عنوان مقاله:

Comparison of the OPLS-UA and TraPPE-UA force fields for prediction of viscosity of methanol and ethanol

محل انتشار:

هفتمین کنگره ملی مهندسی شیمی (سال: 1390)

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خلاصه مقاله:

Equilibrium molecular dynamics simulation combined with Green-Kubo formulation were used to calculate shear viscosity of methanol and ethanol. The accuracy of the Green_Kubo formula for computing viscosity highly depends on the potential model used to describe the intermolecular interactions. In this regard, an investigation has been carried out to study the efficacy of the force fields in predicting viscosity. Two united atom force field models, OPLS (Optimized Potential for Liquid Simulation) and TraPPE (Transferable Potential for Phase Equilibria) were used. All simulations were performed with the DL_POLY_Classic package. The viscosities of the fluids are calculated at different temperatures. Comparison with available experimental data demonstrates that the OPLS force field is more capable of predicting viscosity of alcohols considered in this work.

کلمات کلیدی:

Molecular dynamics simulation, Viscosity, Green-Kubo, TraPPE, OPLS