

ACCOUNTING FOR THE EFFECT OF INTERNAL VISCOSITY IN DUMBBELL MODELS FOR POLYMERIC FLUIDS AND RELAXATION OF DNA

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ABSTRACT. The coarse-graining approach is one of the most important modeling methods in research of long-chain polymers such as DNA molecules. The dumbbell model is a simple but efficient way to describe the behavior of polymers in solutions. In this paper, the dumbbell model with internal viscosity (IV) for concentrated polymeric liquids is analyzed for the steady-state and time-dependent elongational flow and steady-state shear flow. In the elongational flow case, by analyzing the governing ordinary differential equations the contribution of the IV to the stress tensor is discussed for fluids subjected to a sudden elongational jerk. In the shear flow case, the governing stochastic differential equation of the finitely extensible nonlinear elastic dumbbell model is solved numerically. For this case, the extensions of DNA molecules for different shear rates are analyzed, and the comparison with the experimental data is carried out to estimate the contribution of the effect of internal viscosity.

1. Introduction. Modeling the macromolecules is the groundwork to study the bulk rheology of polymeric solutions [1] and to chase the dynamics of a single molecule in detail [2]. The simple version of the elastic dumbbell model (bead-spring-bead model) introduced by Kuhn and Kuhn [3], as well as the finitely extensible nonlinear elastic (FENE) model [4, 5] have been widely employed in the investigations of polymeric solutions and melts. If the entropic springs among the beads are assumed nonlinear and/or other factors are taken into account, in most cases the governing equations of the system can not be solved analytically, and the problem should be attacked with numerical methods. Increasing beads numbers in the molecule chain modeling makes the numerical simulation extremely time-consuming, sometimes completely impractical. The dumbbell model with only two beads is computationally efficient. Also it can yield good results as we underline in this contribution.

It is known that resistance to deformation of the polymer molecule arises from both the friction between the polymer and the solvent, and the polymer molecule itself. There exists a dissipative mechanism producing the resistant force because of the energy consumption of rotations of the molecule bonds and other movements

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contributing to the polymer's configuration. As a result, the connector tension can be represented as a spring, linear or nonlinear, and a linear dashpot in parallel [3].

In this paper the dumbbell model with IV is analyzed for the elongational flows. Further, in steady shear flow, the FENE dumbbell model with IV is used to study the extensions of the molecules. Despite model simplicity, the influence of the IV could be uncovered in the resulting equations and the corresponding curves when time-dependent strain rates are applied to the complex fluid. The FENE dumbbell model with IV is employed to describe the DNA molecules in steady shear flow. The results of molecule extension obtained by numerical computation are compared to those obtained in experiment by Smith et al [6]. The plot of extension for different Weissenberg numbers is superimposed by the data from different models, such as, the bead-spring model with wormlike spring by Jendrejack et al [7] and the classic FENE dumbbell model by Hur and Shaqfeh [8].

The paper is organized as follows. In Section 2, we shall deduce the governing equations for the dumbbell model with IV and discuss the analytical pre-averaging method in the steady-state elongational flow case and the numerical method we apply for the shear flow case. In Section 3, several representative examples are presented, followed by concluding remarks of Section 4.

2. Governing equations. For the dumbbell model with internal viscosity, the spring force is a function of the configuration vector and configuration velocity. This force is the combination of connector force and the IV force, which is a function of the speed of the conformation variation. If we consider also the finitely extensible nonlinear elastic property, we can get the force law acting on the system in the following form:

$$\mathbf{F}\left(\mathbf{Q}, \frac{d\mathbf{Q}}{dt}\right) = \frac{H\mathbf{Q}}{1 - (Q/Q_0)^2} + K\left(\frac{\mathbf{Q}\mathbf{Q}}{Q^2}\right) \frac{d\mathbf{Q}}{dt}, \quad (1)$$

