Finitely Extensible Nonlinear Elastic Model Notes

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What is the FENE Model

The FENE model is used to model long-chained polymers. It simplifies the polymers by connecting a sequence of beads with nonlinear springs. The FENE model is used for shear thinning fluids.

Basic Dumbbell models

- Hookean dumbbell
  - Two beads connected by a Hookean (linear) spring.
  - The beads are often the ends of a the polymer chain.
  - The force between the beads in a Hookean dumbbell is:

$$F = H * Q \tag{1}$$

Where

- F is the force between the beads
- H is the spring constant
- Q is the distance between the beads.

- Hookean spring models are only realistic for small deformations from equilibrium.
- They also put no limit to the extent to which the dumbbell can be stretched. For example in elongational flow, the elongational viscosity at a high strain rate becomes indefinite.

FENE Model

The FENE model incorporates a nonlinear spring into the basic dumbbell model. In its simplest form the connecting force can be found by the following equation:

$$\boldsymbol{F}^{c} = \frac{H\boldsymbol{Q}}{1 - Q^2/Q_0^2}, \tag{2}$$

Where

- F^c is the connector force
- $\boldsymbol{Q}$ (bolded) is the connector vector between the beads
- H is the spring constant
- Q is the extension of the connector vector
- Q_0 denotes the maximum possible spring extension.

Governing Equations of the FENE Model

Eq. (2), is the simplest form of the FENE model. Unfortunately it is not very useful because there is no way to actually measure the elongation of the molecules. We will need to create a larger system of equations to actually measure the properties of the flow.

To find the dynamics and material properties of a flow, I will use the approach based on stochastic differential equations.

First, the time evolution of the internal configuration of a FENE dumbbell is governed by the following stochastic differential equation:

$$\mathrm{d}\boldsymbol{Q} = \left[\boldsymbol{\kappa} \cdot \boldsymbol{Q} - \frac{2}{\zeta} \boldsymbol{F}^{\mathrm{c}} \right] \mathrm{d}t + \sqrt{\frac{4kT}{\zeta}}\, \mathrm{d}\boldsymbol{W}_{(t)} \tag{3}$$

Where

- **Q** (bolded) is the connector vector between the beads
- κ is the transpose of the velocity gradient, $\kappa=(\nabla v)^T$
- ζ is the friction coefficient of a bead,
- F^c is the connector force given by Eq. (2)
- t is the time
- k is Boltzmann’s constant
- T is the absolute temperature
- $\boldsymbol{W}$ represents a three-dimensional Wiener process

The first term incorporates the distortion of the beads due to the velocity field, the second term represents the effect of the restoring spring force, and the last term models the Brownian motion of the beads.

To make the following calculations “simpler” a new unit of time and a new unit of length are used. They are as follows:

$$\lambda_H = \frac{\zeta}{4H} \text{ (Time)} \tag{4}$$

$$\sqrt{\frac{kT}{H}} \text{ (Length)} \tag{5}$$

These new units will be shown in shorthand by the following relationships:

$$\hat{\boldsymbol{Q}} = \boldsymbol{Q} / \sqrt{(kT/H)} \tag{6}$$

$$\hat{t} = t / \lambda_H \tag{7}$$

Using the new relationships Eq. (3) can be rewritten as:

$$\mathrm{d}\hat{\boldsymbol{Q}} = \left[\hat{\boldsymbol{\kappa}} \cdot \hat{\boldsymbol{Q}} - \frac{1}{2} \hat{\boldsymbol{F}}^{\mathrm{c}} \right] \mathrm{d}\hat{t} + \mathrm{d}\boldsymbol{W}_{(\hat{t})}, \tag{8}$$

Where $\hat{\boldsymbol{\kappa}} = \lambda_H \boldsymbol{\kappa},\ \hat{t}$ denotes the dimensionless time and $\hat{\boldsymbol{F}}^{\mathrm{c}}$ is the dimensionless connector force given by

$$\hat{\boldsymbol{F}}^{\mathrm{c}} = \frac{\hat{\boldsymbol{Q}}}{1 - \hat{Q}^2 / b}, \tag{9}$$

Where b denotes the finite extensibility parameter $b = HQ_0^2\,/(kT)$. To recap we have now created the equation that is the derivative of the dimensionless distance between the beads equals the transpose of the velocity gradient times the dimensionless distance between the beads minus one half of the dimensionless connector force all times the derivative of the dimensionless time plus the three-dimensional Wiener process.

