Multi-Scale, Multi-Domain Computational Modeling for Fluidic Transport and Its Applications to Nanomanufacturing

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Goals

- Investigate ion selectivity for carbon nanotube (CNT)-polymer membrane for advances in polymer-membrane based nanomanufacturing.
- Predict effect of AC voltage on catalytic reaction kinetics in micro/nanofluidics based nanomanufacturing.

Mapping to Center’s Objectives

- The objective of this research is to develop a fundamental understanding and the associated computational tools for nanopore-based and tip-based manufacturing processes.
- One of the goals of nano-CEMMS is to develop novel process technologies – for example, nanopore-based printing, electrohydrodynamic writing, tip-based manufacturing, etc.

Fundamental Questions/Challenges

- Predict the ion selectivity of functionalized CNT with and without polymer matrix (e.g. polystyrene) typically used in nanomanufacturing applications.
- Predict the dependence of the chemical reaction rate on the frequency of AC voltage in nanopores with applications in nanomanufacturing.

Research Plan

- Use Molecular Dynamics Simulations.
  - Provides atomistic-level understanding of nanofluidic systems.
- Ion selectivity in CNT-polymer membranes.
  - Calculate the diffusion coefficient and translocation rate of ions through CNT in polymer matrix.

Research Results

- Effect of AC voltage on catalytic reaction kinetics.
  - The reaction rate increases with the increase in frequency until an optimum frequency $= 5kHz$, the rate reaches a maximum and further increase leads to a decrease in reaction rate.
  - Frequency has no effect in fast kinetics since the reaction time scales are so small that they form the products instantly.

Effect of rate constants on optimal frequencies

Confinement effect on product concentration

- Calculate the reaction rate as a function of frequency, amplitude, rate constant

- 35% enhancement in the reaction rates with the application of AC fields when compared with DC voltage alone.
- Increase in rates was due to the increase in the residence time of the species.
- Decrease in diameter increases the rate, since $[A^+]$ increases near the walls with decrease in channel height signifying the importance of nanopores.

Broader Impact

- Multiscale modeling to understand complex physics in nanopore-based manufacturing.

Interaction with Other Projects

- Collaboration between computational and experimental (Shannon, Bohn) groups.
- Interaction with the projects on nano-CEMMS applications (specifically large-scale micro and nanofluidic networks).
- Interaction with the projects in Manufacturing Thrust.

Future Efforts

- Atomistic-level understanding of water and ion transport in CNT-polymer membrane.
- Atomistic-level understanding of DNA transport on surfaces (with applications in tip-based nanomanufacturing).
- Understand the effect of various parameters on catalytic reactions in nanopores.

Micro-Nanofluidics

![Schematic drawing of a functionalized carbon nanotube.](image1)

![Schematic view of the CNTs in polymer matrix.](image2)

![Solvated with water, ions K+ and Cl-](image3)

![Observe the behavior of ions and water (translocation rate and occupancy in CNT)](image4)

![Predict the selectivity of functionalized CNT in polymer matrix.](image5)