PROJECT 41 - NUMERICAL SIMULATIONS OF INTERNAL FLOW IN DUCTS CARRYING CO2, CH4 AND OIL EMPLOYING MOLECULAR DYNAMICS

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Research Centre for Gas Innovation

cleaner energy for a sustainable future

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Material-Specific Boundary Conditions

The main purpose of this project is to investigate and evaluate material-specific boundary conditions at fluid-solid interfaces:

$$\dot{\gamma} = \left. \frac{\partial v_t}{\partial n} \right|_S$$

The shear rate must be regarded as a function of all controllable quantities in a molecular dynamics simulation:

$$\dot{\gamma} = \dot{\gamma}\,(h, T, \rho, U, \ldots)$$

Couette Flow

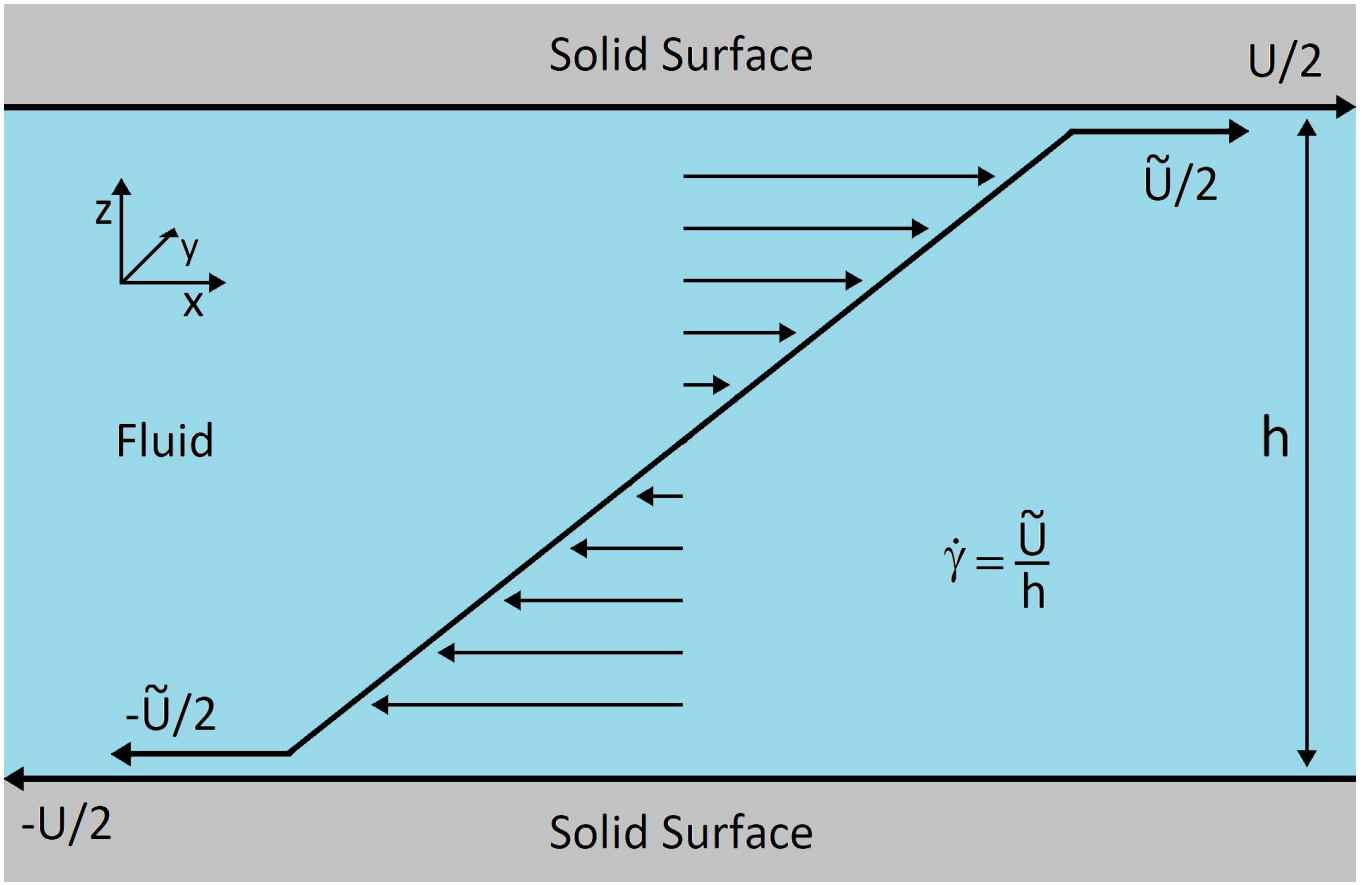

Figure 1: Symmetrical Couette flow.

Molecular Dynamics Simulations

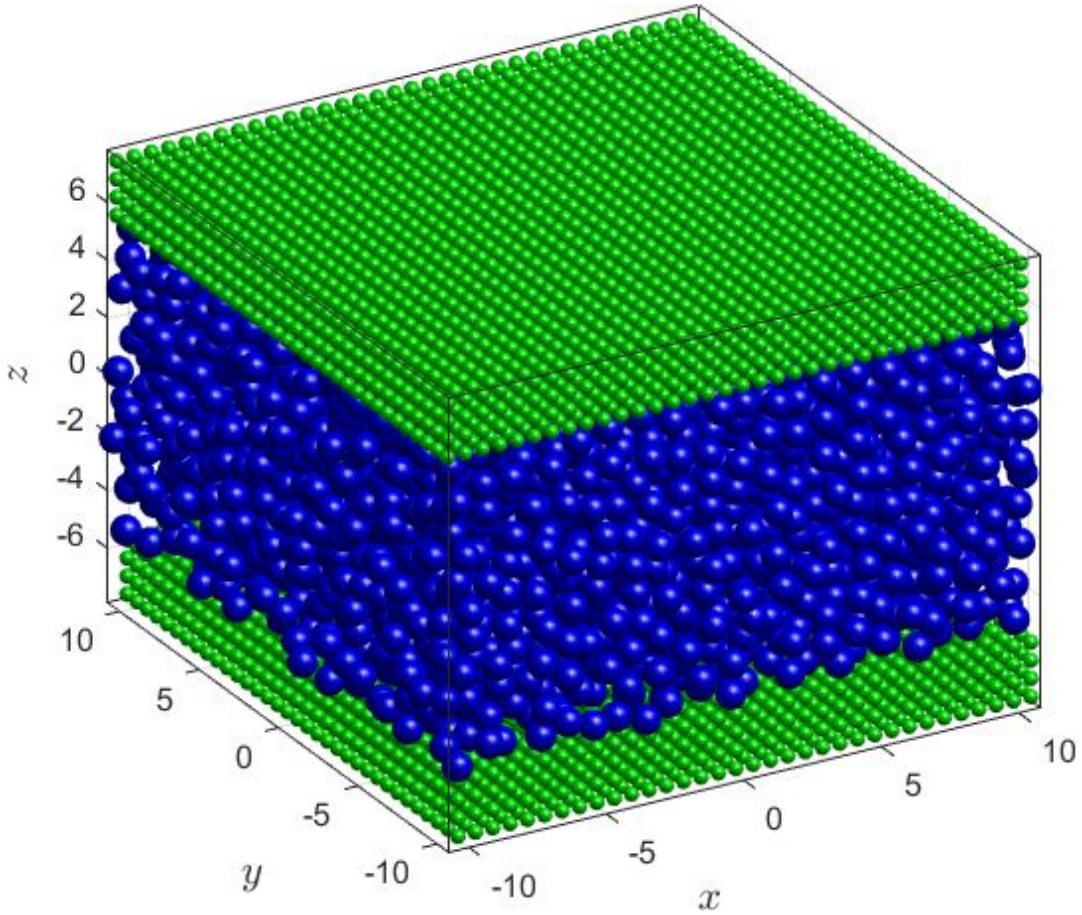

Figure 2: Molecular dynamics simulation of a Couette flow.

