Concentration polarization modeling for high-pressure membranes with engineered surface features

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1: Motivation & Objectives

Motivation

- Concentration polarization reduced performance of membranes in terms of flux and water quality.
- Fouling is more problematic when concentration polarization is high.

Objectives

- Develop a computational framework to predict concentration polarization of patterned membranes.
- Evaluate the effect of hydrodynamics on concentration profiles.
- Explore the performance of different membrane patterns.

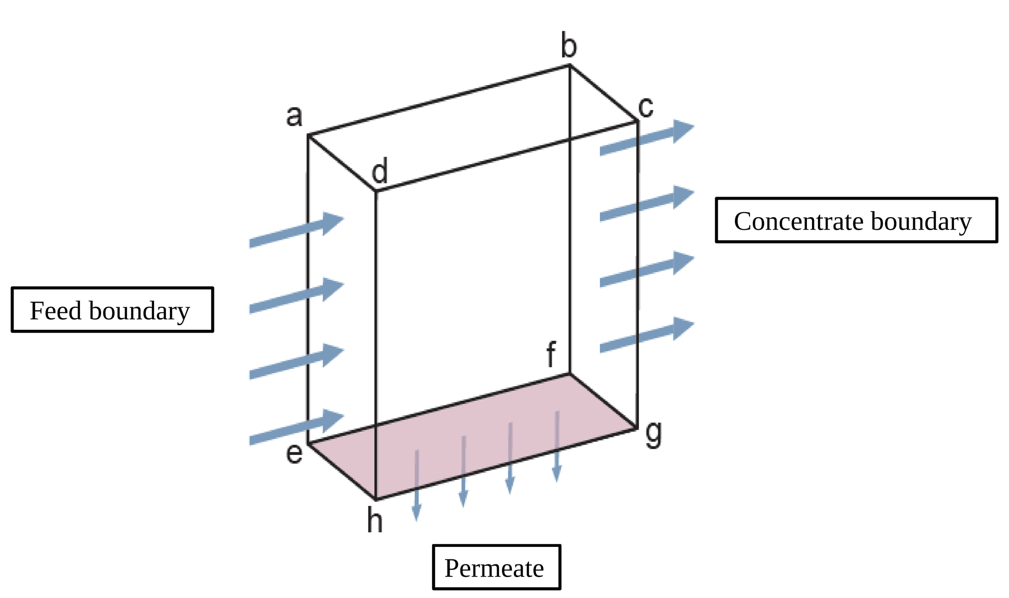
2: Model Introduction

Introduction

- Computational fluid dynamics (CFD) uses numerical analysis to solve and analyze fluid flow problems.
- Models were built with COMSOL Multiphysics (version 5.3).

Geometry

- Block: width 4.096 mm, depth 2.048 mm, height 8 mm.
- Eight geometry types: elementary shapes including line and grooves, pillars, chords, and pyramids. Mesh: boundary layer along the membrane surface due to drastic gradient changes.
- A pattern size of 512 µm was studied first, and then four smaller sizes were studied: 2 µm, 8 µm, 32 µm, and 128 µm. Velocity was normalized in different geometries based on a total channel height of 16 mm.



(Wall abcd: moving wall. Wall abfe and wall dcgh: periodic boundaries. Membranes are located at efgh. Inlet concentration: 0.025 M.)

3: Theoretical Description

Key Governing Equations

- Navier-Stokes

$$\rho(\nabla\cdot\mathbf{u})\mathbf{u} = -\nabla P + \frac{\mu}{2}\nabla\cdot\left(\nabla\mathbf{u}+\nabla\mathbf{u}^T\right)$$

