VISCOSITY OF LIQUID HYDROCARBON MIXTURES: MOLECULAR DYNAMICS SIMULATIONS AND MIXING RULES

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The work presents the results of molecular dynamics calculations of viscosity of liquid mixtures in the methane–n-butane–n-pentane system. The TraPPE-EH forcefield [1] is used for hydrocarbons. The viscosity calculations are made using a nonequilibrium molecular dynamics technique [2].

The viscosities of pure components and mixtures are found to agree with the Batchinski equation $\eta = C/(v-b)$, where η is the viscosity, v is the molar volume, C and b are constant characteristic to a liquid. To predict the viscosities of mixtures with arbitrary composition, Batchinski mixing rule, Arrhenius mixing rule and cubic root mixing rule are tested. The states of pure substances with the same molecular volumes as in mixtures are suggested as the basis states for mixing rules. The Batchinski mixing rule shows the best correspondence between the viscosities predicted by the mixing rules and calculated from direct MD simulations.

The proposed technique allowed us to apply the mixing rules to stable and metastable liquids and liquids with dissolved gas, while typically the mixing rules are only applied to mixtures of liquids.

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2. Müller-Plathe F. // Phys. Rev. E. 1998. V. 415. No. 3. P. 604.