To find the time evolution of the connector vector of a dumbbell (distance between the beads) all you have to do is take the integral of Eq. (8). Simple as can be!

FENE-P

The basic FENE model deals with each bead length individually, while the FENE-P model deals with the average length.

The FENE-P models solution to macroscopic flows is to average out the distance/ maximum distance ratio by using the Peterlin approximation (hence the –P)

$$\boldsymbol{F}^{\mathrm{c}} = \frac{H}{1 - \langle \boldsymbol{Q}^2 / Q_0^2 \rangle} \boldsymbol{Q} \tag{10}$$

First we must find the polymer contribution to the stress, τ^{p}. It is obtained from the Kramers expression:

$$\boldsymbol{\tau}^{\mathrm{p}} / nkT = \langle \hat{\boldsymbol{Q}} \hat{\boldsymbol{F}}^{\mathrm{c}} \rangle - \boldsymbol{1}, \tag{11}$$

Where the brackets denote an averaging over the dumbbell configuration distribution function and *n* is the number of dumbbells per unit volume. When a large number, *N*, of dumbbells are used Eq. (11) can be written as:

$$\boldsymbol{\tau}^{\mathrm{p}}/nkT \approx \frac{1}{N}\sum_{i=1}^{N} \hat{\boldsymbol{Q}}_i \hat{\boldsymbol{F}}_i^{\mathrm{c}} - \mathbf{1}. \tag{12}$$

We can now integrate Eq. (8) using the Euler forward method:

$$\hat{\boldsymbol{Q}}(\hat{t}+\Delta\hat{t}) = \hat{\boldsymbol{Q}}(\hat{t}) + \left[\hat{\boldsymbol{\kappa}}(\hat{t})\cdot\hat{\boldsymbol{Q}}(\hat{t}) - \frac{1}{2}\hat{\boldsymbol{F}}^{\mathrm{c}}(\hat{t})\right]\Delta\hat{t} + \Delta\boldsymbol{W}(\hat{t}), \tag{13}$$

Care must be taken in choosing a $\Delta\hat{t}$. If the time step is too large the dumbbells calculated length may exceed the maximum allowable length. Below, in figure 1, is a graph showing the shear stress verses for different shear rates using both the FENE model, and FENE-P model. Figure 2 shows the first normal stress difference verses time.

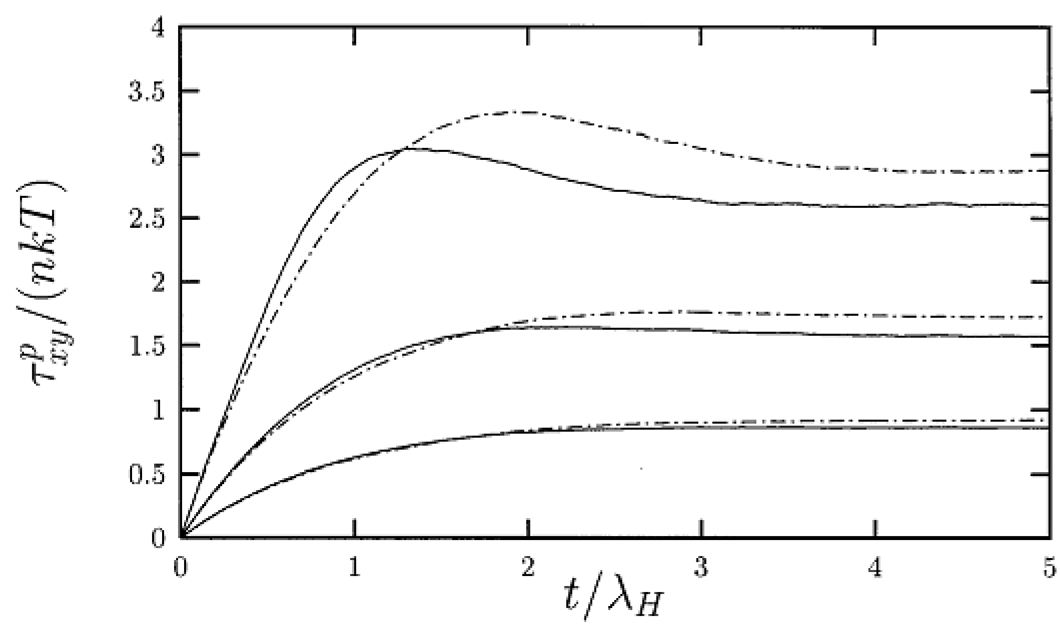

Fig. 1. Brownian dynamics simulations of the shear stress of FENE (solid line) and FENE-P dumbbells (dash-dot line) after inception of shear flow. The results were obtained using ensembles of 64 000 dumbbells with an extensibility parameter $b = 50$. The curves correspond to (dimensionless) shear rates $\dot{\gamma} = 1$ (lower curves), $\dot{\gamma} = 2$ and $\dot{\gamma} = 4$ (upper curves).