- Conservation of momentum

$$\nabla\cdot\mathbf{u} = 0$$

- Convective diffusion

$$\mathbf{u}\nabla c = D_c\nabla^2 c$$

Key Boundary Conditions

- Permeate flux

$$u_m = A(\Delta p - a_{osm}c_w)$$

- Inlet velocity

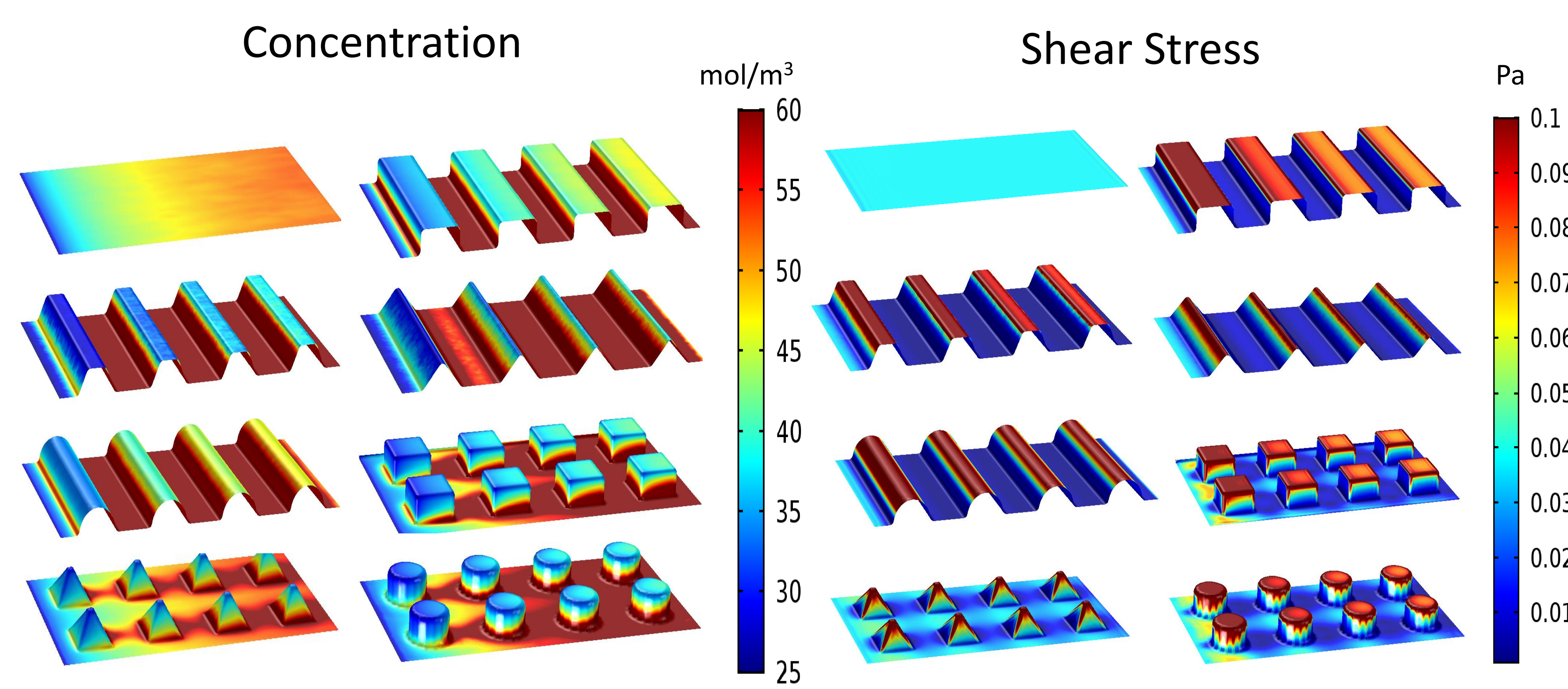
(Adjusted based on v=0.1 m/s in a 16 mm channel)

