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Enhanced Fluid Mixing in Nanochannels: A Molecular Dynamics Study ERIC C.J. OLIVER, GARY W. SLATER, University of Ottawa — The efficient mixing of fluids is of paramount importance in several applications such as lab-on-a-chip and microfluidic devices. The main limitation to efficiency is that on small scales where the Reynolds number of the flow is low, mixing is dominated by diffusion. Purely diffusive motion is very slow and is an inefficient mixing mechanism unless the channel width is extremely small. Starting with the basic result for diffusive mixing of a binary fluid in a Poiseuille flow we explore methods to enhance the level of mixing between the two fluid species. We simulate the system using Molecular Dynamics and model the fluids as assemblies of Lennard-Jones beads. In order to increase the rate of mixing we have forced lateral motion in the fluid using configurations of mid-stream posts. Specifically, posts set in a prism-like structure have proven to be extremely well suited to reducing the channel length required to achieve complete mixing. In order to measure efficiency we have proposed a mathematical function that quantifies the level mixing associated with a fluid element. Furthermore, we have developed a basic theory for the position of the mixing front in a flow with spatially dependent velocity and diffusion coefficient.

Eric C. J. Oliver
University of Ottawa

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