Developing high performance computing model of vapor transition through advanced membranes for applications in 7AC Liquid Desiccant Air Conditioners

HPC4Mfg Program Project – NREL and 7AC Technologies

May 2017 to Mar2019

Jason Woods and Hai Long, NREL
Peter Luttik, 7AC Technologies
Peter Frischmann, Sepion Technologies

U.S. DOE Advanced Manufacturing Office Program Review Meeting
Washington, D.C.

June 11, 2019

Overview

Project Title: Developing high performance computing model of vapor transition through advanced membranes for applications in 7AC Liquid Desiccant Air Conditioners

Timeline:

Project Start Date: 05/01/2017

Budget Period End Date: 03/31/2019

Project End Date: 03/31/2019

Project Budget and Costs:

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%

Barriers and Challenges:

- Effect of porous-membrane morphology on breakthrough pressure and vapor permeability is important for liquid/gas membrane contactor application, but is difficult to predict.

AMO MYPP Connection:

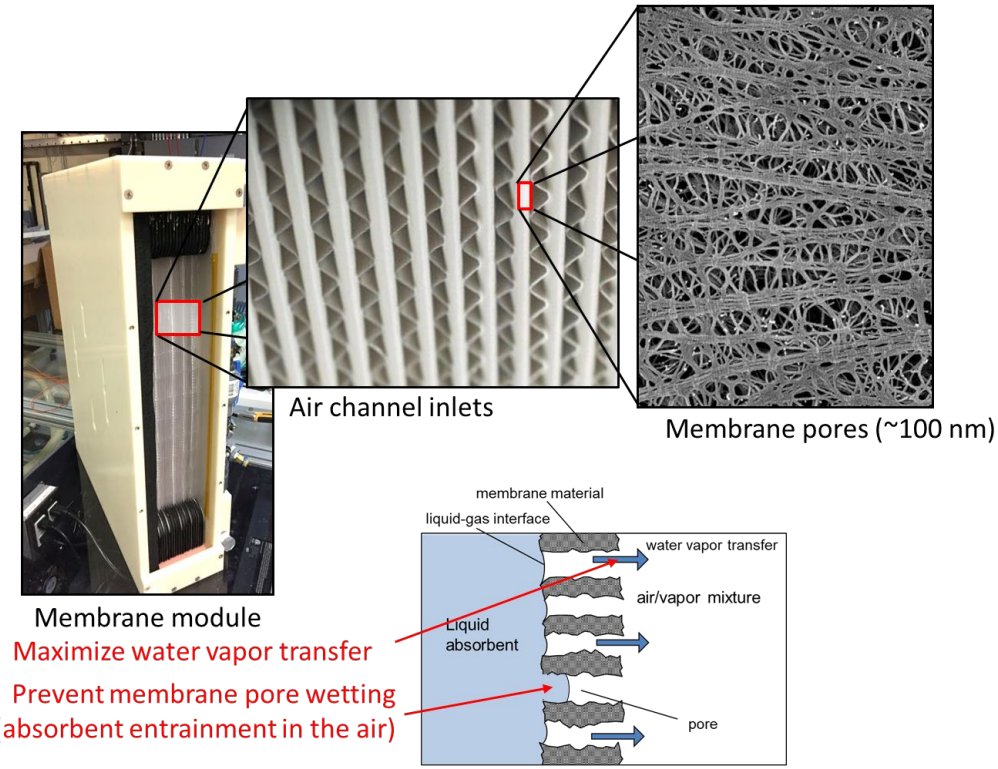
- Advanced Sensors, Controls, Platforms and Modeling for Manufacturing

Project Team and Roles:

- Peter Luttik, 7AC Technologies; Company Sponsor, membrane-module manufacturer
- Jason Woods, NREL, co-PI; heat and mass transfer expert
- Hai Long, NREL; co-PI; molecular dynamic simulations
- Peter Frischmann, Sepion Technologies; membrane consultant

Project Objective(s)

- Liquid/gas membrane contactors require pores that
  - prevent liquid breakthrough
  - maximize vapor transport
- This HPC4Mfg project developed molecular dynamic models to investigate the microscopic effects of membrane pores for this application, to better define membrane parameters for this application.
- The results can be used to guide design of new membranes suitable for this application.



