

Linear alkanes confined between smooth solid surfaces

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We focus here on the behavior of confined n-alkane molecules between solid walls of different kind (mostly metals and oxides). Molecular Dynamic simulations are lead to investigate the structure and rheology of the confined fluid, and the major point of interest is the slip at the wall, depending on both solid and fluid materials and the confinement itself.

The first part of the talk concerns the effects of chain length and surface (nature, orientation) on slip, as well as the role of the wall-fluid interactions. Details can be found in [1].

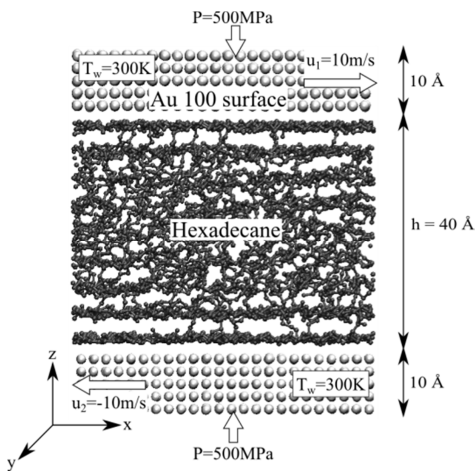


Figure 1 Overview of the molecular dynamics system and the applied operating conditions

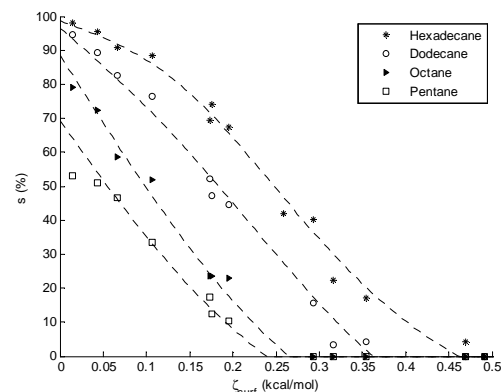


Figure 2 Wall slip values for different linear alkanes as a function of the surface interaction parameter. The points represent results from MD simulations, the dotted lines the predicted values.

A wall slip model based on the competition between these two factors is introduced. A surface parameter accounts for the wall-fluid interaction and commensurability, and is valid for both canonical and complex crystal lattices: this quantity is then linked to the shear stress transferred to the fluid molecules. Finally, a semi-analytical law for wall slip prediction including both the fluid viscosity and the surface characterization parameter is proposed.

The second part of the talk is a highlight on what is happening when the surfaces get closer and nearly touch each other, with a critical amount of fluid in between. Details can be found in [2].

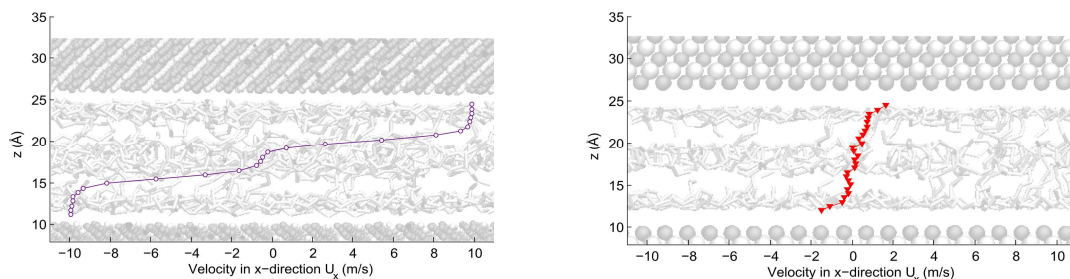


Figure 3 Velocity profiles across the film thickness for different combinations of surface wettability.

[1] Savio et al. Tribol Lett (2012) 46:11–22

[2] Savio et al. Tribol Lett (2013) 50:207–220