Thermal Conductivity and Shear Viscosity of n-Decane and n-Hexadecane with Nanoparticle Suspensions using Molecular Simulations

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Atomistic molecular dynamics simulations were carried out at equilibrium to calculate the constant pressure shear viscosity and thermal conductivity of n-decane and n-hexadecane within the range of ambient to extreme temperature and pressure conditions (i.e. up to 500 ◦F and 35,000 psi). A quantitative comparison of the results was performed against experimental values and values predicted from a high temperature - high pressure perturbed chain - statistically associated fluid theory (HPHT PC-SAFT) model. In addition, the effect of the presence of Lennard-Jones nanoparticle suspensions was also analyzed for volume fractions of up to 1%. Analysis of the intra- and inter-molecular structure of the fluid as well as its dynamical characteristics were also performed.