Predicting the viscosity of hydrocarbons using molecular dynamics and machine learning approach

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Predicting the viscosity of organic liquids and their mixtures in a wide range of pressures and temperatures remains a challenging task. Direct classical molecular dynamics (MD) simulations using the Green–Kubo approach require long trajectories to ensure convergence of the integral.

Quantitative structure-property relationship (QSPR) models using machine learning (ML) serve as a powerful alternative to such calculations. QSPR modelling allows us to obtain relations between the macroscopic properties of substances and molecular descriptors of the individual atoms or molecules.

While obtaining the viscosity as a function of temperature from QSPR was discussed many times in the literature, the pressure-viscosity relationship is more challenging, as the molecular descriptors are less sensitive to the pressure.

In this work, we develop the combined MD–ML model to predict the viscosity of hydrocarbons in a wide range of pressures and temperatures using the pair entropy approach [1]. The efficiency of the created model is analysed by comparing predicted values with the experimental data.

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[1] Nikitiuk B I, Salikova D I, Kondratyuk N D and Pisarev V V 2022 *J. Mol. Liq.* **368** 120714