Numerical Simulations of the Molecular Behavior and Entropy of Non-Ideal Argon

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A numerical model is built, simulating the principles of kinetic gas theory, to predict pressures of molecules in a spherical pressure vessel; the model tracks a single particle and multiplies the force on the spherical walls by a mole of molecules to predict the net pressure. An intermolecular attractive force is added for high-density simulations, to replicate a real fluid; the force is chosen to ensure the fluid matches the Peng-Robinson equation of state as it is compressed to a near supercritical density. The standard deviations of the molecule position and velocity with respect to temperature and density is studied to define the entropy. A parametric study of a Stirling cycle heat engine utilizing near-supercritical densities is modeled, to study how the temperature dependence of the attractive intermolecular Van der Waal forces can affect the net total entropy change to the surrounding environment. - https://arxiv.org/abs/2004.03584- https://doi.org/10.1063/1.5043523