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Macroscopic relations for microscopic properties at the interface between solid substrates and dense fluids

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Abstract-

Strongly confined fluids exhibit inhomogeneous properties due to atomistic structuring in close proximity to a solid surface. State variables and transport coefficients at a solid-fluid interface vary locally and become dependent on the properties of the confining walls. However, the precise mechanisms for these effects are not known as of yet. Here, we make use of nonequilibrium molecular dynamics simulations to scrutinize the local fluid properties at the solid-fluid interface for a range of surface conditions and temperatures. We also derive microscopic relations connecting fluid viscosity and density profiles for dense fluids. Moreover, we propose empirical ready-to-use relations to express the average density and viscosity in the channel as a function of temperature, wall interaction strength, and bulk density or viscosity. Such relations are key to technological applications such as micro-/nanofluidics and tribology but also natural phenomena.

Index Terms-

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