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# Tribologycal Design by Molecular Dynamics Simulation- The Influence of Porous Surfaces on Wall Slip and Bulk Shear

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**Abstract :** Molecular Dynamics (MD) simulation is a proven method to inspect behaviours of lubricant oils in nano-scale gaps. However, most MD simulations on tribology have been performed with atomically smooth walls to determine wall slip and friction properties. This study will investigate the effect of porosity, specifically nano-porous walls, on wall slip properties of hydrocarbon oils confined between two walls in a Couette flow. Different pore geometries will be modelled to investigate the effect on wall slip and bulk shear. In this paper, the Polyalphaolefin (PAO) molecules are confined to a stationary and a moving wall. A hybrid force field consisting of different potential energy functions was employed in this MD simulation. Newton's law defines how those forces will influence the atoms' movements. The interactions among surface atoms were simulated with an Embedded Atom Method (EAM) potential function which can represent the characteristics of metallic arrangements very strongly. We implemented NERD forcefield for intramolecular potential energy function. Also, Lennard-Jones potential was employed for nonbonded intermolecular interaction.

**Keywords :** slip length, molecular dynamics, critical shear rate, Couette flow
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