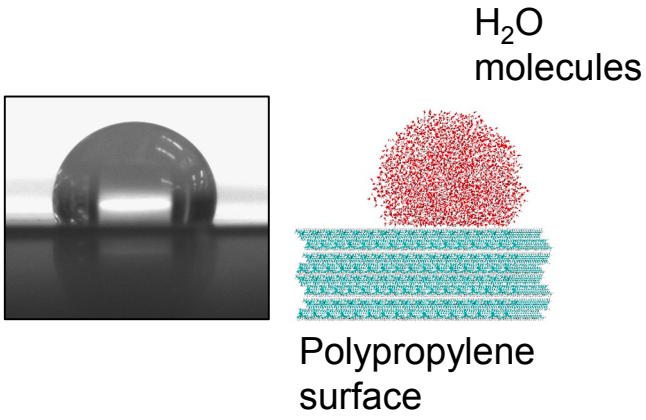
Technical innovation

Membranes are not currently designed for liquid/vapor contactor applications (instead, battery separators or microfiltration membranes are used).

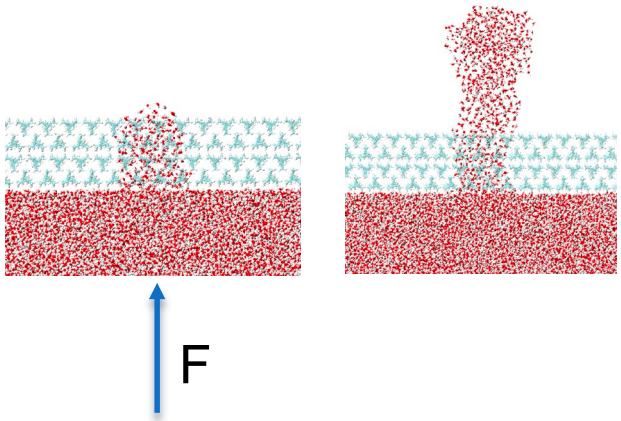
- Limitations:
  - Existing membranes need higher vapor flux
  - Pore breakthrough prevents commercial use
- Proposed approach
  - Use molecular dynamic simulations to study the membrane/liquid interface to better predict the impact of pore morphology on breakthrough pressure, liquid/vapor phase change, and diffusion through pores
- Critical innovations:
  - New method for estimate breakthrough pressure as a function or pore morphology
  - New membrane design with high breakthrough resistance and improved flux for liquid-to-vapor processes

Technical Approach (1)

- Our approach used molecular dynamic simulations (MD) of the membrane and liquid/vapor interface. We calculated:
  - Pore breakthrough pressure
  - Vapor flux through the pore
- Calculating pore breakthrough pressure requires:
  - surface tension effects
  - Simulations of increasing force to achieve breakthrough of liquid into the pore.
- We used the LAMPPS software for our MD simulations, including the SPC/E model for water, and the GAFF force field for interactions of the ions with the membrane.



Droplet showing surface tension compared to measured contact angle

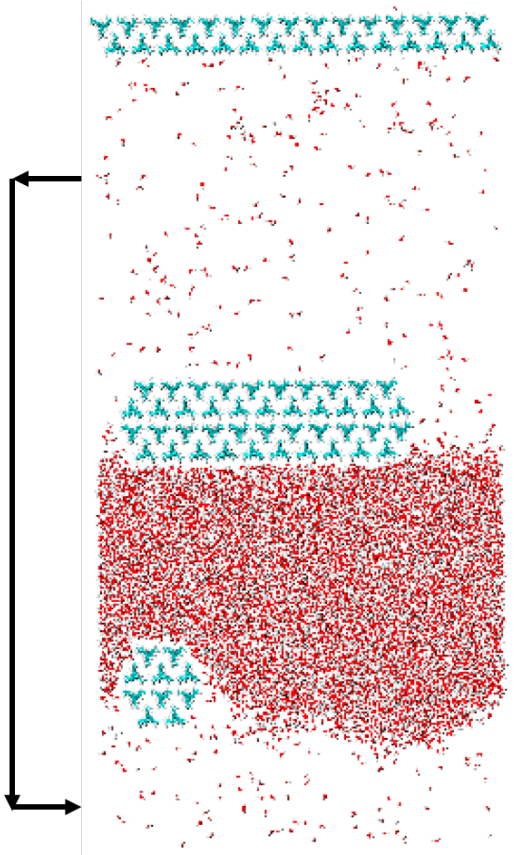


Example setup with force applied to liquid water (left) to cause breakthrough (right). A force is applied directly to the water molecules.

