Comparison of Wall Models' Effects on Liquid Nanoflows in Planar and Cylindrical Geometries. Application to Nanoinjection.

Authors: Nadia Sellami and Dr. Michael M. Micci
Affiliation: Aerospace Engineering Department, The Pennsylvania State University-USA

Molecular simulations of single phase bounded flows especially at high density showed discrepancies from the classical Navier Stokes solutions: the failure of predicting the slip value at the wall, stratification of the density close to the wall and excessive heating which affects the natural thermal fluctuations of the atomistic system (NVE ensemble). To alleviate some of these observed phenomena, the modeling of the solid boundaries progressed from implicit mathematical wall models to explicit multi-layered atomistic structure including temperature/pressure-control mechanisms. The wetting property of those models is either inexistent or can be adjusted through the respective interactive solid-fluid potential and its parameters. Abraham was among the few who tried to compare the effect of different wall models commonly used in molecular simulations and observed differences in the structure of the fluid in the channel (density distribution) which in return is expected to affect the pressure of the bulk fluid. Our objective is to account for the differences that can be observed from the use of different wall models in molecular dynamics simulations for a wide range of densities and temperatures of a single phase Lennard Jones monatomic fluid (Argon) away from the critical point. We study 3 categories of wall models used in literature: the Atomistic model, the Lennard Jones continuous model and the Mathematical model (purely reflective models). We track the effect of these wall models through their interaction with the fluid and the effects of the system size, geometry and cutoff distance on the density, pressure and slip distance in flowing conditions. It is found that these wall models do not naturally provide similar data or profiles and are affected differently by the change of size, cutoff distances fluid density and the wetting property/transition. Application to nanoinjection also shows that even though the initial conditions are fitted to be similar, the jet exit velocity is dependent on the wall model applied to the dense phase.