# The non-equilibrium molecular dynamics calculation of methane viscosity in the COMPASS force field

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The transport properties of hydrocarbons and their mixtures are of great practical interest in the oil and gas extraction industry. The simulations of extraction processes and flows in porous media require models for prediction of viscosities of liquid and gas phases. In this work, the properties of liquid methane $CH_4$ and its mixtures with different hydrocarbons are studied using classical molecular dynamics methods. The interatomic potential is COMPASS [1]. The shear viscosity is calculated using non-equilibrium molecular dynamics [2, 3]. The temperature range is from 300 K to 360 K. The pressures are varied from 500 atm to 10000 atm.

The results calculated using COMPASS force field are compared with the values predicted by the TraPPE-EH [4] force field in the previous work. The TraPPE-EH potential has simpler model of interaction between atoms. The predictive power of both potentials is analyzed.

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