Solving the closure problem for dilute polymer solutions

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ABSTRACT

Typically, rheological models for dilute polymer solutions are obtained via approximate representation of the underlying micro-mechanical model of the individual macromolecules[1]. The most simple micro-mechanical model for a dilute polymer solution is the elastic dumbbell model that consists of two beads connected by an entropic spring. The simplistic Hookean spring force approximation yields an **O**ldroyd-B type fluid which suffers from many fallacies when the distribution is far from Gaussian. While, Warner's finitely extensible non-linear elastic spring (FENE) is more realistic and leads to better rheological predictions, it leads to a closure problem at the macroscopic level. The **F**ENE-P approximation to FENE model allows us to formulate a closed form constitutive equation for the conformation tensor. While this is a good model and qualitatively correct, in strong flows and transient flows it leads to erroneous predictions. In complex flows such as flow past a cylinder, FENE-P approximation predicts stresses that are substantially times larger than FENE, even at a moderate Weissenberg number.

We revisit this question of approximate constitutive models for FENE model and focus our attention on the **tensorial structure** of many closure approximations in literature, and their intrinsic inability to capture the second normal stress difference ($N2$) in simple shear flows. We suggest a simple and elegant approach to correct the tensorial structure of the polymeric stress approximation. This understanding is then carried forward to the framework in the second part of the work, where we focus on the selection of relevant macroscopic variables in the system.

We recognize that the non-linearity of the spring is crucial for predicting correct rheological behaviour. Similar to kinetic theory of gases, one needs more variables to represent highly non-linear situations. We show that this new model FENE-NP, drastically improves the steady state and time dynamics results over FENE-P model, even in strong extensional flows. Finally, we discuss possible coupling of this constitutive model with flow solvers such as lattice Boltzmann.

REFERENCES

In-text citations

For references to documents referred to in the reference list, use superscript sequentially$^{1-6}$. Author names may be used together with a superscript number.

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[1] RB Bird, RC Armstrong, O Hassager., *Dynamics of polymeric liquids. Vol. 2: Fluid mechanics.* (1987).

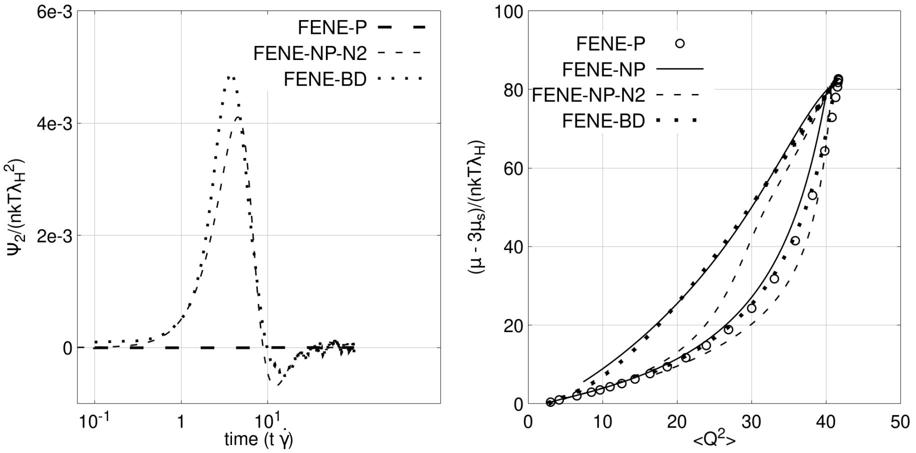

Figure 1: (a)Non-zero N2 for a simple shear flow at Wi=10.
(b)Hysteresis observed in a uniaxial extensional flow.
FENE-P fails to predict a transient non-zero second normal stress difference (**N2**) in simple shear flows and **fails to predict hysteresis** in strong extensional flows. BD : Brownian dynamics

EXAMPLE OF REFERENCE LIST STYLES

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