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Molecular Dynamics Simulations of Nanoscale Gas Flows MURAT BARISIK, BOHUNG KIM, ALI BESKOK, Old Dominion University — Three-dimensional molecular dynamics (MD) simulations of rarefied gas flows confined within nano-scale channels are investigated by introduction of a smart wall model that drastically reduces the memory requirements of MD simulations for gas flows. The smart wall molecular dynamics (SWMD) represents three-dimensional FCC walls using only 74 wall molecules. Linear Couette flow of argon at Knudsen number 10 is investigated using the SWMD utilizing Lennard-Jones potential interactions. Presence of the walls creates an additional length scale based on the Lennard-Jones force field near the walls. This is typically 3 molecular diameters (σ) in the parametric regime studied here. Therefore 3σ region near the walls becomes a critical length scale that admits deviations from the kinetic theory. Our results have shown increase in the gas density and sudden change of the velocity profiles within this region. Kinetic theory solutions based on the Boltzmann equation neglect the wall force field effects, and hence, cannot predict this density increase and the change in the velocity profile. We have shown that the velocity profile within the interface region exhibits self similar behavior regardless of the channel height (provided that $H > 6\sigma$). Overall, the slip velocity is over predicted using kinetic theory solutions.

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