# STOCHASTIC MULTISCALE SIMULATION OF SUPERTHIN MEMBRANES FOR MICROFLUIDIC SEPARATIONS

**Garrison N. Stevens, Enkeleda Dervishi, Stephen L. Yarbro**

**Los Alamos National Laboratory**
**Los Alamos, NM 87545**
**505-695-3978 / garrison@lanl.gov**

## KEYWORDS

Actinide Separation, Computational Fluid Dynamics, Design Optimization, Graphene, Random Pore Model, Stochastic Simulations

## ABSTRACT

Large scale solvent extraction and ion exchange has long been employed for actinide separation. However, new technologies are emerging presenting opportunity to scale these processes down to microfluidic systems. Microfluidic channels, with small length scales and laminar flows, hold potential for high mass transfer rates enabling efficient separation of actinides while also reducing the footprint and potential hazards of current separation apparatuses. Countercurrent flow is achievable in microfluidic devices when a membrane is installed as a divider between organic and aqueous phases in the channel. With channel dimensions less than a tenth of a millimetre and a desire for high transfer rates, the thinness of the membrane becomes critical. Graphene, a unique material with atomic thickness, is an ideal membrane to maintain phase separation yet also allow for high mass transfer through nanoscale pores. During countercurrent operations, the delicate membrane is exposed to relatively high shearing and pressure loads causing large deformation and damage to single-layer graphene, thus requiring a highly porous, nanoscale support structure to be incorporated in the design.

Herein, a multiscale multiphysics numerical model is developed to study the behavior of a microfluidics system for liquid-liquid extraction with a supported graphene membrane providing phase separation. Stochastic simulations reveal the effects of design parameters on the membrane stability and extraction performance. Graphene and formvar as membrane and support materials introduce flexibility to the design, as these materials can be chemically modified during synthesis to provide controllable design parameters such as functional groups, pore size, pore distribution, and thickness. Simulations

couple multiple scales and physics with statistical distributions of design parameters to optimize the microreaction design and operation.

Nanoscale design parameters are first implemented in a random pore model of a unit membrane sample to characterize the porosity and permeability of the membrane for a given fluid. These membrane parameters are then scaled up to a microscale computational fluid dynamics simulation and coupled with chemical reactions to quantify the extraction performance. Additionally, the microscale CFD model predicts pressure and shear loads on the membrane given operational parameters such as fluid density, viscosity, and flow rates. Finally, the predicted loads are applied to the nanoscale membrane model to determine the structural behavior and possible failures of the porous membrane. The multiscale, multiphysics design optimization is demonstrated for the extraction of acetic acid from a kerosene phase into a neutralizing aqueous phase.