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Perspectives on continuum flow models for force-driven nano-channel liquid flows ALI BESKOK, JAFAR GHORBANIAN, ALPER CELEBI, Southern Methodist University — A phenomenological continuum model is developed using systematic molecular dynamics (MD) simulations of force-driven liquid argon flows confined in gold nano-channels at a fixed thermodynamic state. Well known density layering near the walls leads to the definition of an effective channel height and a density deficit parameter. While the former defines the slip-plane, the latter parameter relates channel averaged density with the desired thermodynamic state value. Definitions of these new parameters require a single MD simulation performed for a specific liquid-solid pair at the desired thermodynamic state and used for calibration of model parameters. Combined with our observations of constant slip-length and kinematic viscosity, the model accurately predicts the velocity distribution and volumetric and mass flow rates for force-driven liquid flows in different height nano-channels. Model is verified for liquid argon flow at distinct thermodynamic states and using various argon-gold interaction strengths. Further verification is performed for water flow in silica and gold nano-channels, exhibiting slip lengths of 1.2 nm and 15.5 nm, respectively. Excellent agreements between the model and the MD simulations are reported for channel heights as small as 3 nm for various liquid-solid pairs.

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