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Single polymer in fluid flows: a numerical study ALBERTO PULIAFITO, ANTONIO CELANI, INLN-CNRS, KONSTANTIN TURITSYN, Landau Institute — Thanks to the improvements in experimental techniques, a comprehensive study ofthe motion of single molecules in fluid flows has recently become a reality. The direct comparison of experiments with numerical simulations and theory permits to check and refine the various polymer models, and unveils the role of interactions between different macromolecules and between the molecule and the surrounding fluid. The dynamics of single molecule in fluid flows has been studied in great detail by Chu, Larson, Shaqfeh and coworkers. We show how nontrivial aspects of polymer-fluids interactions may be accounted for and even explained at a semi-quantitative level by means of simple, few degrees of freedom models. We investigate the dynamics of orientation and elongation of a polymer molecule in a laminar shear flow as a function of the flow strength, and we analyze the aperiodic rotational motion of the molecule. In the laminar elongational flow and in the random chaotic flow we investigate the transition time from a given initial condition to the stationary distribution as a function of the flow strength, temperature, and length of the polymer. We give a theoretical explanation for the anomalous increase of relaxation times around the coil-stretch transition.

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