Pressure calculations in nanochannel gas flows

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Abstract
In this research, pressure driven flow within a nanochannel is studied for argon in rarefied gas states. A Molecular Dynamics simulation is used to resolve the density and stress variations. Normal stress calculations are based on Irving-Kirkwood method, which divides the stress tensor into its kinetic and virial parts. The kinetic component recovers pressure based on the ideal-gas law. The particle-particle virial increases with increased density. The kinetic part and the virial part of the pressure is studied from Kn = 0.1 to Kn = 0.5 at 300 K. This pressure calculation was also compared with a simulation for a static fluid. Pressure driven gas flow gives a different result compared to static situation, which has a uniform particle distribution across the system. For a flow situation, the virial part is no longer the same. This can also be predicted from the virial equation and by the fact that the compressible fluid flow causes a temperature and density difference along the flow direction. The relation between the virial and distribution of particles has been studied further to understand the nature of virial component along the flow direction in compressible flows.