Simulating the Diffusion of Nanoparticles through Hydrogels

Austen Brooks Casey[1], Benjamin Beach[2], Taylor Tarlton[2], Divya Elumalai[2], and Pedro Derosa[2,3]

[1]Department of Chemistry and Physics, Warren Wilson College
[2]Institute for Micromanufacturing , Louisiana Tech University
[3]Department of Mathematics and Physics, Grambling State University

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

Motivation

- To create a code that tracks the diffusion of nanoparticles (NPs) through a computational model of a physical hydrogel
- Understand the contribution of various interactions to the diffusion of NP through a polymer network

Introduction

- Physical hydrogels have many uses ranging from cell encapsulation and tissue-scaffolding, to drug delivery.
- These are transient polymer networks that rely on physical entanglements, ionic interactions, and hydrogen-bonding as a means to resist dissolution.
- The degree and method of swelling is dependent upon the polymers that make up the hydrogel; that is, whether thermo-responsive or pH sensitive polymers are present.

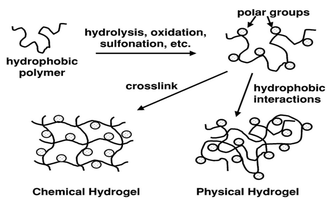

Figure 1: Schematic representation of polymer orientation in physical and chemical hydrogels. Reproduced from ref [1].

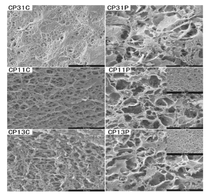

Figure 2: SEM of chemical and physical PVA/cellulose hydrogel cross sections Reproduced from ref [2].

Methodology

- A random walk Monte Carlo algorithm is used to determine the most energetically favorable movements for the NP and polymer chains as the hydrogel swells or contracts.
- The model was executed using MATLAB to simulate the diffusion through a 1 μm^3 partitioned box containing a physical hydrogel.
- Van der Waal and Columbic interactions play in this process.
- A Java code was used to visualize the diffusion process through the polymer network.
- We consider the hydrodynamic radius of the solute/NPs diffusing out of the hydrogels
- The hydrogel considered is a generic physical hydrogel.

Motion of Polymer	Motion of Particles
❖ A new position for the polymer strand is tested, using the force on it as a bias. ❖ Polymer strands are allowed to move if the total energy of the system after the move is less than or equal to the energy of the system before the move. (including the energy associated with bending and stretching). ❖ If the total energy increases, the move is accepted with Boltzmann probability.	For each new configuration NPs are moved as follows: ❖ Particles are allowed to move in any random direction if the total energy of the system after the move is less than or equal to the energy of the system before the move. ❖ If the total energy increases, the move is accepted with Boltzmann probability. ❖ Any move is rejected if the particle overlaps with any other particle or with any polymer strand.