Interaction Potentials

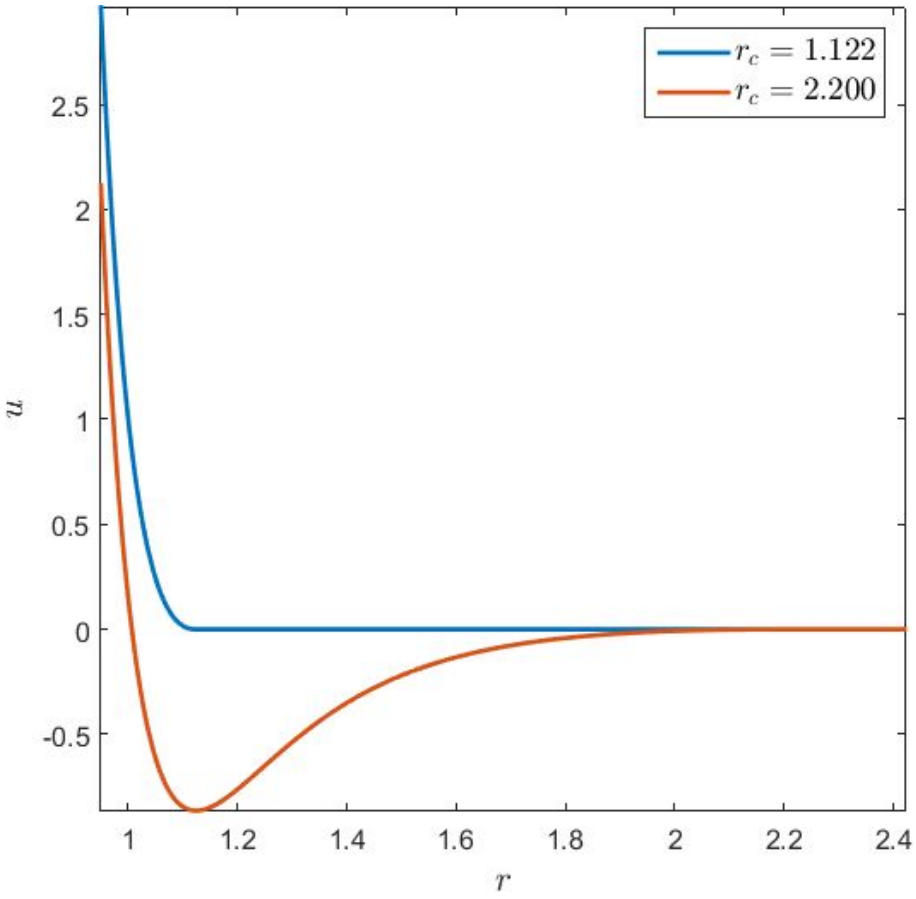

Figure 3: Lennard-Jones potential for different cutoff distances.

