-1}(\mathrm{Id})\mathrm{d}W(t), \qquad X(0) = X,$$

where $X(t) = (r_1(t), r_2(t))^T$,

$$b(X(t)) := \begin{pmatrix} u(r_1(t),t) + \zeta^{-1}F^s(r_2(t) - r_1(t)) \\ u(r_2(t),t) + \zeta^{-1}F^s(r_1(t) - r_2(t)) \end{pmatrix}.$$

The forward Kolmogorov equation gives a partial differential equation, a *Fokker-Planck equation,* for the evolution of the probability density function ψ of the stochastic process $t \mapsto X(t)$, in the form

$$\begin{aligned} &\frac{\partial \psi}{\partial t} + \nabla_{r_1} \cdot [u(r_1,t)\psi + \zeta^{-1}F^s(r_2 - r_1)] + \nabla_{r_2} \cdot [u(r_2,t)\psi + \zeta^{-1}F^s(r_1 - r_2)\psi] \\ &= \frac{k_B T}{\zeta}(\Delta_{r_1} + \Delta_{r_2})\psi. \end{aligned}$$

Rewriting the equation for ψ as a function of x and q and in dimensionless form gives

$$\frac{\partial \psi}{\partial t} + \nabla_x \cdot (u\psi) + \nabla_q \cdot [(\nabla_x u)q\psi - \frac{1}{2\mathrm{We}}F(q)\psi] = \frac{1}{2\mathrm{We}}\Delta_q\psi + \frac{c}{8\mathrm{We}}\Delta_x\psi, \tag{8.2}$$

where We is the Weissenberg number and $c = (l_0/L)^2$ is given by the quotient of the characteristic length of a dumbbell l_0 and of the flow, L. In particular, a Taylor expansion and linearization of $u(r_1) - u(r_2)$ was used, which is appropriate for slow flow, but also otherwise, because the micro- and macro-length scales differ in several orders of magnitude. For given u, the solution ψ of equation (8.2) gives the probability density for finding at time t, a dumbbell with center of mass x and configuration q. From given ψ, an extra stress tensor τ which acts on the fluid through the orientation and stretching of the polymer molecules it contains, can be derived. For a given number density n_p of polymer molecules in the solvent, it is determined by the *Kramers expression*:

$$\tau(t,x) = n_p k_B T \int_D (F^s(q) \otimes q)\psi(t,x,q)\,\mathrm{d}q. \tag{8.3}$$

A motivation for this formula is roughly as follows. Each dumbbell of configuration q carries the force $F^s(q)$. Moreover, it can be shown that the number of dumbbells of configuration q intersecting a plane P with normal n at time t is proportional to

$$\int_P n_p(q \cdot n)\psi(t,x,q)\,\mathrm{d}x. \tag{8.4}$$

In the momentum balance, the stress tensor τ models contact forces F_C in the sense that $F_C = \int_{\partial V} \tau n\,\mathrm{d}(\partial V)$ on every control volume with outer normal n. To get F_C in this case, we multiply (8.4) by $F^s(q)$ and integrate over q. This gives (8.3).

Putting the above equations together, the coupled Fokker-Planck Navier-Stokes equa-

tions for dilute polymer flow in non-dimensional form are given by

$$\begin{cases} \mathrm{Re}(\frac{\partial v}{\partial t} + (u\cdot\nabla)u) - (1-\alpha)\Delta v + \nabla q = \frac{\alpha}{\mathrm{We}}\mathrm{div}\,\tau + f, & \text{in } \mathbb{R}_+\times\Omega,\\ \mathrm{div}\, v = 0, & \text{in } \mathbb{R}_+\times\Omega,\\ \frac{\partial\psi}{\partial t} + (u\cdot\nabla_x)\psi + \nabla_q\cdot[(\nabla_x u)q\psi - \frac{1}{2\mathrm{We}}F(q)\psi] = \frac{1}{2\mathrm{We}}\Delta_q\psi + \frac{c}{8\mathrm{We}}\Delta_x\psi, & \text{in } \mathbb{R}_+\times\Omega\times D,\\ \tau = n_p\int_D F^s(q)\otimes q\psi(q)\,\mathrm{d}q, & \text{in } \mathbb{R}_+\times\Omega,\\ v|_{\partial\Omega} = 0, & \text{on } \mathbb{R}_+\times\partial\Omega,\\ v|_{t=0} = v_0, & \text{on } \Omega. \end{cases} \tag{8.5}$$

8.3 Reduction to UCM and Oldroyd-B models

A special property of the Hookean spring dumbbell model is that, in contrast to the FENE model, it reduces to the closed form of the Upper Convected Maxwell model. This is shown in [10] and also in [1]. To show this, an additional approximation has to be made in (8.2). We set $c = 0$ to ignore the diffusion in x. For a discussion of this approximation, cf. [2]. In particular, this approximation makes the analysis in the FENE case more complicated, because the smoothing term $\Delta_x\psi$ vanishes.

