SHEAR VISCOSITY CALCULATION FOR LIQUID HYDROCARBONS USING MOLECULAR DYNAMICS METHODS

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Modern industry is strongly interested in research of liquid hydrocarbon properties since they are parts of lubricants, insulators and fuels. One of the main properties of such liquids are transport coefficients (diffusivity, viscosity and thermal conductivity).

The calculations of the viscosity of liquid hydrocarbons have demonstrated the applicability of the Green-Kubo method [1] in the case of single-component systems. The obtained values of the viscosity coefficients for the hydrocarbons under study coincide with the experimental data within 10%. The experimental dependence of viscosity on temperature is reproduced using the methods used.

The contributions of various components of the stress tensor to the viscosity integral is analyzed. An approach is proposed for the convenient presentation of data in the form of tables. It is shown that the contributions of individual components can exceed by an order of magnitude the total value of the integral. It was also found that the correlation times increase with the increase of the number of atoms in the hydrocarbon molecule. In this connection, in further calculations, the authors of the project consider it most effective to use the method of nonequilibrium molecular dynamics, since it requires less computational time.

Comparison of the results obtained by the Green-Kubo method with the results of nonequilibrium molecular dynamics [2] is performed. The values coincide within the limits of the computational error for the entire series of n-alkanes under study at different temperatures and pressures.

Three interaction potentials are used: TraPPE-EH, OPLS-AA and COMPASS, unlike TraPPE-EH and OPLS-AA, which takes into account the anharmonicity of bonds and angles. In the case of viscosity, all three potentials give similar results. This can be explained by the calibration of the interatomic interaction potentials during their development.

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2. Bordat P., Müller-Plathe F. // J. Chem. Phys. 2002. V. 116. No. 8. P. 3362.