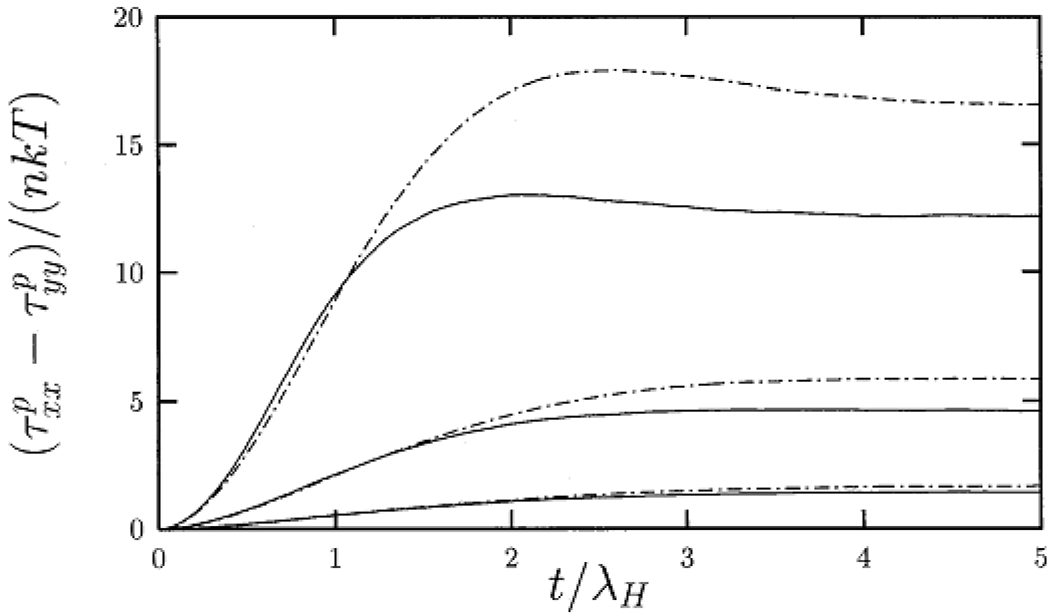

Fig. 2. Brownian dynamics simulations of the first normal stress difference of FENE (solid line) and FENE-P dumbbells (dash-dot line) after inception of shear flow. The results were obtained using ensembles of 64 000 dumbbells with an extensibility parameter $b = 50$. The curves correspond to shear rates $\dot{\gamma} = 1$ (lower curves), $\dot{\gamma} = 2$ and $\dot{\gamma} = 4$ (upper curves).

From the results for the shear stress, shown in Fig. 1 two important observations can be made. Firstly, at the inception flow, the FENE-P model is seen to under predict the FENE shear stress, and its overshoot occurs too late and is too high. Secondly, the Peterlin approximation yields higher steady state values. The results of the first normal stress difference, fig. 2, show that the FENE-P model over predicts the FENE values by a factor of 1.5 for a dimensionless shear rate of 4.

The reason for the different finding is that the meaning of the extensibility parameter *b* in the FENE model is very different from that in the FENE-P model. In the FENE model the length of an individual dumbbell is constrained by the condition $Q^2 < b$, whereas in the FENE-P model only the average dumbbell length is constrained, i.e. $\langle Q^2 \rangle < b$. Thus, in the FENE-P model it will be possible to find dumbbells with a length $Q^2 > b$. A way to combat this is to use the FENE-P* model.

