Predicting hydrocarbons properties at pressures up to 1 GPa using molecular dynamics methods

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The ability to predict the hydrocarbon liquids properties is of great industrial interest, since they are components of oils and fuels. In this work, we apply classical molecular dynamics methods to calculate the equation of state and self-diffusion and viscosity coefficients of the linear and branched alkanes and aromatic compounds [1–4]. The interatomic force fields are compared by their ability to predict the experimental data. The molecular dynamics methods are used to predict the shear viscosities of hydrocarbons in the pressure range from 0.1 MPa to 1 GPa. Blindly predicted viscosity values for isononane match the experimental data measured later. We demonstrate the universal scaling between the viscosity and diffusivity at pressures up to 500 MPa.

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[1] Kondratyuk N D and Pisarev V V 2019 *Fluid Phase Equilib.* **498** 151–159
[2] Pisarev V and Kondratyuk N 2019 *Fluid Phase Equilib.* **501** 112273
[3] Kondratyuk N, Lenev D and Pisarev V 2020 *J. Chem. Phys.* **152** 191104
[4] Kondratyuk N D, Pisarev V V and Ewen J P 2020 *J. Chem. Phys.* **153** 154502