Velocity Profile

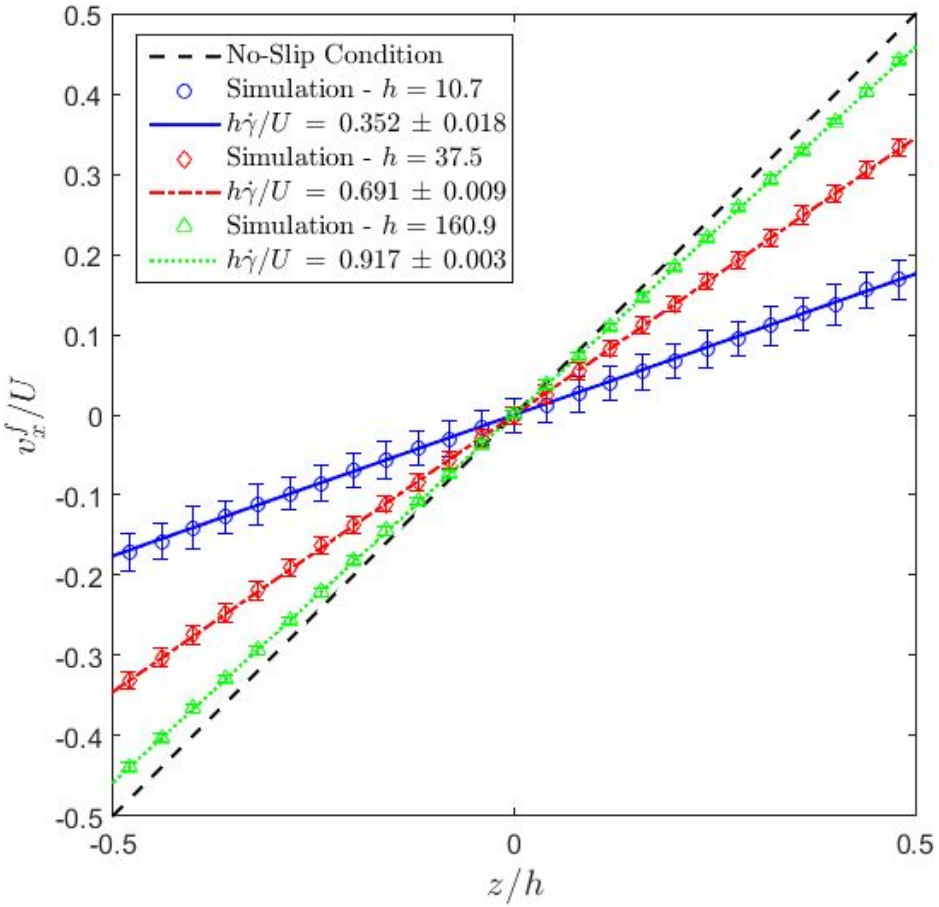

Figure 4: Velocity profile for different separation distances.

