Henry's Coefficient Simulator

A tool to simultaneously calculate Henry's coefficients of several n-alkanes for a nanoporous material.

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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 algorithm.

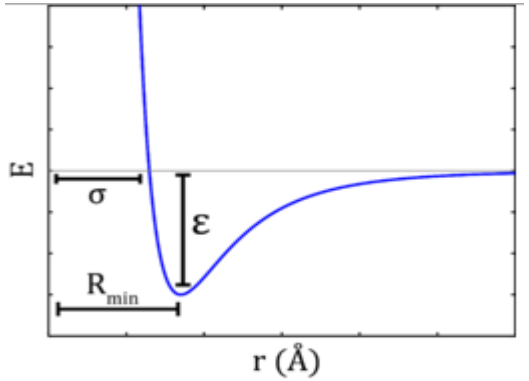
Every simulation is performed with 5000 production cycles.

- No initialization cycles are required, because Widom insertions do not require equilibration.
- The data is collected during production cycles.

Transferrable Potential for Phase Equilibria (TraPPE) forcefield is used to define the molecular interactions for every molecule in this tool.

Molecule	Forcefield	Reference
n-pentane (C5)	TraPPE	M.G. Martin, and J.I. Siepmann, "Transferable potentials for phase equilibria. 1. United-atom description of n-alkanes", J. Phys. Chem. B, 1998, 102, 2569-2577
n-hexane (C6)	TraPPE	
n-heptane (C7)	TraPPE	
n-octane (C8)	TraPPE	
n-nonane (C9)	TraPPE	

Lennard-Jones Potential



https://upload.wikimedia.org/wikipedia/commons/thumb/f/fe/Schematic_of_the_Lennard-Jones_6-12_Potential.png/255px-Schematic_of_the_Lennard-Jones_6-12_Potential.png

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

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

The tool uses Widom insertion to calculate Henry's coefficients for multiple n-alkanes on a nanoporous material. The Widom insertion probe is only a test insertion to evaluate the energy. The tool allows the option of selecting the material from a drop list. Using a pre-calculated ideal gas Rosenbluth weight and Temperature, it performs the calculation.

The temperature used for the simulation is 573 K and the nanoporous materials used for this tool include IRMOF-1, IRMOF-16 and MFI_SI.

Sample simulation run for IRMOF-1 at temperature 573 K gives the Henry's coefficients in mol/(kg-Pa): 3.69409e-07 for n-pentane, 3.77874e-07 for n-hexane, 3.83747e-07 for n-heptane, 3.92102e-07 for n-octane, and 4.00566e-07 for n-nonane.