Technical Approach (2)

- Calculating vapor flux through the membrane requires:
  - surface tension effects
  - Vapor pressure estimates
  - Calculation of vapor flux through the pore

For vapor flux calculations, we designed a steady state method for evaporation by moving evaporated water molecules from the gas phase back into the liquid phase.



Evaporation rate measured from pore, with driving force set by removing atoms from space above pore, and replacing them within the liquid phase with a separate larger pore at the bottom.

Results and Accomplishments (1)

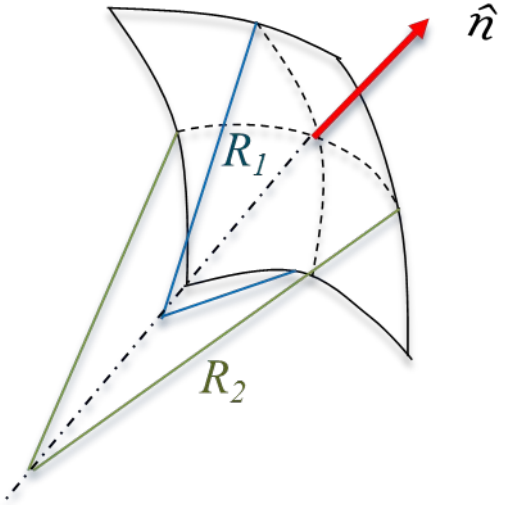
This project resulted in two key accomplishments:

1) New guidance on an empirical geometric coefficient for breakthrough pressure calculation.
2) Potential membrane design for high breakthrough resistance and high vapor flux.

Results and Accomplishments (2)

1) New guidance on an empirical geometric coefficient for breakthrough pressure calculation.

Existing practice uses the Young-Laplace Equation to predict pore breakthrough pressure, but requires a geometric factor to determine the impact of pore shape.



Young-Laplace Equation

$$\begin{aligned}\Delta p &= -\gamma \nabla \cdot \hat{n} \\ &= 2\gamma H \\ &= \gamma\left(\frac{1}{R_1}+\frac{1}{R_2}\right)\end{aligned}$$

Breakthrough pressure calculation (derived from Young-Laplace):

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

$\boldsymbol{B}$ = empirical geometric factor for non-cylindrical pores

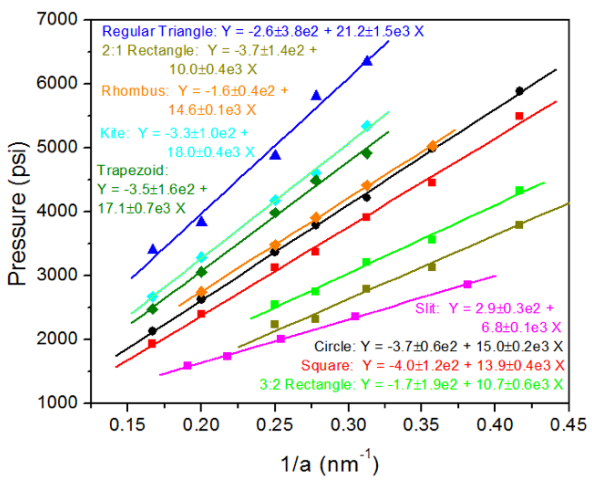
$\boldsymbol{B}$ = 1 for cylindrical pores