Soft-Sphere Particles

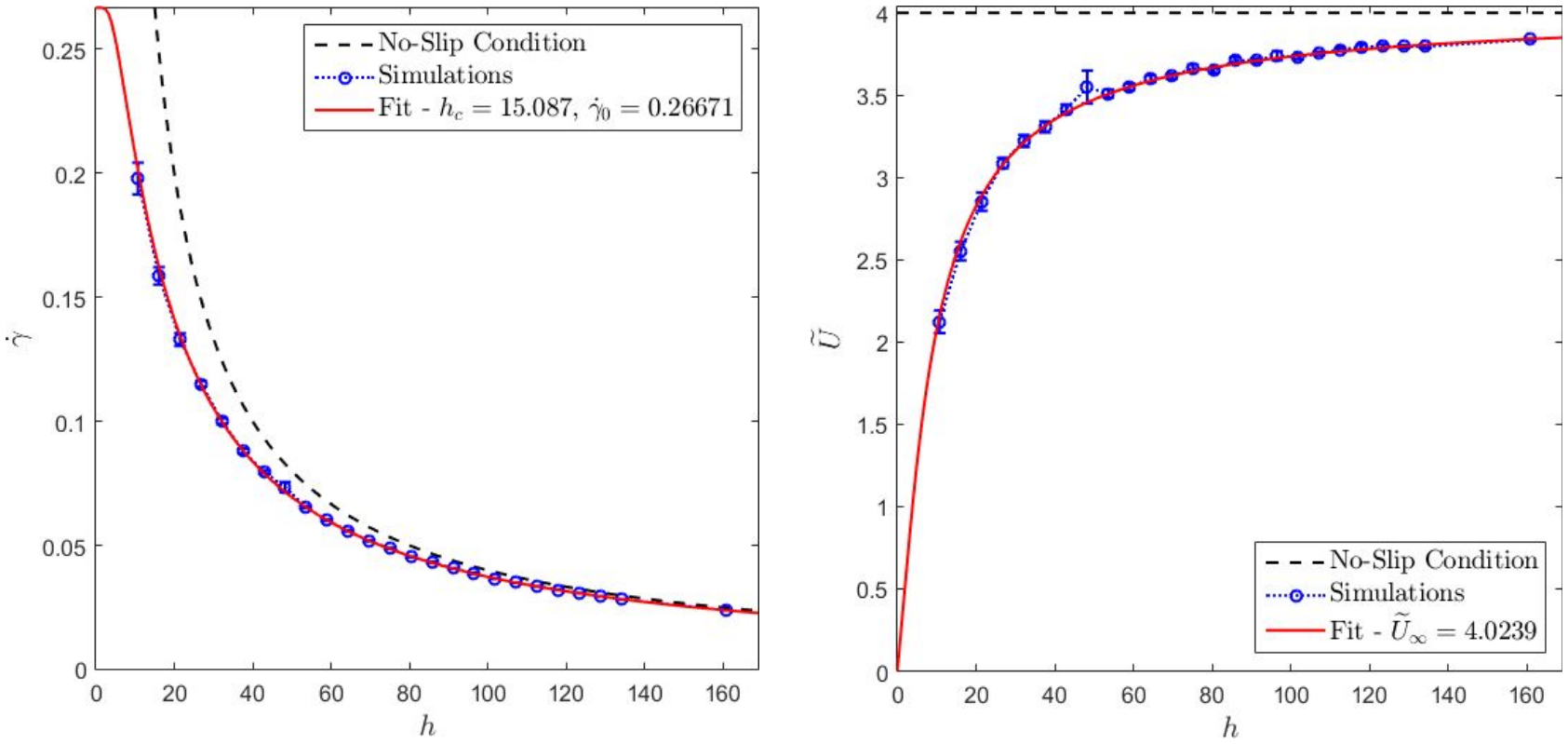

Figure 5: Shear rate and fluid velocity variation as functions of the separation distance.

