A comparison between the FENE-P and sPTT constitutive models in Large Amplitude Oscillatory Shear (LAOS) - Supplementary Material

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1. Effect of β on 1D modelling results

Figure 1 shows the viscous Lissajous curve (for $\tau_{p,12}$) for the FENE-P ($L^2 = 100$) response obtained using the 1D MOL simulations for various values of β where $N_y = 128$. There is virtually no change in the Lissajous curves between $\beta = 1 \times 10^{-4}$ and $\beta = 9.99 \times 10^{-4}$, indicating that the results are insensitive to β at $\beta = 1 \times 10^{-4}$, which is the value we used in this study.

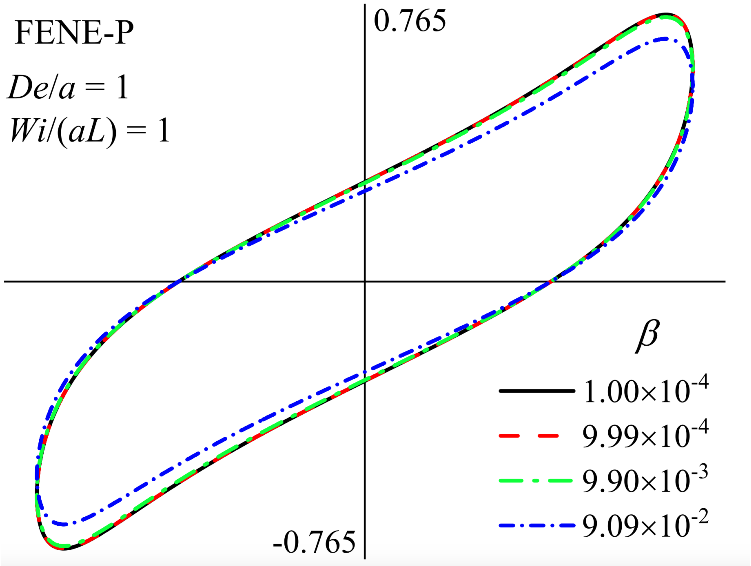

Figure 1: Viscous Lissajous curves for FENE-P ($L^2 = 100$) with varying β. Results obtained for the 1D MOL simulations. $N_y = 128$ for these simulations.

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2. Effect of N_y on 1D modelling results

Figure 2 shows the viscous Lissajous curve (for $\tau_{p,12}$) for the FENE-P ($L^2 = 100$) response obtained using the 1D MOL simulations for various values of N_y. There is no change in the model response under LAOS between $N_y = 64$ and $N_y = 256$, indicating that the results are insensitive to N_y (provided there is no shear-banding) at $N_y = 128$, which is the value we used in this study.

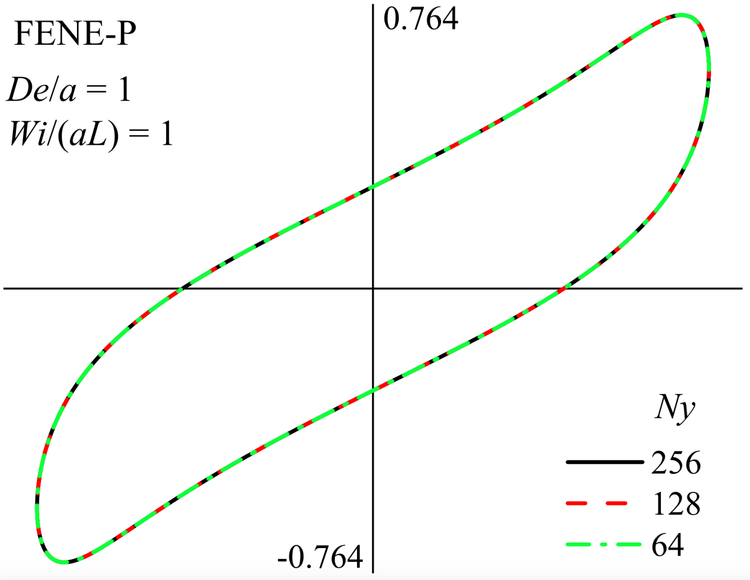


Figure 2: Viscous Lissajous curves for FENE-P ($L^2 = 100$) model response with varying N_y. Results obtained for the 1D MOL simulations. $\beta = 1/1001$ for these simulations.