FENE-P* Model

The FENE-P* model is made to more closely match the results from the FENE model by constraining the shear modulus and the zero-shear-rate viscosity to the values found in the FENE model. Shown below is a plot comparing the three models:

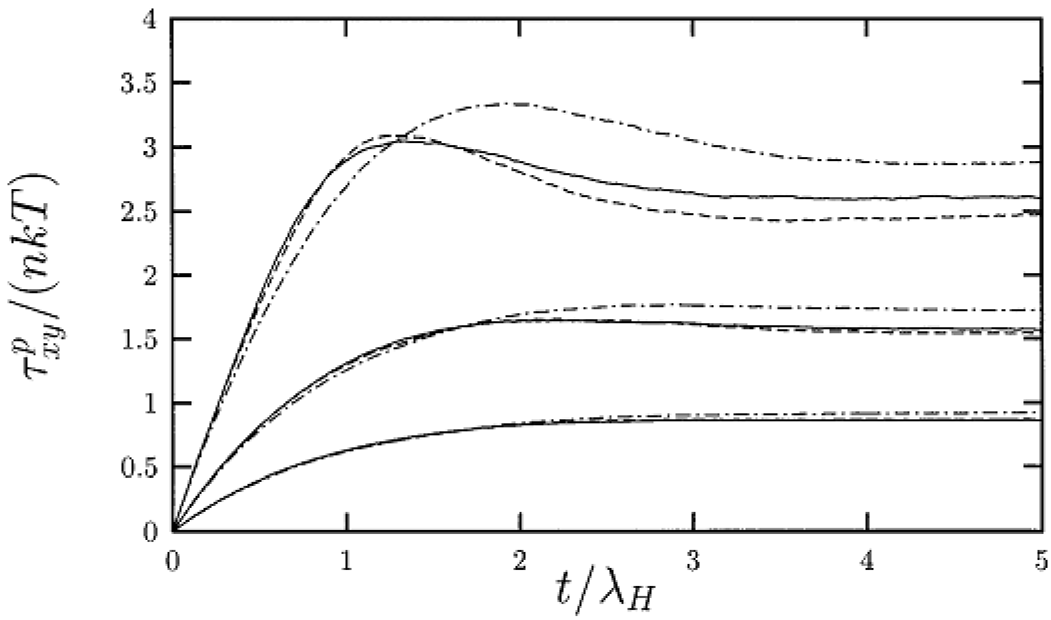

Fig. 5. Shear stress FENE (solid line), FENE-P (dash-dot line) and FENE-P* model (dashed line) in start-up of shear flow. The extensibility parameter in the FENE and FENE-P calculations is $b = 50$. In the FENE-P* model we use $b^* = 20.57$ and $(nkT)^* = 1.04nkT$. The results were obtained using ensembles of 64 000 dumbbells. The curves correspond to shear rates $\dot{\gamma} = 1$ (lower curves), $\dot{\gamma} = 2$ and $\dot{\gamma} = 4$ (upper curves).

Calculation of the FENE Shear Modulus

When calculating the FENE shear modulus we use the following

- Large and constant velocity gradient
- Very small period of time, δt

- Therefore because of the delta-like behavior of the velocity gradient
  - The effects of the connector force are negligible
  - Effects of the Brownian motion during the deformation process are negligible

Eq. 8 can simplify to the following ordinary differential equation:

$$\boldsymbol{Q}^{+} = \boldsymbol{Q} + \boldsymbol{\kappa} \cdot \boldsymbol{Q}\,\delta t, \tag{14}$$

Where

- **Q** (bolded) is the dumbbell connector vector in equilibrium
- $\mathbf{Q}^{+}$ denotes the connector vector of the dumbbell at $t=\delta t$ (immediately after deformation has been applied).

The polymer contribution to the stress immediately after the deformation is given by:

$$\boldsymbol{\tau}^{+}/nkT = \left\langle \frac{\boldsymbol{Q}^{+}\boldsymbol{Q}^{+}}{1-(Q^{+})^{2}/b} \right\rangle^{+} - \mathbf{1}. \tag{15}$$

After more math involving tensors this transforms into:

$$\boldsymbol{\tau}^{+}/nkT = \frac{b}{b-2}(\boldsymbol{\kappa}+\boldsymbol{\kappa}^{\mathrm{T}})\,\delta t. \tag{16}$$

Then noting that the infinitesimal strain tensor γ is given by $\boldsymbol{\gamma} = (\boldsymbol{\kappa}+\boldsymbol{\kappa}^{\mathrm{T}})\,\delta t$, we obtain

$$G_0 = \frac{b}{b-2}nkT. \tag{17}$$

Eq. 17 is valid for the FENE model, for the FENE-P model b/(b-2) is set equal to 1.