## Molecular dynamics simulations of flow in nanopores

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A no-slip boundary condition is usually assumed when estimating the velocity of fluid in a channel of continuum flow dimensions. However, at the nanoscale, molecular roughness has a large impact on fluid behavior at surfaces and in pores [1]. With increasing roughness, the no-slip boundary condition arises naturally. However, at lower fluid densities slip appears [2]; a non-zero velocity arises at the wall of the channel. If slip is not taken into account then the mean velocity in the channel can be underestimated dramatically. This can be a problem when dealing with flow in porous structures where the nanoporosity is non-negligible, such as engine deposits and gas shales. Quantifying the amount of slip in a channel of given material-fluid combination is a challenge that requires simulation techniques such as Molecular Dynamics (MD). However, MD is limited to relatively small simulation boxes, commonly only a few nanometres. As such, there is a need for a procedure for calculating flow in nanopores for larger geometries than just single pores.

This study is specifically aimed at understanding transport of hydrocarbons in nanoporous engine deposits. Engine deposits are complex carbonaceous materials accumulating on the inner surfaces of car engines that can act as a "sponge" and adsorb fuel components [3]. The presence of these deposits may lead to adverse engine performance such as power loss, slow acceleration, poor drivability, a poor cold start and increased emissions. The mechanisms strongly depend on the porous nature of the deposits and may or may not depend on the surface roughness of pores. A previous study found that the equilibrium adsorption capacity is certainly sufficient to perturb the combustion process, however a method is needed for finding credible adsorption within a realistic time frame, i.e. that of an engine cycle (circa 1 ms).

Equilibrium [5] and non-equilibrium Molecular Dynamics (MD) are used to study slip within slit pores. An MD package known as GROMACS [4], primarily designed for biomolecular systems such as proteins and lipids, is used here. The effects of the solid surface structure, wettability and method of restraining the surface on the observed slip length are investigated as well. The study is then extended to include the effect of surface geometry on the relation between the planar slip length and slip velocity and a model produced based on the surface curvature. Furthermore, surface roughness is quantified and included in the model. Finally, the geometry dependent model for slip is implemented as a boundary condition in a multi-phase multi-component Lattice Boltzmann (LB) code, for simulating flow in larger scale systems such as the porous structures that exist in engine deposits. LB method is an efficientsolution for simulations of complex flow in porous media, due to its statistical physics background, easy implementation, strength of dealing with complex geometries and inherent parallelism [6]. The LB code is then validated against MD simulations on complex geometries.

With adaptations implemented within the LB model and the model validated, MD simulations are performed on surfaces representative of engine deposits in order to extract slip lengths for use in LB. Future work will include imaging these carbonaceous deposits for use as geometries in the model, for flow and spontaneous imbibition calculations.

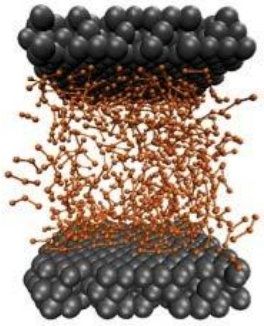

Figure 1: Snapshot of model nano-pore in MD simulation

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