where \mathbf{Q} is the connector vector of the two beads of the dumbbell and its extension is denoted by Q . In equation (1), Q_0 is the maximum spring extension, and when the extension of the dumbbell approaches this value, the spring force tends to be infinite; H and K are Hookean constant and interval viscous coefficient. The first term of the right hand side in equation (1) is responsible for the FENE spring force proposed by Warner[5]. Considering the forces described above, the equation of motion for one bead can be obtained if the inertial term is neglected. It is assumed that there is no interaction among the beads of different dumbbells and the viscous drag coefficient is due to the resistance of the flow denoted further by ζ . According to the phase-space theorem [9], the equation of motion can be represented by the equation of the dumbbell configuration vector \mathbf{Q} :

$$\frac{d\mathbf{Q}}{dt} = \left(\boldsymbol{\delta} - \frac{1}{(\zeta/2K) + 1} \frac{\mathbf{Q}\mathbf{Q}}{Q^2}\right) \cdot \left([\boldsymbol{\kappa} \cdot \mathbf{Q}] - \frac{2kT}{\zeta} \frac{\partial}{\partial \mathbf{Q}} \ln \psi - \frac{2}{\zeta} \frac{H}{1 - (Q/Q_0)^2} \mathbf{Q}\right), \quad (2)$$

where ψ is the configuration distribution function of \mathbf{Q} changing with time. The fluid velocity is given by specifying transpose of imposed fluid velocity gradient $\boldsymbol{\kappa}$, and $\boldsymbol{\delta}$ is a unit matrix.

2.1. Pre-averaging methodology for elongational flows. Consider the Hookean spring dumbbell model with IV, the evolution of the configuration distribution function ψ governed by the Smoluchowski equation can be obtained by the diffusive

theorem:

$$\frac{\partial \psi}{\partial t} = -\frac{\partial}{\partial \mathbf{Q}} \left(\delta - \frac{1}{(\zeta/2K) + 1} \frac{\mathbf{Q}\mathbf{Q}}{Q^2} \right) \cdot \left([\boldsymbol{\kappa} \cdot \mathbf{Q}] - \frac{2kT}{\zeta} \frac{\partial}{\partial \mathbf{Q}} \ln \psi - \frac{2}{\zeta} H \mathbf{Q} \right) \psi. \quad (3)$$

The explicit solution to equation (3) is difficult to obtain. However, we can average the coefficient of the viscous term of equation (1) about the configuration distribution in equilibrium in advance:

$$\eta_i = \frac{1}{(\zeta/2K) + 1} \cdot \left\langle \frac{\mathbf{Q}\mathbf{Q}}{Q^2} \right\rangle_{eq} = \frac{1}{(\zeta/2K) + 1} \cdot \int \frac{\mathbf{Q}\mathbf{Q}}{Q^2} \psi_{eq} d\mathbf{Q}, \quad (4)$$

where the distribution function in equilibrium is defined as in [9]

$$\psi_{eq} = \frac{e^{-H\mathbf{Q}^2/2KT}}{\int e^{-H\mathbf{Q}^2/2KT} d\mathbf{Q}}. \quad (5)$$

From the Smoluchowski equation we can obtain the differential equation written with respect to the average value of conformation tensor $\mathbf{Q}\mathbf{Q}$

$$\frac{d\langle \mathbf{Q}\mathbf{Q} \rangle}{dt} = (1 - \eta_i) \cdot \left(\boldsymbol{\kappa} \cdot \langle \mathbf{Q}\mathbf{Q} \rangle + \langle \mathbf{Q}\mathbf{Q} \rangle \cdot \boldsymbol{\kappa}^T + \frac{4kT}{\zeta} \boldsymbol{\delta} - \frac{4}{\zeta} H \langle \mathbf{Q}\mathbf{Q} \rangle \right). \quad (6)$$

