

Modelling the nonlinear shear response of linear polymer melts with tube models

M. Dalne^a, L.G.D Hawke^a, C. Hannecart^a, E. van Ruymbeke^a

^a*Bio and Soft Matter, Institut de la Matière condensée et des Nanosciences, UCLouvain, Belgium*

Email of corresponding author: maxime.dalne@uclouvain.be

This poster focuses on describing the transient response of the stress growth coefficient of monodisperse linear polymer melts. Specifically, we want to improve the understanding of the polymer chains behavior during the overshoot. To this end, we use the Time Marching Algorithm developed by the UCLouvain group and we study the orientation and the stretch state of the polymer chains. Flow-induced disentanglement is introduced in the model, taking place in addition to reptation, contour length fluctuation and constraint release [1]. A first assumption is to consider that at very early times, the polymer chains are fully entangled while at longer times (at steady-state regime) the chains are partially entangled. This affects the relaxation time of chain strands and thus, influences their orientation. We also assume that the chain can adopt different stretch levels depending on the size of a shear blob [2].

By adapting the constitutive equations of McLeish and Larson [3] to the concepts introduced with the TMA, we observed that we can capture either the overshoot or the steady regime depending on the stretch relaxation time imposed in the model.

[1] H. Taghipour, S. Costanzo, D. Vlassopoulos, E. van Ruymbeke, and L. G. D. Hawke, "Entangled linear polymers in fast shear flows: Comparison of tube-model predictions and experimental data." *J. Rheol.* **2021**, *65*, 1111–1137.

[2] C. Hannecart, T. Shahid, D. Vlassopoulos, F. Oosterlinck, C. Clasen, and E. van Ruymbeke, "Decoding the steady elongational viscosity of monodisperse linear polymers using tube-based modeling." *J. Rheol.* **2022**, *66*(1), 197-218.

[3] T. C. B. McLeish, and R. G. Larson, "Molecular constitutive equations for a class of branched polymers: The pom-pom polymer." *J. Rheol.* **1998**, *42*(1), 81-110.