Optimized Force Field for Sulfur Hexafluoride (SF_6)

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Phase equilibria and transport properties represent the basis to design many industrial processes. Both can be estimated by different molecular simulation techniques, where macroscopic properties of matter are obtained from interactions occurring at atomic level. This explains the interest on proposing simple and reliable force fields for substances with relevant technological applications. In this work a new force field for SF_6 is proposed. This study is justified due to the many applications of SF_6, for example, as insulator gas in electromechanical devices. In a previous work[1], we calculated the liquid vapour coexistence curve of SF_6 using the six-sites interaction model of Pawley[2], which considers SF_6 molecules as rigid units. We concluded that disregarding molecular flexibility gives a wrong description of the liquid vapour coexistence region. The force field provided in this work contains two terms. The first one, following the nature of Pa wley's model, consists on a LJ potential that deals with F atoms intermolecular interactions. The second takes into account flexible features of SF_6 molecule by including six harmonic stretching for S-F bonds and twelve harmonic bending for F-S-F angles. The four parameters of the force field were optimized following the procedure of Ungerer and co-workers[3]. Such procedure allows the simultaneous parameters optimisation by minimizing an objective function, in which molecular simulation results and experimental values for several properties are compared. As an important contribution, transport and interfacial properties were used at the same time to adjust the parameters. The resulting force field was validated using MD simulations to calculate the liquid vapour coexistence curve, the surface tension and transport properties (self-diffusion and shear viscosity) at different conditions. Results reveals that including flexibility features into a six-sites interact ions model of SF_6 improves the prediction of both liquid-vapour coexistence curve and transport coefficients.

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