Using the elementary physical derivation, the stress tensor can be expressed by the Kramers equation where the solvent viscosity is neglected for concentrated solution. Wedgewood [12] discovered that in some cases the Kramers equation for the spring model and spring-and-dashpot model yields the similar results. Here, we adopt the Kramers equation with spring model for simplicity,

$$\boldsymbol{\tau} = -nH \langle \mathbf{Q}\mathbf{Q} \rangle + nkT \boldsymbol{\delta}. \quad (7)$$

Although the internal viscosity is not considered in the Kramers equation, the effects of the internal viscosity have been incorporated in equation (6). In this model the stress tensor does depend on the internal viscosity force as indicated by Wedgewood [12]. Applying the convected differentiation operation to Kramers equation and substituting equations (6) and (7) into the result yield

$$\boldsymbol{\tau}_{(1)} + \frac{4H(1 - \eta_i)}{\zeta} \boldsymbol{\tau} + \eta_i \boldsymbol{\kappa} \cdot \boldsymbol{\tau} + \eta_i \boldsymbol{\tau} \cdot \boldsymbol{\kappa}^T = (\eta_i \boldsymbol{\kappa} + \eta_i \boldsymbol{\kappa}^T) nkT \boldsymbol{\delta} - nkT \boldsymbol{\gamma}_{(1)}, \quad (8)$$

where notations

$$\boldsymbol{\tau}_{(1)} = \frac{\partial \boldsymbol{\tau}}{\partial t} - \boldsymbol{\kappa} \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \boldsymbol{\kappa}^T \quad (9)$$

and

$$\boldsymbol{\gamma}_{(1)} = \dot{\boldsymbol{\gamma}} = \boldsymbol{\kappa} + \boldsymbol{\kappa}^T \quad (10)$$

are used. Using equations (9) and (10), equation (8) could be simplified to

$$\frac{\partial \boldsymbol{\tau}}{\partial t} - (1 - \eta_i) (\boldsymbol{\kappa} \cdot \boldsymbol{\tau} + \boldsymbol{\tau} \cdot \boldsymbol{\kappa}^T) + \frac{4H(1 - \eta_i)}{\zeta} \boldsymbol{\tau} = -(1 - \eta_i) nkT \boldsymbol{\gamma}_{(1)}. \quad (11)$$

For steady-state elongational or shear flows, the material equation (11) degenerates into the constitutive equation without the internal viscosity. It is abnormal to find that internal viscosity pays no contribution in the steady state flow. However, we have used the Kramers equation of stress tensor to demonstrate the effect of IV in the steady state flows [10]. In this contribution, for the time-dependent deformation case, the influence of IV is discussed qualitatively in the absence of accurate stress tensor expressions. We will discuss this issue in the next section.

2.2. Numerical methodology for shear flows. Equation (2) can be solved numerically. We introduce dimensionless parameters

$$\bar{\mathbf{Q}} = \frac{\mathbf{Q}}{\sqrt{kT/H}}, \quad \bar{t} = \frac{t}{\lambda} = \frac{4Ht}{\zeta}, \quad (12)$$

so that equation (2) could be cast into the dimensionless form as follows:

$$\frac{d\bar{\mathbf{Q}}}{d\bar{t}} = \left(\delta - \frac{1}{(\zeta/2K) + 1} \frac{\bar{\mathbf{Q}}\bar{\mathbf{Q}}}{\bar{Q}^2} \right) \cdot \left([\lambda\boldsymbol{\kappa} \cdot \bar{\mathbf{Q}}] - \frac{1}{2} \frac{\partial}{\partial \bar{\mathbf{Q}}} \ln \psi - \frac{1}{2} \frac{\bar{\mathbf{Q}}}{1 - (\bar{Q}/\bar{Q}_0)^2} \right), \quad (13)$$

where $\lambda = \zeta/4H$ is the relaxation time of the molecules and $\sqrt{kT/H}$ is the root-mean-square average size of the Hookean dumbbell in one dimension at equilibrium. For convenience, the bars over the dimensionless parameters are omitted thereafter without causing confusion.

