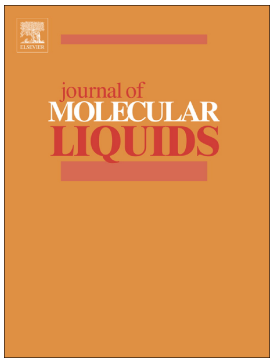

Polydispersity influence in rheological behavior of linear chains by Molecular Dynamics

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Polydispersity influence in rheological behavior of linear chains by Molecular Dynamics

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Abstract

Non–equilibrium molecular dynamics simulations were performed to study the effect of the polydispersity index (PDI) on the rheological behavior of linear chains. Four distributions were studied, in which the number average molecular weight was kept constant and the weight average molecular weight was varied. The rheological behavior was obtained by using the SLLOD equation of motion at 450 K. All flow curves show three regions: a first Newtonian plateau, a shear–thinning, and a second Newtonian plateau. The weight average molecular weight exhibited a strong influence in the shear–thinning behavior. Also, at higher shear–rates, some larger chains suffer instabilities in their conformation, causing the presence of the second Newtonian plateau at the lowest apparent viscosity, which is an indicative that potential flow-induced entanglements may occur.

Keywords: Linear chains, Molecular Dynamics, Rheological behavior, Polydispersity

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