RDF Calculator

A tool to calculate the radial distribution function (RDF) of fluids.

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 Molecular Dynamics algorithm with the canonical (NVT) ensemble.

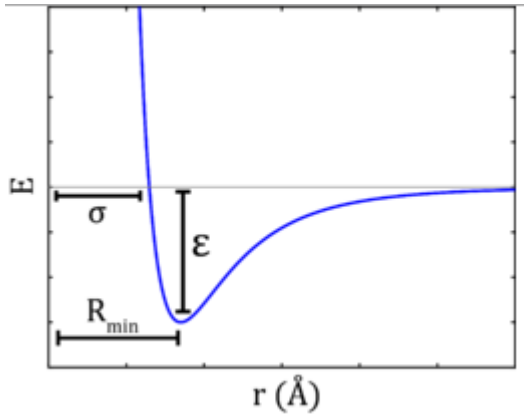
Every simulation is performed with initialization, equilibration and production cycles of 50000, 50000 and 100000 respectively.

- Initialization cycles set the configuration for the start of equilibration.
- Equilibration 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 every molecule in this tool.

Molecule	Forcefield	Reference
Methane	TraPPE	*J. Phys. Chem. B*, 1998, 102, 2569-2577
Ethane	TraPPE	
Propane	TraPPE	
Butane	TraPPE	
Nitrogen	TraPPE	*Theor. Chem. Acc.* 2006, 115, 391–397
Carbon dioxide	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

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

RDF contains a significant amount of information about the local structure and correlation between molecules. It describes how density varies as a function of distance from a reference particle.

The tool allows the option of selecting the molecule and the temperature and then it outputs the radial distribution function, self diffusion constant of the molecules as well as the density which is fixed by the simulation tool.

RDF, *g(r)*, may be described as the probability of finding a particle at a distance away from a reference particle relative to that of an ideal gas. “To define RDF, the configurational distribution function is integrated over the positions of all atoms except two. The function gives the probability of finding a pair of atoms at a distance *r* apart relative to the probability expected for a completely random distribution at the same density.” (Reference 1, Day 2, pg 1)

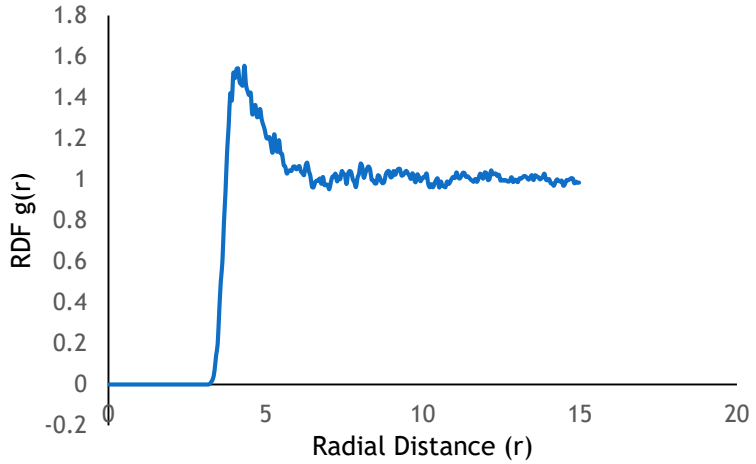
It is given by the equation (1);

$$g^{(n)}(r_1,\ldots r_n) = \frac{V^n N!}{N^n\,(N-n)!}\frac{1}{Z_{NVT}}\int \ldots \exp\int\left[-\beta U(r_{n+1,\ldots,}rn)\right] d_{r3},\ldots,r_N$$

“Where *N* is the number of particles, *V* the volume, … β the inverse temperature, Z_{NVT} the canonical partition function, r_i the position of the particles (with *i* = 1,…,*N*), *U* (r_1,…,r_N) the potential energy between the particles …” (Reference 1, Day 2, pg 1)

Reference 1: D. Dubbledam, R. Snurr, S. Calero, and T. J. H. Vlugt, Raspa Workshop Module, Evanston, July 10-13, 2018.

Graph of RFD against radial distance



The plots above is the RDF and the self diffusion graphs of Methane at 300 K and a density of 98.6635 kg/m^3.

Einstein's equation of diffusion is used to calculate the self diffusivity

MSD = 6 D t + C

Where;

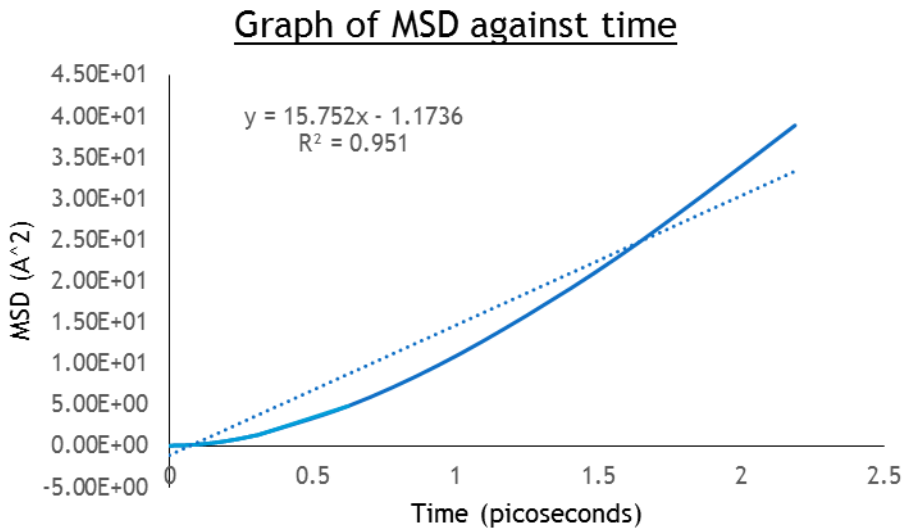
MSD = mean square displacement

msd = $\frac{1}{N}\sum_{j=1}^{n}([r_j(t) - rj(0)]^2)$

D = diffusion constant

t = time

C = constant



The diffusion constant is obtained from the $\frac{slope}{6}$ of the mean square displacement against time graph.

The initial and final few points were omitted and the center points fitted to a straight line.

Its unit is in squared angstrom per picosecond (A^2/ps).

In the graph above, the slope is 5.0903 and diffusivity is $\frac{15.752}{6}$ = 2.625 A^2/ps