Next, we can get the dimensionless Smoluchowski equation for this dumbbell model:

$$\begin{aligned} \frac{\partial \psi}{\partial t} = & - \frac{\partial}{\partial \mathbf{Q}} \cdot \left[\left(\delta - \frac{1}{\varepsilon + 1} \frac{\mathbf{Q}\mathbf{Q}}{Q^2} \right) \cdot \left(\lambda\boldsymbol{\kappa} \cdot \mathbf{Q} - \frac{1}{2} \frac{\mathbf{Q}}{1 - (Q/Q_0)^2} \right) \psi \right] + \\ & \frac{1}{2} \frac{\partial}{\partial \mathbf{Q}} \left(\delta - \frac{1}{\varepsilon + 1} \frac{\mathbf{Q}\mathbf{Q}}{Q^2} \right) \cdot \frac{\partial}{\partial \mathbf{Q}} \psi, \end{aligned} \quad (14)$$

where the internal viscosity parameter is defined as $\varepsilon = 2K/\zeta$.

With the Ito interpretation we can obtain the equivalent stochastic differential equation of equation (14), following details given in Appendix A of [11]:

$$\begin{aligned} d\mathbf{Q} = & \left[\left(\delta - \frac{\varepsilon}{\varepsilon + 1} \frac{\mathbf{Q}\mathbf{Q}}{Q^2} \right) \cdot \left(\lambda\boldsymbol{\kappa} \cdot \mathbf{Q} - \frac{1}{2} \frac{\mathbf{Q}}{1 - (Q/Q_0)^2} \right) - \frac{\varepsilon}{\varepsilon + 1} \frac{\mathbf{Q}}{Q^2} \right] dt \\ & + \left[\delta - \left(1 - \sqrt{\frac{1}{\varepsilon + 1}} \right) \frac{\mathbf{Q}\mathbf{Q}}{Q^2} \right] \cdot d\mathbf{W}_t, \end{aligned} \quad (15)$$

where

$$\begin{aligned} \langle d\mathbf{W}_t \rangle &= \mathbf{0}, \\ \langle d\mathbf{W}_t d\mathbf{W}_t \rangle &= \delta(t - t') \delta dt. \end{aligned} \quad (16)$$

If $\varepsilon = 0$ in equation (15), the stochastic differential equation degenerates into the case for the classic FENE dumbbell model as described in the references [8] and [13].

The steady state simple shear flow in the Cartesian coordinate system has the velocity in three dimensions, $v_x = \dot{\gamma}y$, $v_y = 0$, $v_z = 0$, where $\dot{\gamma} = dv_x/dy$ is the shear rate. In such flow, $\boldsymbol{\kappa}$ can be expressed as a linear function of shear rate $\dot{\gamma}$

$$\boldsymbol{\kappa} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \dot{\gamma}. \quad (17)$$

So we can adjust the parameter $\lambda\boldsymbol{\kappa}$ in equation (17) by tuning Weissenberg number W_i defined by $W_i = \lambda\dot{\gamma}$.

Based on Euler's method, equation (15) can be discretized as follows:

$$\begin{aligned} \mathbf{Q}_{t+\Delta t} = & \mathbf{Q}_t \left[\left(\delta - \frac{\varepsilon}{\varepsilon+1} \frac{\mathbf{Q}_t \cdot \mathbf{Q}_t}{Q_t^2} \right) \cdot \left(W_i \cdot \mathbf{Q}_t - \frac{1}{2} \frac{\mathbf{Q}_t}{1 - (Q_t/Q_0)^2} \right) - \frac{\varepsilon}{\varepsilon+1} \frac{\mathbf{Q}_t}{Q_t^2} \right] \Delta t \\ & + \left[\delta - \left(1 - \sqrt{\frac{1}{\varepsilon+1}} \right) \frac{\mathbf{Q}_t \cdot \mathbf{Q}_t}{Q_t^2} \right] \cdot \Delta \mathbf{W}_t, \end{aligned} \quad (18)$$

where Δt is the constant time step and the components of increments $\Delta \mathbf{W}_t = \mathbf{W}_{t+\Delta t} - \mathbf{W}_t$ are all independent real-valued random variables with mean 0 and variance Δt .

