PERFORMANCE OF A NEW FORCE FIELD FOR SULFUR HEXAFLUORIDE (SF_6) IN CONFINED GEOMETRIES

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Sulfur hexafluoride is a synthetic molecule with an octahedral structure, where six
fluorine atoms are symmetrically located around a central sulfur atom. This compound
is widely used for several industrial applications. Its wide range
of industrial applications and the special symmetrical geometry of the molecule have
created a raising interest for studying its properties.
We have recently published[1] molecular dynamics (MD) simulations of a rigid model of SF_6
proposed by Pawley[2] to obtain the vapor-liquid coexistence curve, the surface tension
and self-diffusion coefficients. The model provided good results for diffusion properties,
while the phase envelope and the surface tension were poorly captured. We have then proposed
a new force field for this molecule in which the flexibility is explicitly considered.

We present here GCMC simulation results of both, the rigid and the flexible models
of SF_6 confined on cylindrical pores of different diameters. Results for adsorption
capacities and monolayer completion are presented as a function of temperature,
pressure and pore diameters. Density and energetic profiles along pore radius are also provided here.

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[1] Olivet A. et al, *Sulfur hexafluride's liquid-vapor coexistence curve, interfacial properties, and diffusion coefficients as predicted by a simple rigid model*, J. Chem. Phys., 123,194508, 2005.

[2] Pawley G. S. et al, *Molecular dynamics simulation of the plastic phase; a model for sulfur hexafluoride.* Mol. Phys, 43,1321-1330,1981.