If the spring is Hookean, i.e. $F^s(q) = Hq$ for some constant $H > 0$, the extra stress τ from (8.3) is given by

$$\tau_p = n_p H\int_{\mathbb{R}^3} q\otimes q\psi(q)\,\mathrm{d}q.$$

We use the notation $\langle f\rangle := \int_{\mathbb{R}^3} f(q)\psi(q)\,\mathrm{d}q$ and $C := \langle q\otimes q\rangle$. Equation (8.2) is multiplied by $q\otimes q$ and integrated with respect to q. We use that by integration by parts,

$$\int_{\mathbb{R}^3}(\Delta_q\psi)(q\otimes q) = \int_{\mathbb{R}^3}\psi\Delta_q(q\otimes q) = 2\mathrm{Id},$$

$$\begin{aligned} [\int_{\mathbb{R}^3}\nabla_q\cdot(-(\nabla_x u\cdot q)\psi)q\otimes q]_{ij} &= [\sum_{k,l}\int_{\mathbb{R}^3}(\partial_k u_l)q_k\psi(\partial_l(q\otimes q))]_{ij}\\ &= \sum_{k,l}\int_{\mathbb{R}^3}(\partial_k u_l)q_k\psi(\delta_{li}q_j + \delta_{lj}q_i)\\ &= [(\nabla u)C + C(\nabla u)^T]_{ij} \end{aligned}$$

and

$$\int_{\mathbb{R}^3}\nabla_q\cdot(q\psi)q\otimes q = -\int_{\mathbb{R}^3}\psi q\nabla_q(q\otimes q) = -2C$$

to get the equation

$$\partial_t C + (u\cdot\nabla)C = \frac{1}{\mathrm{We}}\mathrm{Id} - \frac{H}{\mathrm{We}}C + (\nabla u)C + C(\nabla u)^T.$$

Multiplying by $n_p H$ gives

$$\partial_t \tau_p + (u \cdot \nabla)\tau_p - (\nabla u)\tau_p - \tau_p(\nabla u)^T = \frac{1}{\mathrm{We}}\mathrm{Id} - \frac{H}{\mathrm{We}}\tau_p.$$

By substituting $\tau_p = \frac{1}{H}\mathrm{Id} + \tau$, we get the equation

$$\partial_t \tau + (u \cdot \nabla)\tau - (\nabla u)\tau - \tau(\nabla u)^T + \frac{H}{\mathrm{We}}\tau = \frac{2}{H}D(u),$$

which is the Upper Convected Maxwell model, cf. Section 6.2, so that (8.5) is equivalent to the Oldroyd-B model.

9 Literature and results

In this chapter, there is a short review of related literature in analysis. The results are very new. Again, the list of references is not complete, but compared to the other subjects, not as many authors are involved. I tried to quote very new papers from different authors, so that the references in the cited paper can be used.

In the mathematical approaches to well-posedness of the generalized Newtonian models and the Oldroyd-B/Maxwell-type models, we encountered an iteration scheme or fixed point argument of some kind. For the viscoelastic models, it was always about moving back and forth from Newtonian to non-Newtonian parts, so this works for the Hookean dumbbell. If it is known how to solve the Fokker-Planck equation (8.2), cf. the paper by Jourdain and Lelievre [6], a similar approach can be used. More precisely, one can solve (8.2) for $\psi_{(n)}$ from given $u_{(n)}$, and then calculate $\tau_{(n)}$ from the Kramers expression. From $\operatorname{div} \tau_{(n)}$ as a right-hand side, a new $u_{(n+1)}$ is calculated as the solution of the Navier-Stokes equation. This yields $\psi_{(n+1)}$ and $\tau_{(n+1)}$. To get local-in-time existence, as for the previous models, it has to be shown that the iteration is contractive or has a compact image. Recently, well-posedness results were shown by a method of this kind by E, Li and Zhang [5] and Zhang and Zhang [11]. I think that the proofs are difficult. In 2000, Renardy wrote that "the solution of the Fokker-Planck equation is a formidable task,"[10, p. 20].

The fact that the Fokker-Planck equation is high-dimensional, i.e. "7D" for the three-dimensional problem, makes the problem also numerically very challenging. This is an even much stronger problem if instead of dumbbells, chains of beads are considered. There are algorithms and results in Barrett and Süli [3], Knezevic and Süli [7] and the references therein, as well as an earlier work on the two-dimensional problem by Lozinski and Chauviere [9].

The global existence and regularity of weak solutions for the two-dimensional problem is shown in [4] and [8]. In three dimensions, the existence of global weak solutions was shown under additional regularizing assumptions on the extra-stress τ, cf. [1] and [2].

9.1 Related questions

- In general, boundary conditions for this model are somehow a difficult subject, if the molecules are allowed to touch the boundary or in general for the Fokker-Planck equation. There is some discussion of this in the literature.

- In the context of the seminar, it is natural to ask whether using a non-Newtonian solvent would give a good model?

- The section on the Fokker-Planck equation above is really short. A full derivation could be the topic of a seminar talk.
- What are the predictions of the FENE model for simple flow? What would then be the density ψ?

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