

Abstract Submitted
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Gas Flows in Nano-Scale Confinements ALI BESKOK, Southern Methodist University, MURAT BARISIK, Izmir Institute of Technology — Most studies on gas transport in nano-scale confinements assume dynamic similarity with rarefied gas flows, and employ kinetic theory based models. This approach is incomplete, since it neglects the van der Waals forces imposed on gas molecules by the surfaces. Using 3D molecular dynamics (MD) simulations of force driven gas flows, we show the significance of the wall force field in nano-scale confinements by defining a new dimensionless parameter (B) as the ratio of the wall force-penetration length to the channel height. Investigation of gas transport in different nano-channels at various Knudsen numbers show the importance of wall force field for finite B values, where the dynamic similarity between the rarefied and nano-scale gas flows break down. Molecularly structured walls determine the bulk flow physics by setting a proper tangential momentum accommodation coefficient, and also determine transport in the near wall region. Gas nano-flows with finite B exhibit significant differences in the local density and velocity profiles, affecting the mass flow rate and the behavior of Knudsen's minimum in nano-channels.

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