

Supplementary Information

Mechanical and Transport Properties of the Poly (Ethylene Oxide) – Poly (Acrylic Acid) Double Network Hydrogel from Molecular Dynamic Simulations

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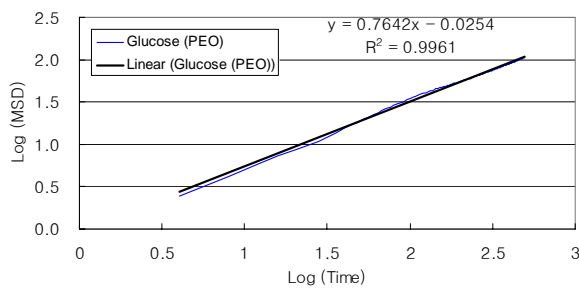
Howard Hughes Medical Institute & Stanford University Institute of Regenerative Medicine & Stem Cell Biology and the Department of Neurosurgery
Stanford, CA 94305

1. Diffusion of Solutes in SN or DN Hydrogel

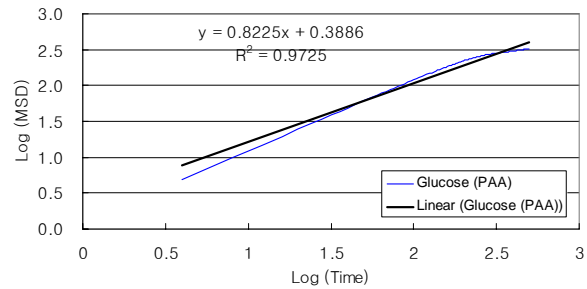
Log-Log plot of Equation (5)

The values of the slope of these plots (0.74~0.82) indicate that the diffusion of the solutes studied in our simulations do not reach the Fickian regime yet.

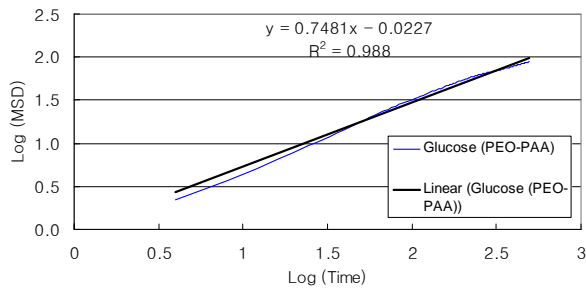
1.1 D-Glucose



(a) PEO SN hydrogel

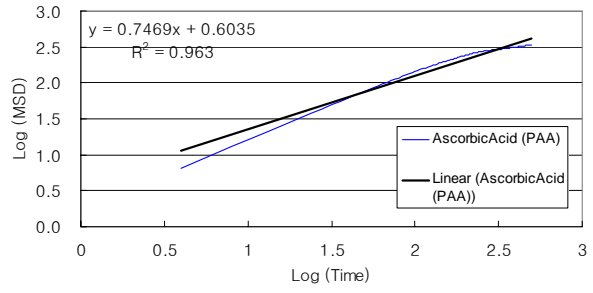
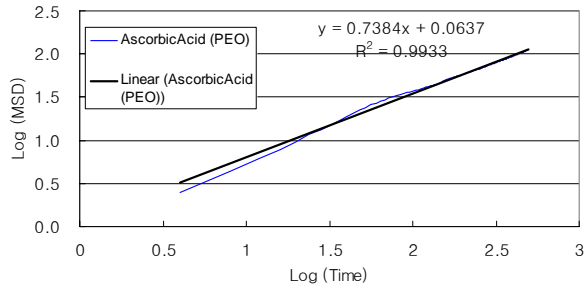


(b) PAA SN hydrogel



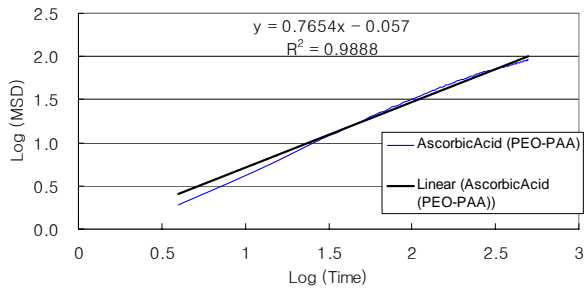
(c) PEO-PAA DN hydrogel

1.2 Ascorbic Acid



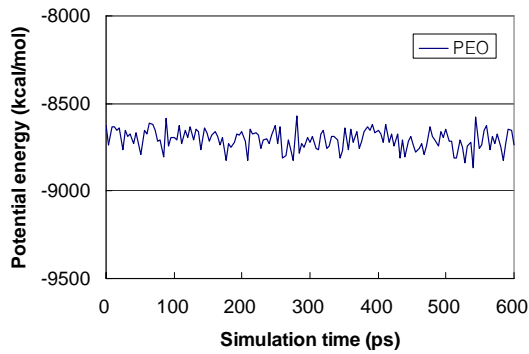
(a) PEO SN hydrogel

(b) PAA SN hydrogel

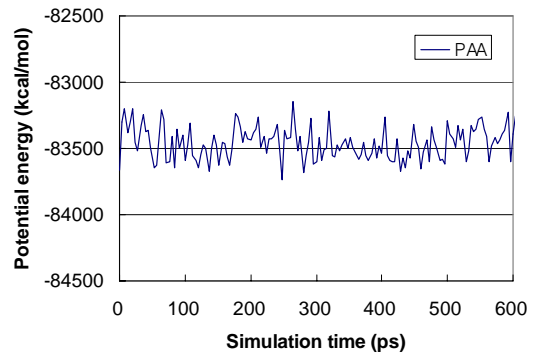


(c) PEO-PAA DN hydrogel

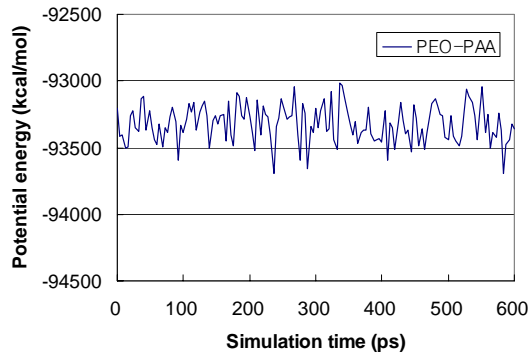
2. Convergence of Energy in Equilibration Procedure (using 600 ps NPT MD simulation)



(a) PEO SN hydrogel



(b) PAA SN hydrogel



(c) PEO-PAA DN hydrogel