For the FENE dumbbells, at any finite time step, there exists a certain probability that the simulation extension values exceed the maximum allowed extension Q_0 . Hence, we adopt the rejection method that all moves larger than a fixed big value are rejected. Because the extension that is very close to the maximum allowed value will bring bad results, as proposed by Öttinger [13], we reject all moves which lead to a value of Q^2 larger than

$$\left(1 - \sqrt{\Delta t} \right) Q_0^2, \quad (19)$$

where all the variables here are in dimensionless form.

3. Results and examples. In this section, the contribution of IV to rheological properties of polymeric fluids in time-dependent elongational flows will be demonstrated by an example presented in Subsection 3.1. In Subsection 3.2, a numerical method will be applied to the calculation of molecule extension for λ -phage DNA solutions in shear flows.

3.1. Polymeric fluids in time-dependent elongational flows. If a polymeric fluid is considered in the Cartesian coordinate system $Oxyz$ and the time-dependent simple elongational flow is along the z direction, the velocity components in the 3D case can be assumed as $v_z = \dot{\varepsilon}(t)z$, $v_x = -\frac{1}{2}\dot{\varepsilon}(t)x$, $v_y = -\frac{1}{2}\dot{\varepsilon}(t)y$, where $\dot{\varepsilon}(t)$ is a scalar time-dependent function describing the coefficient of the velocity gradient. So the rate of strain could be expressed as

$$\dot{\boldsymbol{\gamma}} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \dot{\varepsilon}(t). \quad (20)$$

Substitution of equation (20) into equation (11) yields

$$\begin{aligned} & \left(1 + \frac{\lambda_H}{1-\eta_i} \frac{\partial}{\partial t} \right) \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \tau_{yy} & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \tau_{zz} \end{pmatrix} - \lambda_H \begin{pmatrix} -\tau_{xx} & 0 & 0 \\ 0 & -\tau_{yy} & 0 \\ 0 & 0 & 2\tau_{zz} \end{pmatrix} \dot{\varepsilon}(t) \\ & = -nkT\lambda_H \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \dot{\varepsilon}(t), \end{aligned} \quad (21)$$

where λ_H is defined as $\lambda_H = \zeta/4H$.

The solution to equation (21) can be obtained by equating every element of the tensor. The elongational stresses can be obtained as

$$\tau_{zz} = -2nkT(1-\eta_i) \int_{-\infty}^t \dot{\varepsilon}(t') \exp \left\{ -\frac{1-\eta_i}{\lambda_H} \int_{t'}^t [1 - 2\lambda_H \dot{\varepsilon}(t'')] dt'' \right\} dt', \quad (22)$$

$$\tau_{xx} = \tau_{yy} = nkT(1 - \eta_i) \int_{-\infty}^t \dot{\varepsilon}(t') \exp \left\{ -\frac{1 - \eta_i}{\lambda_H} \int_{t'}^t [1 + \lambda_H \dot{\varepsilon}(t'')] dt'' \right\} dt' \quad (23)$$

while all shear stresses vanish.

Comparing to the stress history function of the elongational flow mentioned in the case without IV [9], a new introduced variable η_i appears before the integral symbols. It is clear that this new variable pays no contribution to the general trend of the stress history in time t . It only affects the transient values of stresses quantitatively.

