Thermophysical properties of molecular liquids from simulation, experiment, and equation of state

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Molecular Dynamics (MD) simulations are used to investigate thermophysical properties of molecular liquids such as 1-chloropropane, 2-chloropropane and water as a function of temperature and pressure. Investigated properties include the density, the constant pressure and constant volume heat capacities, the isobaric thermal expansion coefficient, the isothermal compressibility and the speed of sound. For chloropropanes, experimental data for density have been reexamined [1-3] and used together with other experimental data [4] to fit the Span-Wagner equation of state (EoS). For water, an extensive MD study is performed with the SPC/E model and compared to prediction of a Span-Wagner-type EoS and to experimental results [5].

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FIGURES

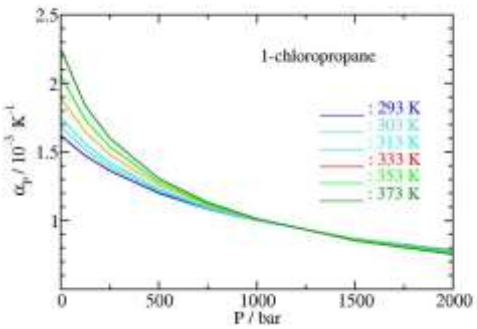

Figure 1: Isobaric thermal expansion coefficient of 1-chloropropane from MD simulation results