

Molecular Dynamics Computations of Temperature and Concentration Profiles in Highly Confined Planar Poiseuille Flows of Colloidal Suspensions

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We present the results of molecular dynamics simulations of model colloidal suspensions in highly confined planar Poiseuille flows with channel widths of the order of a few colloidal particle diameters up to around 80 particle diameters. The temperature and concentration profiles are compared with those predicted by using linear transport equations with the thermal conductivity, viscosity, thermal and mutual diffusion coefficients and other data from molecular dynamics simulations on the corresponding homogeneous fluids. The concentration profiles show an increase in colloid concentration at the walls. The temperature profiles cannot be accurately described without considering thermal diffusion. At higher flow rates, and for narrower channels, the description in terms of linear non-equilibrium thermodynamics breaks down, and we suggest possible extensions of the linear treatment that will be required for very narrow channels and high velocity gradients.