Mixed Gas Adsorption Calculator

A tool to calculate the adsorption of a mixture of two gas molecules onto a metal organic framework

By Julian C. Umeh

This tool uses RASPA for its backend simulation. RASPA is a molecular simulation software for performing adsorption and diffusion calculations in nanoporous materials. It implements state-of-art algorithms for Molecular Dynamics and Monte Carlo for various ensembles. In this simulation, we used Monte Carlo with the grand canonical ensemble (μVT).

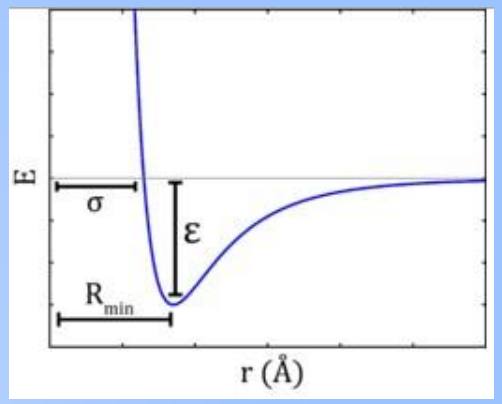
Every simulation is performed with initialization and production cycles of 5000 and 10000 respectively.

- Initialization cycles warm up the simulation. The data is collected during production cycles.

- Transferrable Potential for Phase Equilibria (TraPPE) forcefield is used to define the molecular interactions for helium and methane.

Mol	Def	Reference
CH_4	TraPPE	*J. Phys. Chem. B,* 1998, 102,2569-2577
Ar	TraPPE	*J. Am. Chem. Soc.,*1992, 114, 10024-10035

Lennard-Jones Potential



en.wikibooks.org/wiki/Molecular_Simulation/The_Lennard-Jones_Potential

- For the MOF, forcefield parameterized by the developers of RASPA were used. IRMOF-1 was used for the simulation

Dubbledam D., Walton K. S., Ellis D. E., Snurr R. Q., Exceptional Negative Thermal Expansion in IsoreticularMetal–Organic Frameworks, Angew. Chem. Int. Ed. 2007, 46, 4496–4499

MOF	Void Fraction (%)	Forcefield
IRMOF-1	82.62	Dubbledam2007FlexibleIRMOF-1

- Lorentz-Berthelot's model was used as the general mixing rule for the Lennard-Jones potentials

$$\sigma_{ab} = \frac{\sigma_a + \sigma_b}{2} \qquad \varepsilon_{ab} = \sqrt{\varepsilon_a \varepsilon_b}$$

- Adsorption also known as loading are of two types;

  Absolute Loading

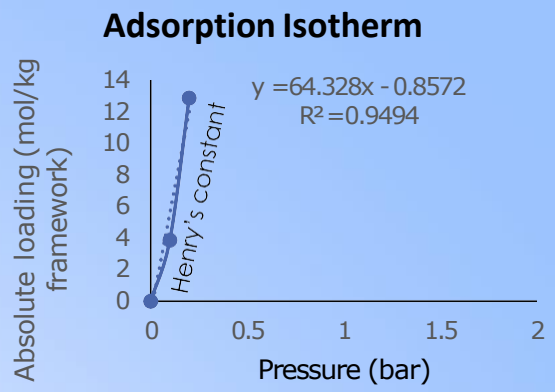
  Excess Loading

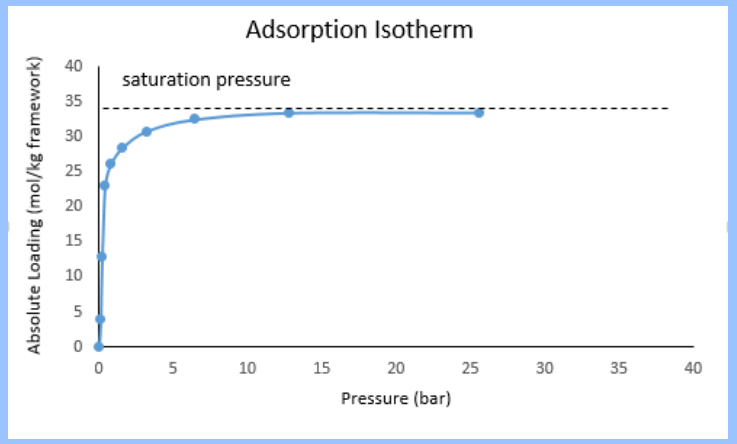
  Absolute loading is the total number of molecule adsorbed onto the material

  Excess loading is the amount by which the molecule adsorbed is greater than that of an ideal gas.

Calculation of Adsorption Isotherm

- The adsorption isotherm is shown by plotting a graph of the absolute adsorption against pressure. The simulation would need to be run a number of times, and each time at the same temperature and different pressure.





The graph of the pressures against the absolute adsorption is used to calculate Henry's constant which is given by the slope of the graph at the lower pressures (left panel). The saturation loading is the maximum amount adsorbed at high pressure (right panel).

The simulation was carried out using IRMOF-1 and methane at a temperature of 150 K and different pressures.

- Gases in nature almost never exist in a pure state, therefore it is important to run simulations of the adsorption of gas mixtures. The results from these simulations will differ from the results of the pure gas especially at higher pressures where one gas may occupy the adsorption sites thereby changing the adsorption of the other gas.

- A good example would be the adsorption of methane at 300K and 50.0e5 Pascal from a gas mixture of helium and methane at 50% mole fraction each; The average absolute adsorption for the methane gas is 11.933 mol/kg framework, and 0.4114 mol/kg framework for helium. The average absolute adsorption for a pure methane at 300K and 25.0e5 Pascal is 12.1916 mol/kg framework. The average absolute adsorption for a pure helium at 300K and 25.0e5 Pascal is 0.683 mol/kg framework. Both simulations were run using IRMOF-1.