Parameterization of H_2S, SO_2 and NO_2

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Data pertaining to compounds such as H_2S, SO_2 and NO_2 are of enormous interest to the petrochemical industrial sector where these species occur as troublesome impurities. As such, they must be removed and effectively dealt with before the final products may be used or sold. An additional complication when dealing with these compounds is their effect on the environment. Hydrogen sulfide is extremely corrosive, especially when exposed to metals. It can also contaminate water supplies and has a high toxicity to both aquatic and terrestrial life forms. Sulfur dioxide forms sulfuric acid in the atmosphere, which is the main component of acid rain. Nitrogen dioxide is harmful to vegetation (it also contributes to acid rain formation) and whilst not itself a greenhouse gas, NO_2 exacerbates their effect through interaction with hydroxyl radicals present in the atmosphere.

A new set of parameters for the Lennard-Jones 12-6 potential are proposed for the polar molecules H_2S, SO_2 and NO_2 based on fitting of the experimental saturation densities. Force fields for simulating H_2S have already been put forward by Kristof and Liszi and Nath, however, in this work explicit determination of the unlike interaction parameters provides a substantial improvement in the saturated vapor pressure and vapor density predictions. SO_2 and NO_2 have not previously been parameterized for the Lennard-Jones 12-6 potential, and the proposed model reproduces the experimental data exceptionally well for SO_2. However, the NO_2 saturated vapor pressure predictions show significant deviation from the available experimental data due to the extensive dimerization that is known to occur in both phases.

A sensitivity analysis was carried out on the Lennard-Jones parameters and showed that even small parameter adjustments produced significant deviations in the simulation results. This highlights the need for careful consideration in the selection of combining rules for unlike interactions.