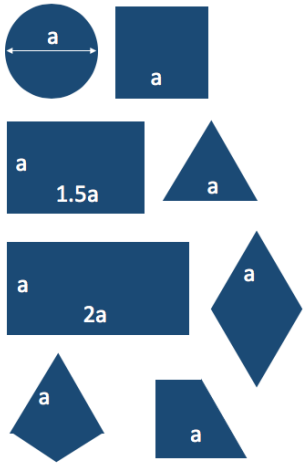
0 < $\boldsymbol{B}$ < 1 for non-cylindrical pores

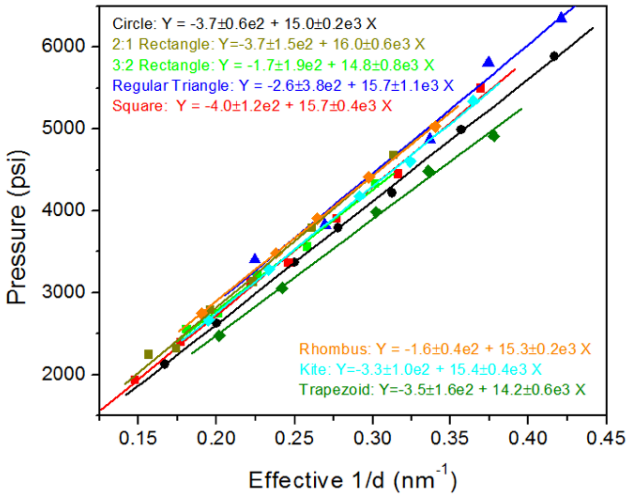
Results and Accomplishments (3)

1) New guidance on an empirical geometric coefficient for breakthrough pressure calculation.

With MD simulations, we determined an *effective diameter* that collapses the breakthrough pressure to a single line. This can be used to predict the impact of pore shape in the pore breakthrough equation (empirical constant B).







Results and Accomplishments (4)

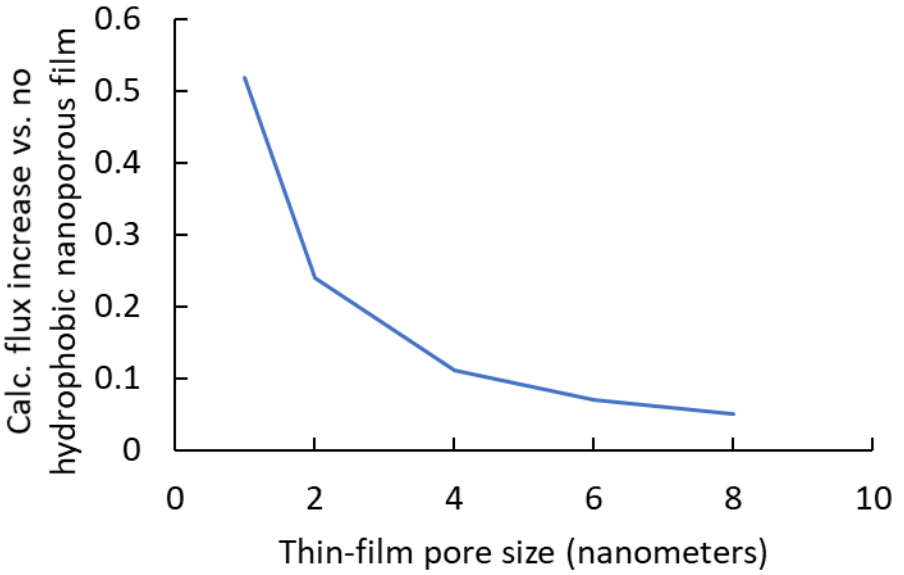
2) Potential membrane design for high breakthrough resistance and high vapor flux.

A new membrane design with two layers:

- A large-pore support layer (~20 microns thick)
- A thin, hydrophobic coating with small pores (~100-nm thick with pores < 10 nm)

The increased vapor pressure due to the Kelvin Equation will increase the vapor pressure of the liquid, giving higher driving forces for evaporation, and therefore higher vapor fluxes

(Add Kelvin eq'n)



Transition

- Results, simplified models, and suggested membrane designs were provided to 7AC Technologies (sponsoring company)

- NREL is continuing to work with 7AC Technologies under a separate CRADA, focused on modeling and experimental characterization of their membranes and membrane modules.