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A Nanoscale Hydrodynamical Model for Transport of Water RAVI BHADAURIA, TARUN SANGHI, N. R. ALURU, Univ of Illinois - Urbana — We present here a one-dimensional isothermal hydrodynamic transport model for SPC/E water. Two separate mechanisms of flow, viz. viscous and slip are incorporated in the present formulation. Spatially varying viscosity is modeled using the local average density method. Slip velocity is provided as a form of the boundary condition which in turn depends upon the macroscopic interfacial friction coefficient. The friction coefficient bridges the atomistic and continuum descriptions of the problem. The value of this friction coefficient is computed using particle-based wall-fluid force autocorrelations and wall-fluid force-velocity cross correlations, where the particle trajectory is generated using a Generalized Langevin Equation formulation. To test the accuracy of the model, gravity driven flow of SPC/E water confined between graphene and silicon slit shaped nanochannels are considered as examples for low and high friction cases. The proposed model yields good quantitative agreement with the velocity profiles obtained from non-equilibrium molecular dynamics simulations. Furthermore, we demonstrate that the slip length is constant for different channel widths for a fixed thermodynamic state under the linear response regime.

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