3. Shear-banding in the Rolie-Poly model in LAOS

Here,we verify that the 1D MOL methodology used in this study is capable of capturing shear banding using the Rolie-Poly (ROuse LInear Entangled POLYmers) model, which has a non-monotonic stress-strain rate relationship for low enough values of the entanglement ratio Z and the convective-constraint release parameter β_{CCR}, and therefore does shear band in both steady-shear and in LAOS. The version of the Rolie-Poly model used here (with the added polymer diffusion term) contains a FENE-type extensibility function, derived by Kabanemi & Hétu (2009), and is given as

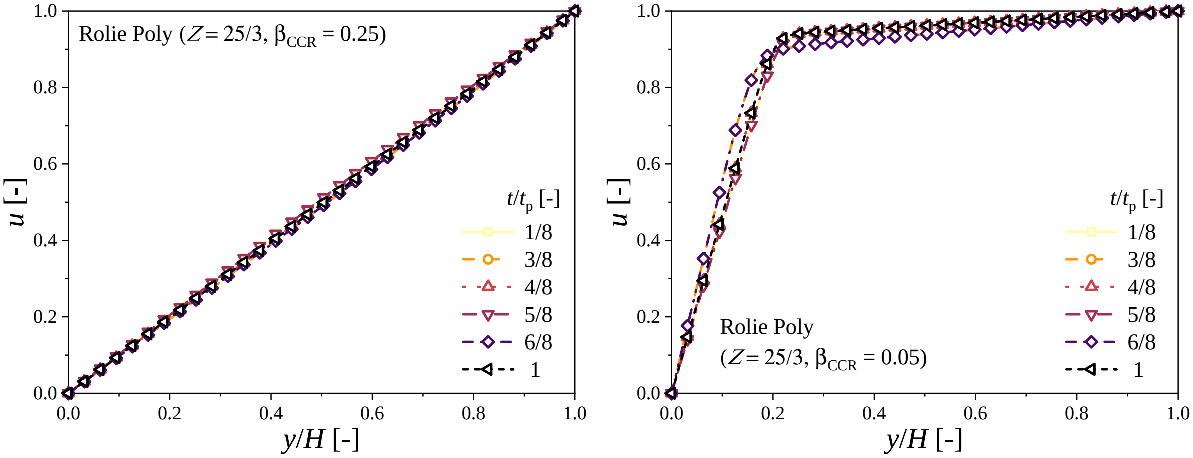
$$
\begin{aligned}
De_D \frac{\partial}{\partial t}\mathbf{A} - Wi_D(\mathbf{A}\cdot\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^{\mathrm{T}}\cdot\mathbf{A} - \boldsymbol{u}\cdot\nabla\mathbf{A}) = -(\mathbf{A}-\mathbf{I}) \\
- 2k\frac{\lambda_D}{\lambda_R}\left(1-\sqrt{3/\mathrm{tr}(\mathbf{A})}\right)\left[\mathbf{A} + \beta_{\mathrm{CCR}}\left(\frac{\mathrm{tr}(\mathbf{A})}{3}\right)^{\delta}(\mathbf{A}-\mathbf{I})\right] \\
+ \kappa\nabla^2\mathbf{A} \quad (1)
\end{aligned}
$$

where De_D and Wi_D are the Deborah and Weissenberg numbers based on the reptation relaxation time, λ_D, λ_R is the Rouse relaxation time, and δ is a parameter usually taken to be $-1/2$ (Reis & Wilson, 2013). Z relates the two relaxation times as $Z = \lambda_D/3\lambda_R$. k is the non-linear spring coefficient which is given by the normalized Padé inverse Langevin function (Cohen, 1991)

$$
k = \frac{\left(3 - \frac{\chi^2}{\chi_{\max}^2}\right)\left(1 - \frac{1}{\chi_{\max}^2}\right)}{\left(1 - \frac{\chi^2}{\chi_{\max}^2}\right)\left(3 - \frac{1}{\chi_{\max}^2}\right)} \tag{2}
$$

