

MANUFACTURING

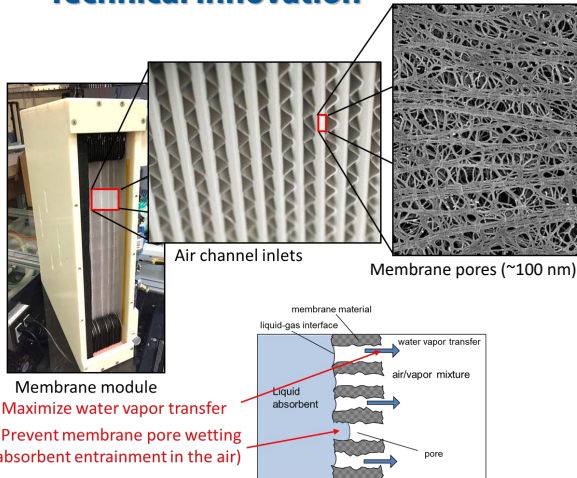
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Project Objectives

- Liquid/gas membrane contactors require pores that:
 - Prevent liquid breakthrough
 - Maximize vapor transport
- This HPC4Mfg project developed molecular dynamic (MD) models to investigate the microscopic effects of membrane pores, to better define membrane parameters for this application.

Technical Innovation

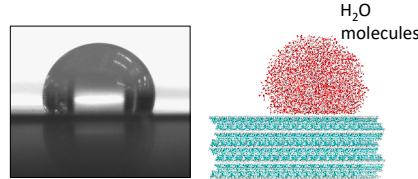


We developed molecular dynamic simulations of the membrane/liquid interface to study the impact of pore morphology on:

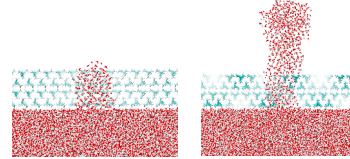
- Breakthrough pressure
- Liquid/vapor phase change
- Diffusion through pores

Technical Approach

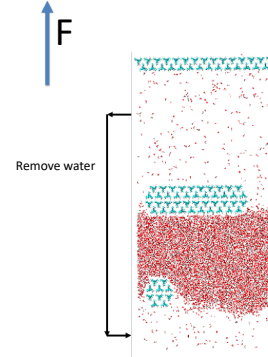
Surface tension simulations confirmed by contact angle measurements



Breakthrough pressure measured with MD simulations



Evaporation and vapor flux simulations used newly-developed steady-state method, where a constant driving force is maintained and flux is measured



Results and Accomplishments

A new membrane design with two layers:

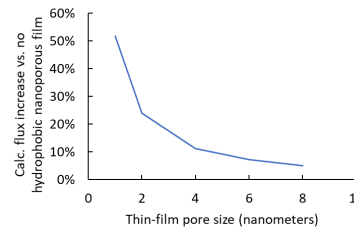
100-nm thick hydrophobic coating with pores < 5 nm

20 μm thick porous support with pores ~100 nm

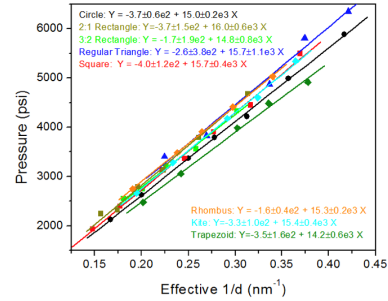
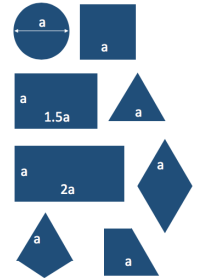
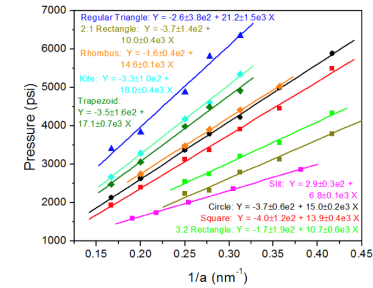
Kelvin Equation

$$\ln \frac{p}{p_{sat}} = \frac{2\gamma V_m}{rRT}$$

Vapor pressure ↑ as pore radius ↓ for non-wetting liquids



Results and Accomplishments (cont.)



$$\Delta p = \frac{2B\gamma\cos\theta}{r_{pore}}$$

Transition

- Results, simplified models, and suggested membrane designs were provided to 7AC Technologies
- NREL continues to work with 7AC Technologies under a CRADA, focused on modeling and experiments on membranes and membrane modules.

Budget/Timeline

Timeline:

Project Start Date: 05/01/2017

Budget Period End Date: 03/31/2019

Project End Date: 03/31/2019

Budget	DOE Share	Cost Share	Total	Cost Share %
Overall Budget	\$300,000	\$75,000	\$375,000	20%
Costs as of 3/31/19	\$300,000	\$75,000	\$375,000	20%