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Hydrodynamically Enhanced Brownian Motion in Flowing Polymer Solutions

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Diffusion of a molecule in solution typically occurs via thermally driven Brownian motion, with solvent collisions leading to a random-walk trajectory for the solute. This physical principle guides our understanding of molecular transport in a wide variety of situations, ranging from protein diffusion in biological systems and mixing in solution processes to charge transport in polyelectrolyte solutions. Thermal diffusion represents a “speed limit” for molecular transport, which can typically only be surpassed by imposing a directional, external field. The other way particles expedite diffusion is via self-propulsion. This “active Brownian motion” is famously seen in some single-cell organisms and can also be shown in some colloidal systems, but because it requires self-propulsion, this is not seen at the molecular level. We show that it is possible to dramatically increase the diffusion of small molecules in a way that mimics active Brownian motion, instead driven by the disturbance flows of highly stretched polymers in strong flows to induce propulsion at a distance. We use molecular simulations that account for these hydrodynamic disturbances to demonstrate that it is possible to increase the effective diffusion constant by more than an order of magnitude, and we provide a mechanistic model for how the interplay of polymer concentration, flow-induced polymer stretching, and chain length gives rise to hydrodynamically enhanced Brownian motion. This effect has important implications for molecular transport, and we show that strong flows and a low concentration of stretched polymers can be used to promote rapid diffusion.

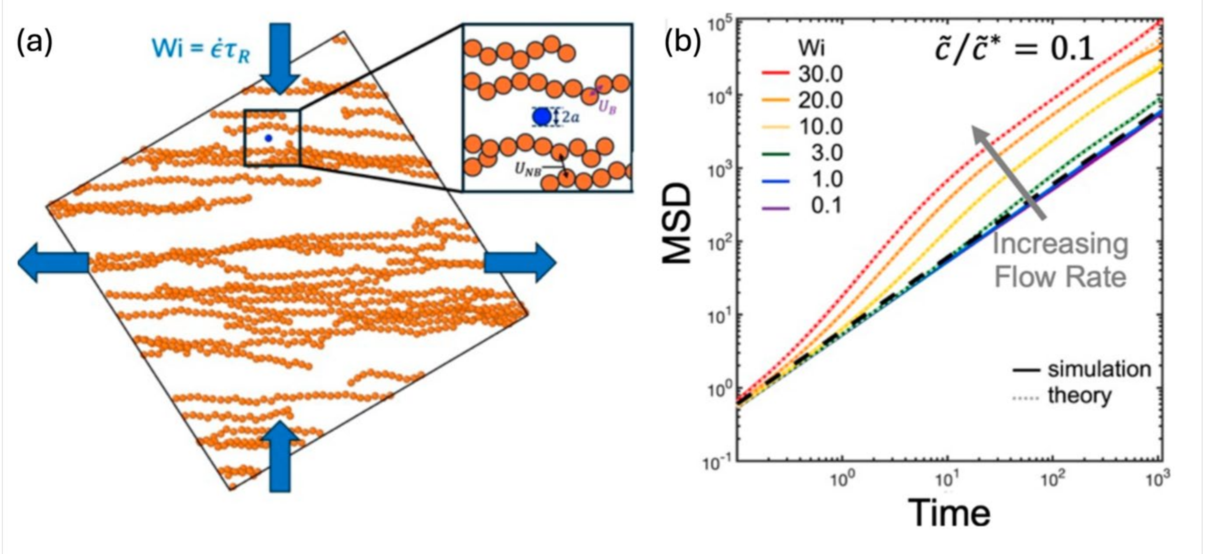

Fig. 1. (a) Simulation snapshot of a semidilute polymer solution at a concentration c = 0.1c* and a flow strength Wi = 6. All particles are characterized by a radius a and nonbonded interactions U_{NB}, while polymer monomers are connected by a bonded potential U_B. (b) The mean-square displacement versus time for several flow strengths showing a super diffusive regime.

References

[1] N. Tyagi, D. W. Walker, C. D. Young, C. E. Sing, Hydrodynamically enhanced Brownian motion in flowing polymer solutions, ACS Macro. Lett. 14 (2025), 464-471.

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