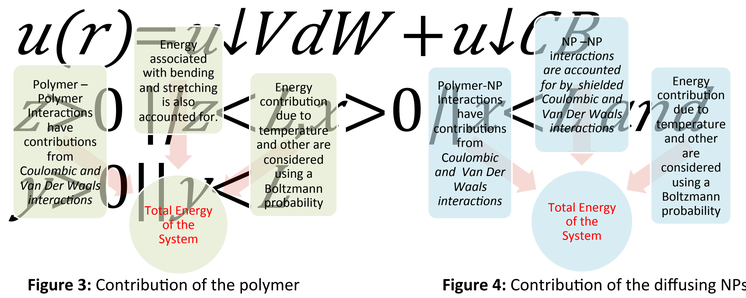

Figure 3: Contribution of the polymer strands to the total energy of the system

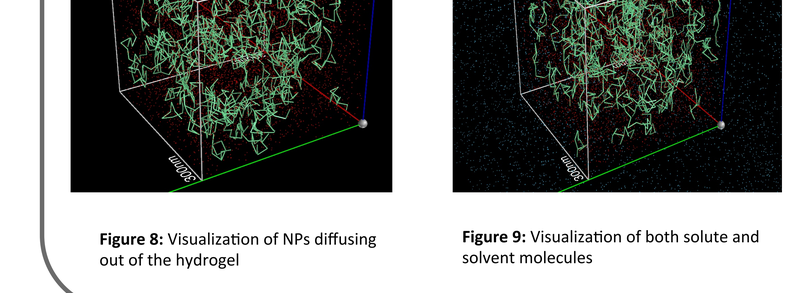

Figure 4: Contribution of the diffusing NPs to the total energy of the system

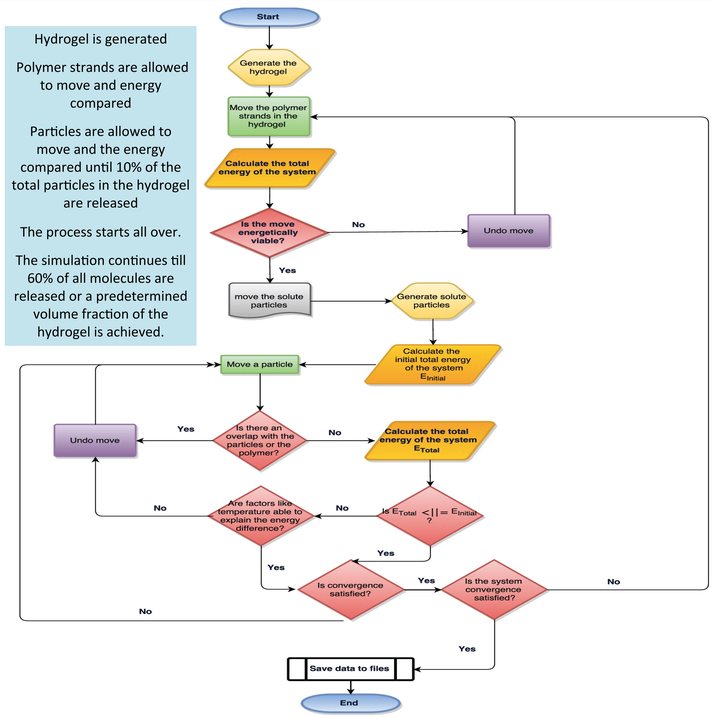

Figure 5: Flowchart detailing the methodology of the model used in this study

Results

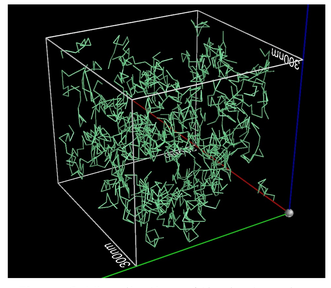

Figure 6: Visualization of the hydrogel model

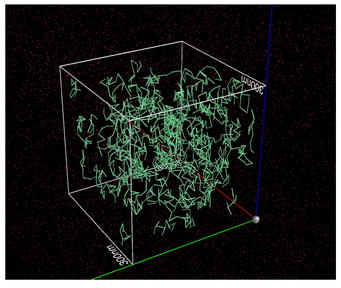

Figure 7: Visualization of NPs diffusing into of the hydrogel

Figure 8: Visualization of NPs diffusing out of the hydrogel

Figure 9: Visualization of both solute and solvent molecules

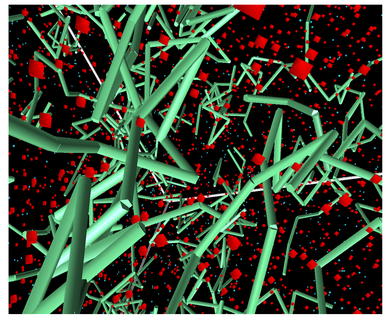

Figure 9: Visualization of a hydrogel sample

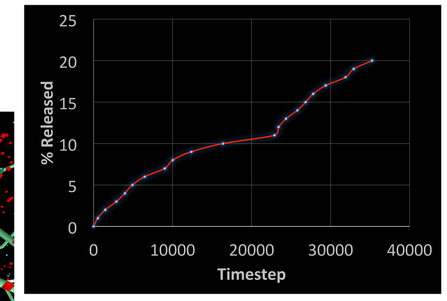

Figure 10: Release profile for the first 20% of NPs from a generic physical hydrogel.

Conclusions

- A 3-D coarse grain Monte Carlo model based on the Boltzmann transport was used to simulate the release profiles and diffusion of molecules into and out of physical hydrogels.
- In the case studied 20% of total NPs were released.
- The NPs undergo molecular diffusion in the system considered.
- The model developed is a promising alternative to the computationally intensive molecular dynamics approach to simulating diffusion.

Future Work

- Validate simulations with experimental data
- Build a model for cross-linked hydrogels
- Extend model for pH, temperature, and electromagnetic fields responsive hydrogels.
- Derive coefficients such as the molecular weight between crosslinks (M_c) and determine a predictive model to estimate these coefficients
- Calculate how a change in coefficients, such as M_c, influences diffusion through a hydrogel

Acknowledgements

This material is based upon work supported by the National Science Foundation under the NSF EPSCoR Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents.

References

1. Hoffman, Allan S. "Hydrogels for biomedical applications." *Advanced drug delivery reviews,* 64 (2012): 18-23.
2. Chang, Chunyu., Ang, Lue., and Lina, Zhang., "Effects of crosslinking methods on structure and properties of cellulose/PVA hydrogels." *Macromolecular Chemistry and Physics,* 209.12 (2008): 1266-1273.

Institute for Micromanufacturing
WARREN WILSON COLLEGE