By analyzing the stress relaxation of polymeric liquids subjected to a sudden intense stretch lasting for very short time, we note that the situation can be modeled by a silent flow subjected to a sudden infinite elongational displacement at $t = 0$. The function measuring the velocity gradient can be expressed by:

$$\dot{\varepsilon}(t) = \varepsilon_0 \delta(t), \quad (24)$$

where $\delta(t)$ is the Dirac delta function and ε_0 is an arbitrary constant. Substituting equation (24) into equations (22) and (23), respectively, yields the stress relaxation history functions

$$\tau_{zz} = -2nkT\varepsilon_0 \exp \left[(1 - \eta_i) \left(-\frac{t}{\lambda_H} + 2\varepsilon_0 \right) \right], \quad (25)$$

$$\tau_{xx} = \tau_{yy} = nkT\varepsilon_0 \exp \left[(1 - \eta_i) \left(-\frac{t}{\lambda_H} - \varepsilon_0 \right) \right]. \quad (26)$$

The contribution of the IV to the stress is transient. The effect will disappear in a long time limit. Figure 1 demonstrates the stress history curves for different internal viscosities. The IV increases initial value of the stress along elongational direction but decreases those of the stresses in other directions. Comparing figures (a) and (b), we can also find that the contribution of IV along elongational direction is much stronger.

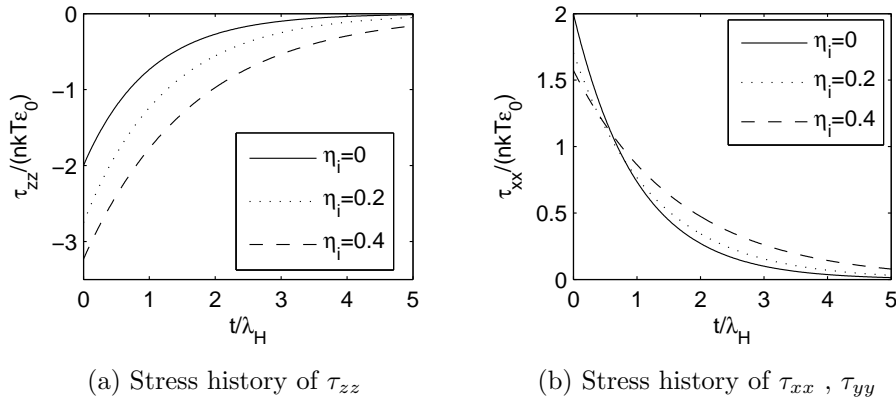


Figure 1. The contribution of the IV in the sudden elongational case.

The ratio of $\langle Q^2 \rangle$ to its value at equilibrium [9] could be expressed by

$$\frac{\langle Q^2 \rangle}{\langle Q^2 \rangle_{eq}} = 1 - \frac{\text{tr} \boldsymbol{\tau}}{3nkT}, \quad (27)$$

where tr is the trace of the corresponding tensor. Substituting equations (25) and (26) into equation (27) yields

$$\frac{\langle Q^2 \rangle}{\langle Q^2 \rangle_{eq}} = 1 - \frac{2}{3} \varepsilon_0 \left[e^{-(1-\eta_i)\varepsilon_0} - e^{2(1-\eta_i)\varepsilon_0} \right] e^{-\frac{1-\eta_i}{\lambda_H} t}. \quad (28)$$

From equation (28) it can be found that the internal viscosity has twofold effects on the transient phenomena of the change of configuration and that of the evolution of stresses in time. First, the IV decreases the initial extension of the dumbbell (Figure 2). On the other hand, the IV makes the curve flatter, which means the IV lets the system reach its steady state more slowly (Figure 3).

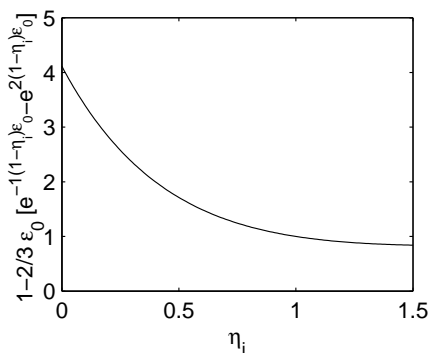


Figure 2. IV effect on the initial value of the extension.

