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Modelling polymer-obstacle collisions: Molecular Dynamics simulations and theory MARTIN KENWARD, GARY W. SLATER, University of Ottawa — We present results from Molecular Dynamics (MD) simulations that explicitly include a Lennard–Jones solvent and therefore hydrodynamic interactions. We utilize these MD simulations to explore the collision of single polymers with obstacles in three specific cases: i) a polymer in the presence of an external force colliding with a fixed obstacle, ii) a polymer in a laminar flow colliding with a fixed obstacle and iii) a polymer in the presence of an external force colliding with a free obstcale. We focus on the limit where the applied force, during a collision, is able to fully elongate the polymer (in the direction of the force) to a length on the order of its contour length. To complement the MD simulations we present a general set of equations which describe these polymer-obstacle collisions. In certain cases of interest these equations yield analytical results for the observed escape dynamics. The data describing the escape of the molecules as a function of chain length, can be collapsed onto a single universal curve. We also show that the molecules undergo a non–neglible compression during the final stages of the escape process which modifies the resulting dynamics. In the case of the inclusion of a laminar flow we also examine qualitatively how the presence of the both the obstacle and the polymer modify the resulting flow profile and the forces dictating the escape of the molecules.

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