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A multiscale transport model for binary Lennard Jones mixtures in slit nanopores. RAVI BHADAURIA, N. R. ALURU, University of Illinois at Urbana-Champaign — We present a quasi-continuum multiscale hydrodynamic transport model for one dimensional isothermal, non-reacting binary mixture confined in slit shaped nanochannels. We focus on species transport equation that includes the viscous dissipation and interspecies diffusion term of the Maxwell-Stefan form. Partial viscosity variation is modeled by van der Waals one fluid approximation and the Local Average Density Method. We use friction boundary conditions where the wall-species friction parameter is computed using a novel species specific Generalized Langevin Equation model. The transport model accuracy is tested by predicting the velocity profiles of Lennard-Jones (LJ) methane-hydrogen and LJ methane-argon mixtures in graphene slit channels of different width. The resultant slip length from the continuum model is found to be invariant of channel width for a fixed mixture molar concentration. The mixtures considered are observed to behave as single species pseudo fluid, with the friction parameter displaying a linear dependence on the molar composition. The proposed model yields atomistic level accuracy with continuum scale efficiency.

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