Axial Transport of Simple Gases in Nanochannels

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It is proposed that at low density and temperatures less than 600 K, argon gas molecules in a carbon nanotube oscillate with in a potential well of -5 kJ/mol depth. With increase temperature, it is expected that molecular diffusivity will increase more quickly than predicted by Knudsen diffusion models. Axial transport occurs in two domains; a near wall domain, in which there is a significant retardation of flow due to wall interaction, and a ballistic domain, in which axial motion is unaffected by the wall potential. Molecular dynamics simulations have been performed to determine the trajectory and momentum loss that a gas molecules experiences when impacting a wall. It was found that a strong dependence on incident angle exists in which collisions are nearly specular at low angle and grow more diffuse until the incident angle reaches 30^{o}. At that point, all incoming momentum is effectively lost before a molecule is reemitted. The shape of the nanochannel has a significant effect on tranport processes.

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