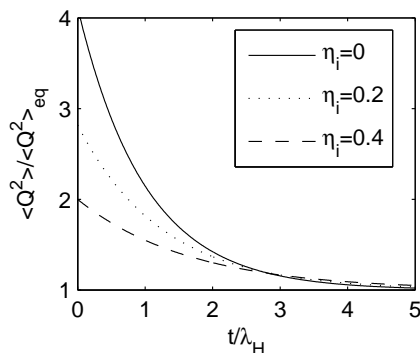


Figure 3. IV effect on the transient extension.

3.2. Molecule extension in steady shear flows. To solve equation (18) numerically, we need to give the values of Weissenberg number, W_i , and the maximum spring extension, Q_0 . For convenience of comparison with the experimental results of [6], the Weissenberg numbers, decided by shear rate of the solvent and relaxation time of DNA molecules, are chosen in the range between 0 to 80. The contour length of λ -phage DNA is taken as extensibility parameter. So, the maximum spring extension can be expressed as $Q_0 = (N - 1)a$, where N and a are the number of beads and the length of a rod of the corresponding bead-rod chain, respectively. All the parameters used in our computation can be found in [6] and [8]. In the computation, the initial values of extension are chosen randomly according to the Gaussian distribution.

Using the numerical method described above, we study the mean extension of 1000 molecules for different Weissenberg numbers. In the simulation, the molecular extension is projected onto the x - y plane to match Smith's experimental data obtained by fluorescence microscopy with intensified video camera perpendicular to the flow-vorticity plane. Every simulation with different W_i has given a specific mean extension value after 10^6 time steps when the average molecular extension appears steady.

In Figure 4, we compare our simulation based on the FENE dumbbell model with internal viscosity with the experimental data by Smith et al [6]. The results from the dumbbell model without IV by Hur & Shaqfeh [8] and the wormlike model with hydrodynamic interactions by Jendrejack et al [7] are also superimposed in the plot. The classic FENE dumbbell model can not predict the extension result when the Weissenburg numbers are high. Our dumbbell model and wormlike model have given better values at high Weissenberg numbers.

When $W_i = 0$, that is, the shear rate of the solvent vanishes, the fluctuations of molecular extension are caused only by the Brownian force bombarding on DNA molecules of small solvent molecules. When W_i increases, the extension reaches an asymptotic plateau as found by Smith et al [6] and Hur & Shaqfeh [8]. Our simulation results have better agreement with the experimental data compared to the other two simulations presented in Figure 6, especially when the values of the Weissenberg numbers are high. The good agreement with the experimental results has demonstrated that the computational efficiency of dumbbell model with internal viscosity is rather high, given its simplicity.

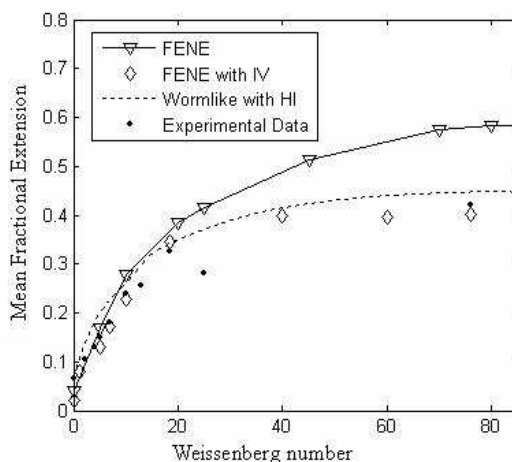


Figure 4. Extension versus W_i

4. Conclusions. In this paper, the analytical pre-averaging method and the developed numerical method are applied to the dumbbell model with IV for polymeric fluids in elongational and shear flows. The contribution of IV to the stress tensor has been discussed for time-dependent elongational flows. The Brownian dynamics simulation has been used to study the extension between the two beads of the dumbbell in shear flows. The results are in agreement with the experimental data, in particular for high Weissenberg numbers. This qualitative and quantitative agreement has demonstrated the efficiency of the dumbbell model with internal viscosity in the analysis of the rheological properties and dynamics of single DNA molecules.

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