Lennard-Jones Particles

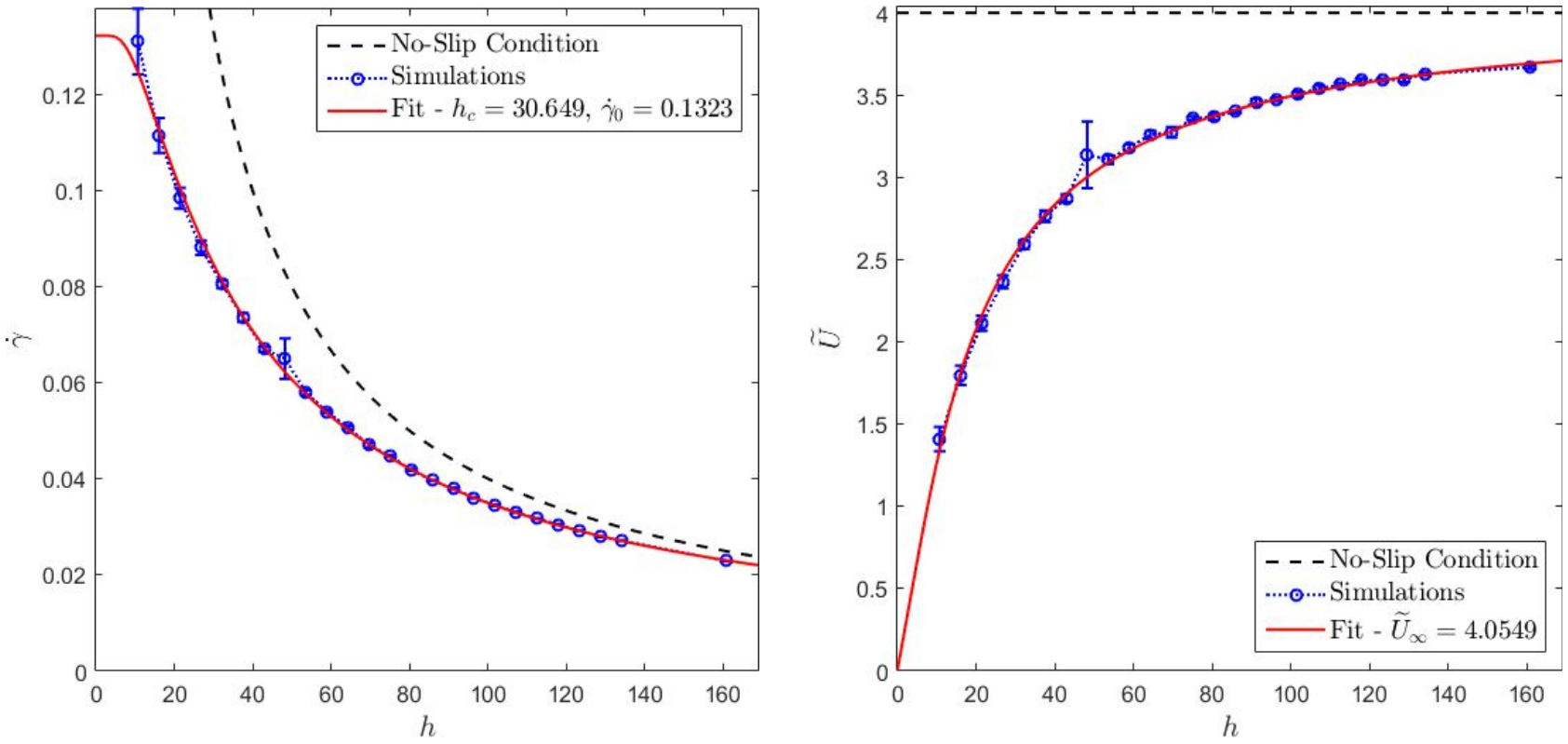

Figure 6: Shear rate and fluid velocity variation as functions of the separation distance.

Universal Behavior

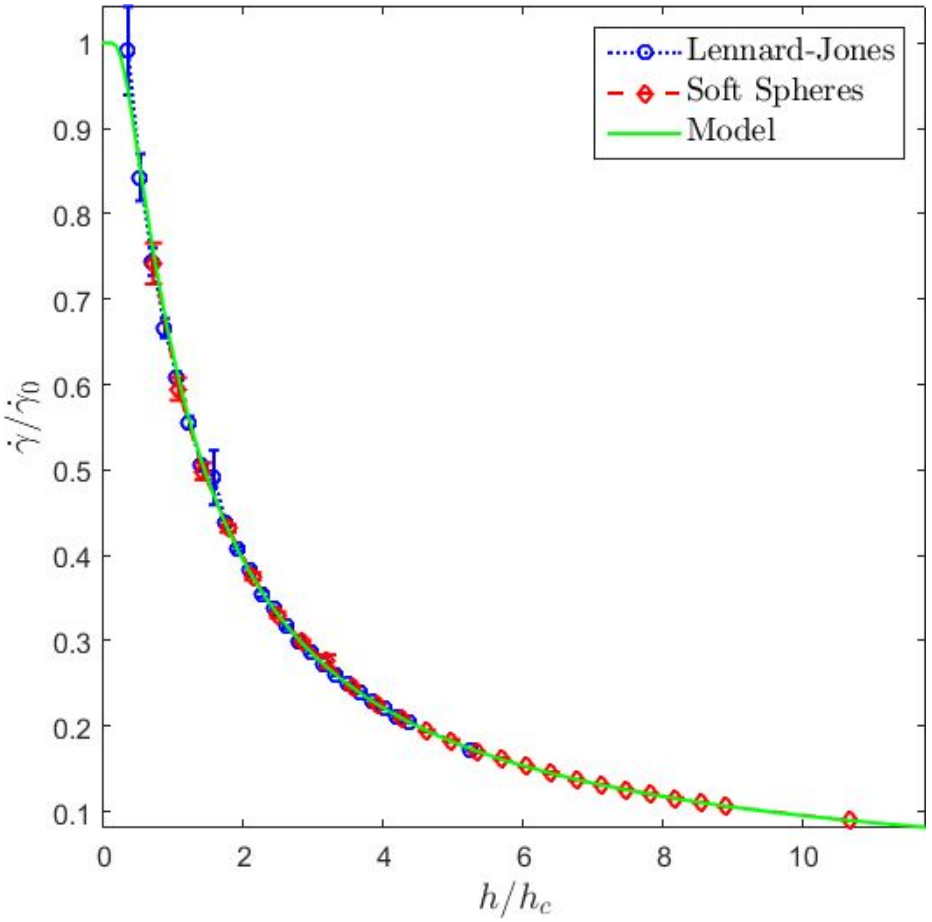

Figure 7: Shear Rate as a function of the separation distance.

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