Molecular Dynamics Simulations of surface roughness effects on monatomic liquid flows

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Flows through micro- and nanochannels are governed by interfacial effects whose description is beyond the capabilities of the continuum Navier-Stokes equations. The Molecular Dynamics method, which treats systems from first principles, has been effective in treating micro and nanofluidic environments. Such atomistic simulations have been embedded in numerous studies of nanochannel flows over the last years. Although flow through such structures is a topic of academic interest, the majority of investigations deal with smooth or periodically patterned surfaces [1-7]. The present study investigates the effect of realistic 3-D fractal roughness on the flow behaviour of monatomic liquids.

Realistic surfaces demonstrate self-affinity; that is, they exhibit a repeating pattern which can be displayed in every scale. The ultimate way of representing this type of topographies incorporates the use of the Weierstrass-Mandelbrot function, which has been used over the last years for the characterisation of fractally rough surfaces. A fractal surface reproduced by the Weierstrass-Mandelbrot function is depicted in Fig. 1.

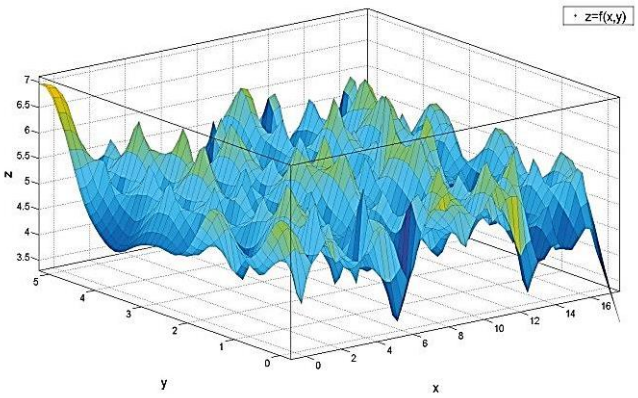

Figure 1: Representation of a fractally rough surface

In our model, fluid particles are confined by two rough walls, while periodic boundary conditions are applied in the *x*, *z* dimensions of the computational domain. The wall particles are placed on a Face Centered Cubic (FCC) lattice and attached to their equilibrium position using a nonlinear spring potential. Interactions between wall and fluid particles are being described by the shifted Lennard-Jones potential. A Poiseuille flow is imposed to the model and temperature, density and velocity profiles are studied. Results indicate that the slip length and shear viscosity can be correlated to the oscillatory pattern of the surface roughness.

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