

Molecular Simulation of Thermodynamic Properties and an Equation of State for the Lennard-Jones Truncated and Shifted Model Fluid

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Recent progress in molecular simulation has shown that molecular models (force fields) have powerful predictive capabilities for thermodynamic data [1]. Such data are also accessible for states which are difficult or impossible to investigate experimentally. Moreover, molecular simulation allows for the generation of large and consistent data sets of arbitrary thermodynamic properties at low cost. As there is a dire need for thermodynamic raw data to optimize equations of state, the idea to develop a new generation of equations of state which are partly based on molecular simulation data is natural. The underlying dataset was generated by the molecular simulation tool ms2 [2]. It contains thermodynamic properties for the Lennard-Jones truncated and shifted interaction model at 718 state points including temperature, density, pressure, residual internal energy, first volume derivative of the residual internal energy and residual isochoric heat capacity. Based on these simulation data an equation of state was developed in form of the Helmholtz energy. It can be used for the calculation of any thermodynamic property, including density, heat capacity, speed of sound, energy, saturation properties, etc. The new equation is valid for temperatures $0.64 < T^* < 11$ and for pressures up to $p^* = 6.8$ corresponding to $0.6 < T^*/T_c^* < 10$ and $p^*/p_c^* = 70$. Comparisons to available simulation data establish the accuracy of calculated properties. The extrapolation behavior for low temperatures and high temperatures, densities and pressures is reasonable.

[1] <http://www.fluidproperties.org>, Industrial Fluid Properties Simulation Collective, 2011

[2] S. Deublein et al., *Comp. Phys. Comm.*, 182, 2350-2367, 2011