The Industrial Fluid Properties Simulation Challenge: Force field parameterized with isooctane REFPROP equation of state

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ABSTRACT

Accurate prediction of viscosity (η) at high pressures (P) necessitates an extremely reliable force field for at least two reasons. First, the viscosity at a given density (ρ) is highly sensitive to the non-bonded function form and associated parameters. Second, the viscosity depends strongly on the predicted density, which is also very sensitive to the force field.

Since the challenge compound is 2,2,4-trimethylhexane (TMH), we chose 2,2,4-trimethylpentane (TMP, a.k.a. isooctane) as a surrogate molecule. Specifically, the optimal non-bonded parameters are obtained empirically by minimizing the deviation between the predicted and REFPROP $P\rho T$ and caloric properties for TMP. The CH_3, CH_2, CH, and C non-bonded parameters are optimized simultaneously. This high-dimensional parameterization is possible by reweighting configurations using Multistate Bennett Acceptance Ratio (MBAR) and by including several properties over a wide range of state points.

Uncertainties in the estimated TMH viscosity are obtained using three complementary methods. First, we use the deviation between the simulated and REFPROP η values for the surrogate compound, TMP, at the target temperatures and pressures. Second, we account for the uncertainty in η that is associated with uncertainties in ρ for a given P. Third, we propagate the uncertainty in the force field non-bonded parameters using Bayesian inference.