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Report:

Gibbs Ensemble Monte Carlo (GEMC) is a simulation technique used to study the coexistence and phase equilibrium of multiple phases in a system. It is commonly employed to investigate systems with different chemical species or phases, such as gas-liquid, liquid-liquid, or solid-liquid equilibria.

Ensemble: GEMC in the NPT ensemble allows the simulation of phase equilibria at constant number of particles (N), pressure (P), and temperature (T).

GEMC involves multiple simulation boxes, each representing a different phase or region of interest. These boxes can have different compositions, pressures, and temperatures.

Here in this problem, we have two boxes.

Box1 contains Zeolite

Box 2 contains CO2 and CH­4­ gas molecules.

The towhee input file contains every detail about each and every atom.

It has been modified accordingly for each of the following pressures:

1, 10, 50, 100, 500, 1000, 2000 kPa.

The force fields for 3 different components have also been defined.

The towhee coords file also have been generated from pdb file of the zeolite.

After running each simulation, the data for 10 steps have been displayed and recorded(in excel sheet1). Through the data, we are able to conclude the following results

Results:

**Selectivity Curve**