

Abstract Submitted
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Surface Effects on Nanoscale Gas Flows ALI BESKOK, MURAT BARISIK, Old Dominion University — 3D MD simulations of linear Couette flow of argon gas confined within nano-scale channels are performed in the slip, transition and free molecular flow regimes. The velocity and density profiles show deviations from the kinetic theory based predictions in the near wall region that typically extends three molecular diameters (s) from each surface. Utilizing the Irwin-Kirkwood theorem, stress tensor components for argon gas confined in nano-channels are investigated. Outside the $3s$ region, three normal stress components are identical, and equal to pressure predicted using the ideal gas law, while the shear stress is a constant. Within the $3s$ region, the normal stresses become anisotropic and the shear stress shows deviations from its bulk value due to the surface virial effects. 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 calculated to be 0.75; this value is independent of the Knudsen number. Results show emergence of the $3s$ region as an additional characteristic length scale in nano-confined gas flows.

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