Poster Example

India-Japan Cooperative Programme
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Properties of gas diffusion in polymer aqueous solution by MD simulation

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Abstract

In chemical engineering, diffusion is responsible for mass transfer. It is an important transport property which plays a vital role in diffusion controlled chemical reactions and mass transfer processes at the micro-scopical level. Diffusion behavior of oxygen in water and oxygen in polymer aqueous solution were investigated using Molecular Dynamic (MD) Simulation with AMBER software. The data was analyzed to determine the diffusion coefficient of those molecules in polymer aqueous solution using Einstein-Smoluchowski relation. This relation is based on Mean Squared Displacement (MSD) method, the slope of MSD vs. time is proportional to diffusion coefficient of certain atoms. The result shows that by addition of poly ethylene glycol (PEG) in water, the diffusion coefficient of oxygen decrease. By changing the number of monomers of PEG, the MSD behavior of oxygen molecules also observed.

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Introduction

MD simulation: is a computer simulation method for analyzing the physical movements of atoms and molecules.

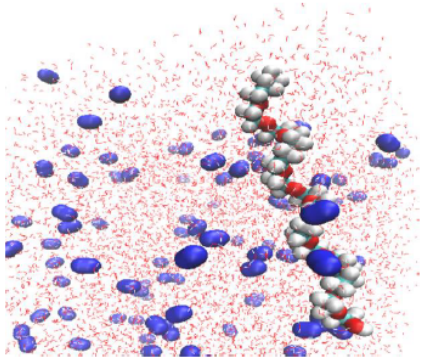

Fig1. O2 diffusion in PEG solution

Objective

Determination of diffusion Coefficient of oxygen molecule:

(1) In water
(2) In presence of (polymer) PEG in water
(3) By changing the number of monomers of PEG

Models & Methods

Diffusion Coefficients

↓

Mean-Squared-Displacement (MSD) method

Einstein Equation

$$D = \lim_{t\to\infty} \frac{\langle |\boldsymbol{r}(t) - \boldsymbol{r}(0)|^2 \rangle}{6t}$$

Results and Discussion

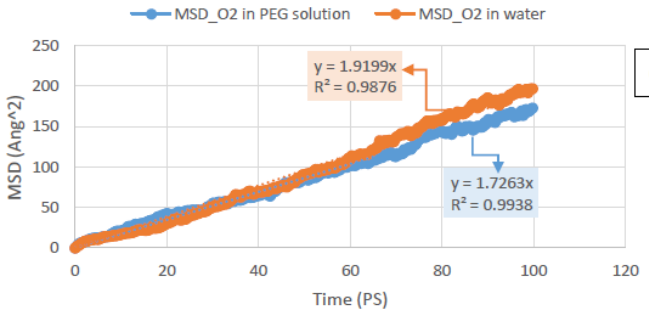

Fig2. MSD of oxygen in water and polymer aqueous solution

Calculation Conditions

Temperature: **300K**
Pressure: **1 bar**
Calculation time: **100 ps**
Calculation Interval: **0.002 ps**
Water molecules: **8600**
Oxygen molecules: **100**
polymer (PEG): **1 chain (n=15)**
NPT ensemble
Periodic Boundary Condition

- Diffusion Coefficient of O_2 in H_2O = 3.1998*10^{-9} (m^2/s)
- Diffusion of O_2 in (PEG+H_2O) = 2.8776*10^{-9} (m^2/s)

✓ From the result, it can be concluded that by addition of polymer, the Diffusion Coefficient of oxygen decrease

No. of monomers n	MSD slope	Oxygen diffusion coefficient [*10^{-9} m^2/s]
9	1.7072	2.8453
15	1.7263	2.8771
34	1.6727	2.7878

Table1: Effect of degree of polymerization on diffusion coefficient of O2 (n= 9, 15 and 34)