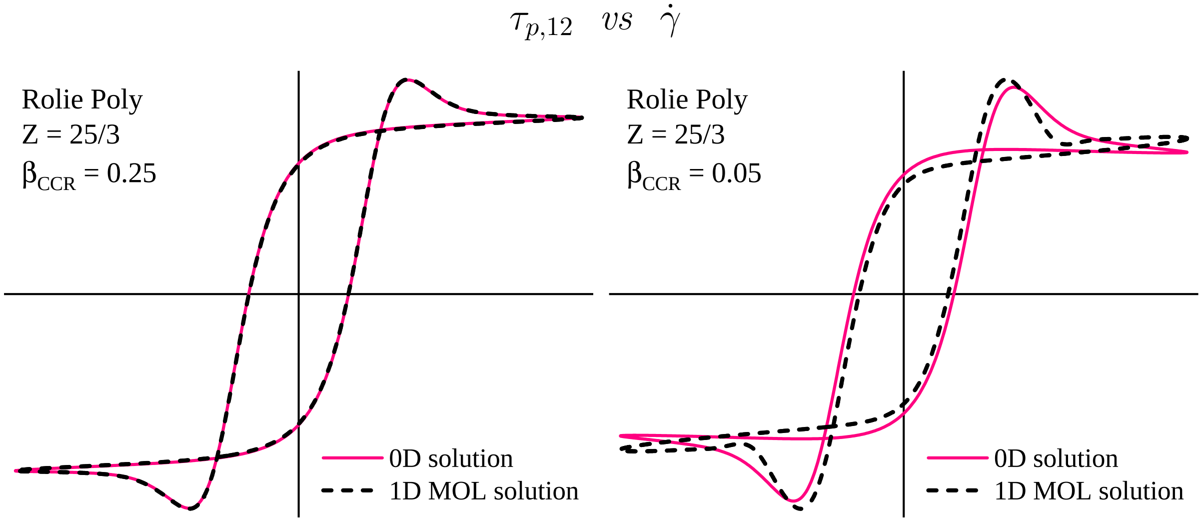
where $\chi = \sqrt{3/\mathrm{tr}(\mathbf{A})}$ and $\chi_{\max}$ is the maximum stretch ratio (similar to L^2 in the FENE-P model). The stress is recovered from the Rolie-Poly model, in a similar manner to the FENE-P model, by

$$
\boldsymbol{\tau}_p = \frac{(1-\beta)}{Wi_D}k(\boldsymbol{A}-\boldsymbol{I}) \tag{3}
$$



(a) (b)

Figure 3: Velocity profile in the gap at various times during the oscillation period during the 1D MOL simulations using the Rolie Poly model for (a) $\beta_{\text{CCR}} = 0.25$ and (b) $\beta_{\text{CCR}} = 0.05$. $De_D = 0.5$ and $Wi_D = 20$. Shear banding is observed for $\beta_{\text{CCR}} = 0.05$. $N_y = 128$.



(a) (b)

Figure 4: Lissajous-Bowditch plot (viscous projection) showing the 1D MOL solution (black dashed lines) and the 0D simulation (pink solid line) using the Rolie Poly model for (a) $\beta_{\text{CCR}} = 0.25$ and (b) $\beta_{\text{CCR}} = 0.05$. $De_D = 0.5$ and $Wi_D = 20$. The stress plotted for the 1D MOL simulations is the stress at the top boundary of the gap. $N_y = 128$.

In Figures 3 and 4 we show, respectively, for the Rolie-Poly model, the velocity profiles in the gap during one oscillation with period t_p and the corresponding viscous Lissajous curves where the stress is computed at the top boundary, as would be the case in most experiments using a plate/plate or cone/plate rheometer. It is evident that with $\beta_{\mathrm{CCR}} = 0.05$, shear banding is predicted with the MOL technique. The shear banding causes a significant difference in the viscous Lissajous curve when the 1D solution and 0D solutions are compared, particularly in the region following the stress overshoot, which was also observed in the study of Adams & Olmsted (2009) during start-up flow.

References

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