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Surface-Gas Interaction Effects on Nanoscale Flows MURAT BARISIK, ALI BESKOK, Old Dominion University — Three-dimensional molecular dynamics (MD) simulations of linear Couette flow of argon gas confined within nano-scale channels are investigated as a function of the surface-gas interaction strength ratio (ISR). Simulations are performed in the slip, transition and free molecular flow regimes by keeping the base pressure constant for different ISR cases. Near-wall gas density increases with increased ISR and eventually results in adsorption of argon on the surfaces. Although the velocity profiles agree with the kinetic theory predictions in the bulk of the channel, they show sudden increase in the near wall region, resulting in decreased velocity slip at the interface. High ISR values are shown to induce velocity stick. Increase in the ISR results in stronger surface–particle interactions. Hence, the surface virial becomes more dominant in the near wall region, resulting in increasingly anisotropic normal stresses. Utilizing the kinetic theory and MD predicted shear stress values, the tangential momentum accommodation coefficient for argon gas, interacting with FCC structured walls (100) plane facing the fluid, is shown to increase with increased ISR.

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