

Abstract Submitted
for the DFD07 Meeting of
The American Physical Society

A continuum approach to reproduce molecular scale slip behavior

NEELESH A. PATANKAR, HUA-YI HSU, Northwestern University — In this work we ask the question: Is it possible to reproduce molecular scale slip behavior by using continuum equations? To that end we note that: i) near the wall, the fluid experiences a potential, ii) the fluid density responds to the wall potential, hence, fluid compressibility is relevant, and iii) the fluid can lose momentum to the wall. To incorporate these features we simulate shear flow of a *compressible* fluid between two walls *in the presence of a wall potential*. Compressibility is important only in the near wall region. The slip length is calculated from the mean velocity profile. The slip length vs. shear rate trend is similar to that in molecular dynamic calculations. First, there is a constant value of slip length at low shear rates. Then, the slip length increases beyond a critical shear rate. Lastly, the slip length reaches another constant value if the wall momentum loss parameter is non-zero. The scaling for the critical shear rate emerges from our results. The value of the slip length increases if the wall potential is less corrugated and if the momentum loss to the wall is low. An understanding of the overall force balance during various slip modes, suggested previously, emerges from the governing equations. This work could be useful to develop continuum simulation tools for nanoscale problems without the need for expensive hybrid computations.

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Date submitted: 01 Aug 2007

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