

Abstract Submitted
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Modeling the thermal conductivity and shear viscosity of mixtures of methane and n-decane under high pressure and high temperature conditions using molecular simulations JOHN SHELTON, Carnegie Mellon Univ — Atomistic molecular dynamics simulations were carried out at equilibrium to calculate the shear viscosity and thermal conductivity of various mixtures of methane and n-decane within the range of ambient to extreme temperature and pressure conditions (i.e. up to 500 degree F and 35,000 psi). Both a computationally efficient united-atom force field and an all-atom force field were employed in this investigation. 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. Analysis of the intermolecular structure of the fluid as well as its dynamical characteristics were performed.

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