- Outlet pressure

$$p_{out} = 400 \text{ psi}$$

3: Results & Discussion

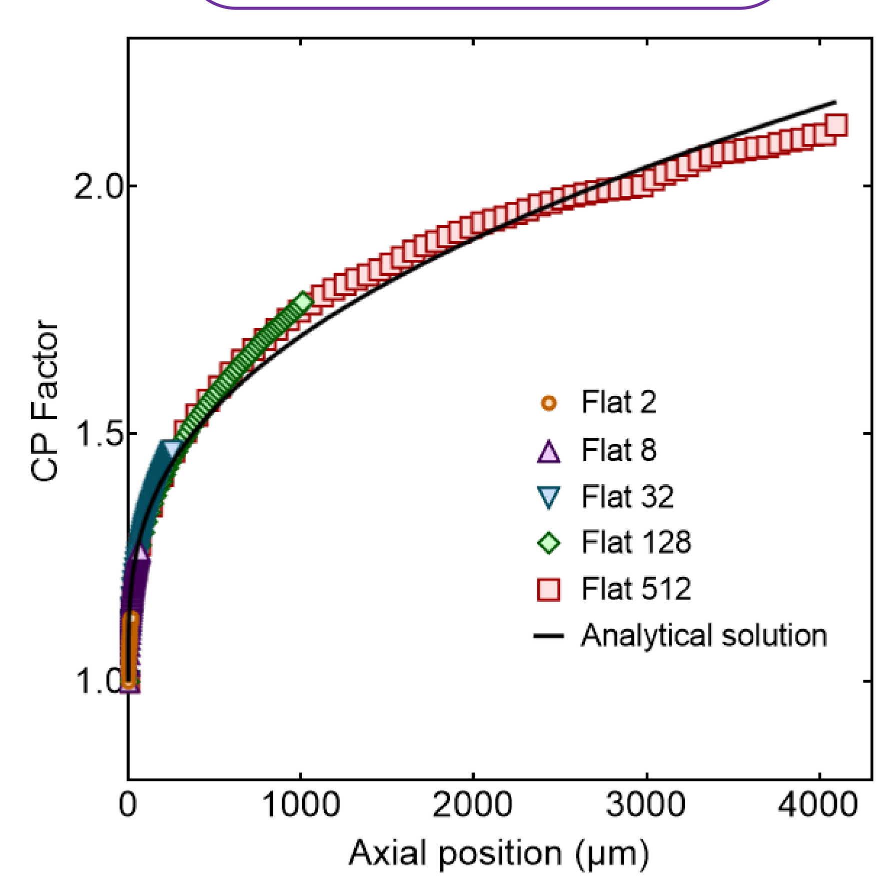
CONCENTRATION AND SHEAR PROFILES



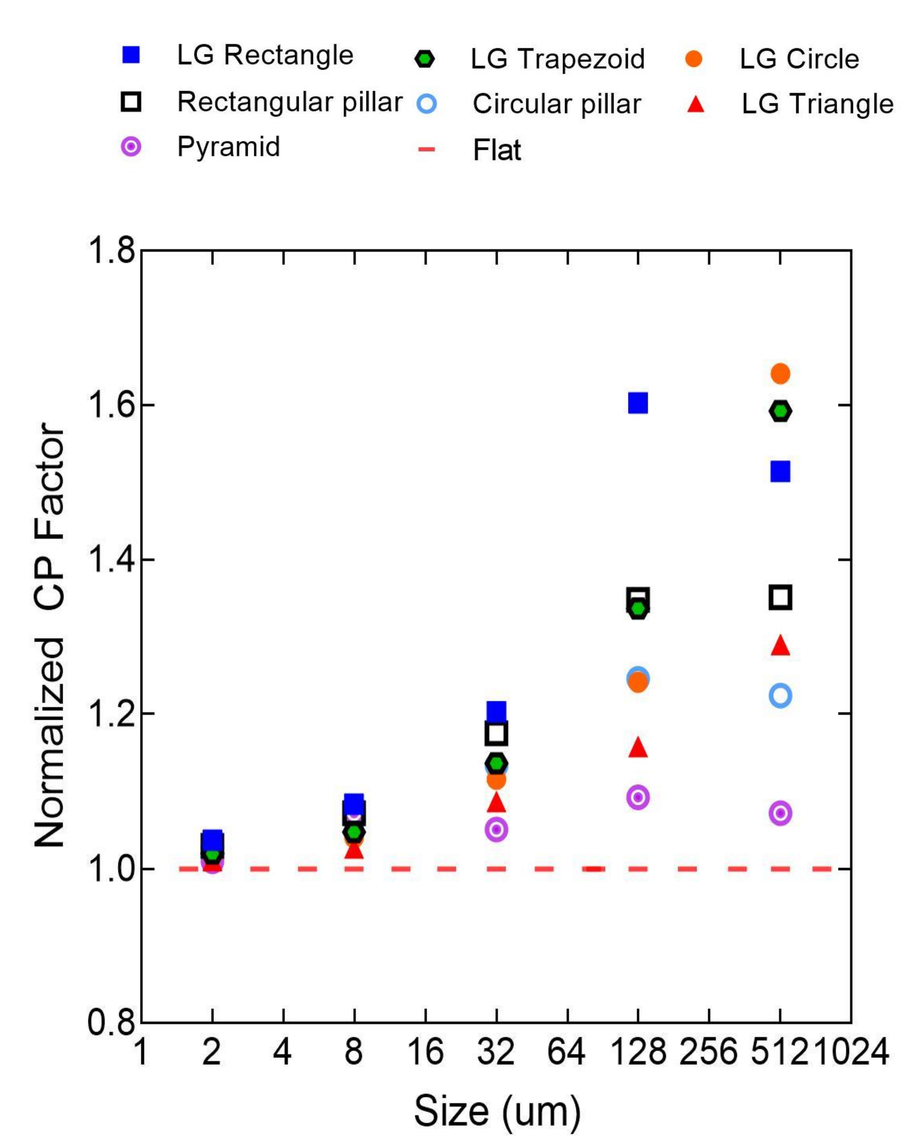
ANALYTICAL VS. NUMERICAL SOLUTIONS

$$Sh = 1.85\left(Re\cdot Sc\cdot\frac{d_h}{L}\right)^{0.275}$$

$$k = \frac{Sh\cdot d}{d_h} \qquad \frac{c_m}{c_b} = \exp\left(\frac{J}{k}\right)$$



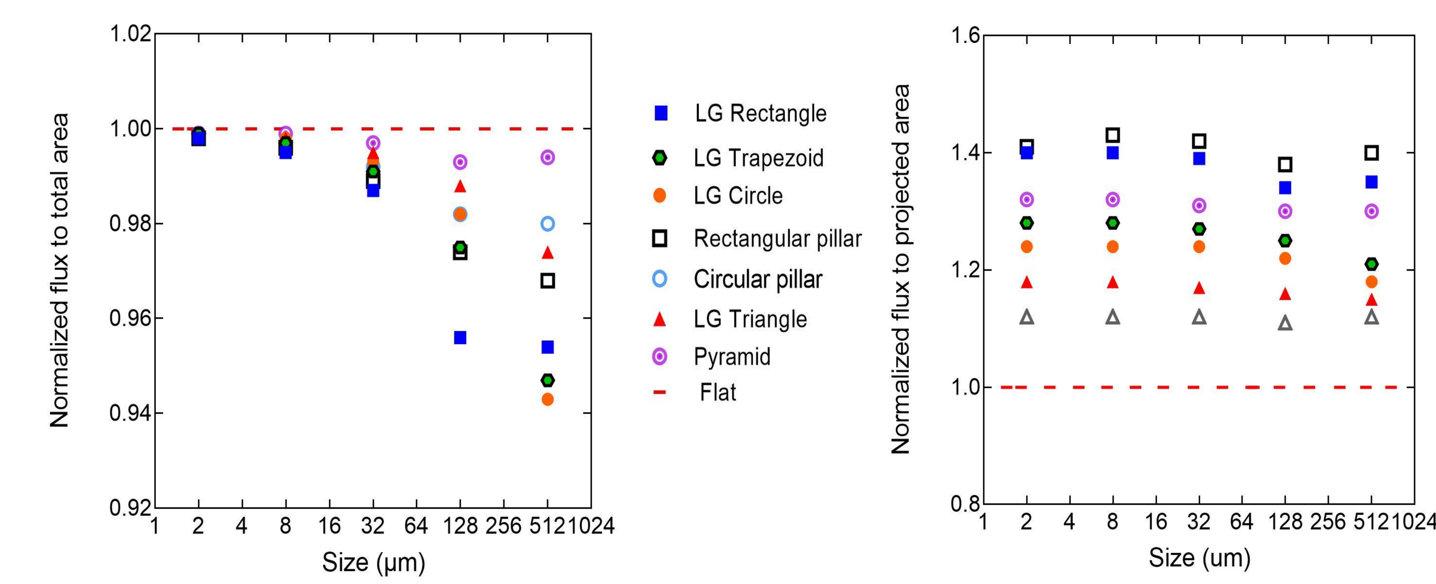
CP RESULTS



3: Results & Discussion

PERMEATE FLUX VS PATTERN SIZES

Feature Length (µm)	Feature Height (=0.5·Length) (µm)	Between-Feature Distance (=Length) (µm)	Fillet (=0.2·Height) (µm)
2 µm	1 µm	2 µm	0.2 µm
8 µm	4 µm	8 µm	0.8 µm
32 µm	16 µm	32 µm	3.2 µm
128 µm	64 µm	128 µm	12.8 µm
512 µm	256 µm	512 µm	51.2 µm



4: Conclusions and Looking Forward

- Analytical solutions were used to validate modeling results among all the flat membranes.
- Seven membranes with different surface features were scrutinized and compared with flat membranes. None of the patterns reduced CP.
- Patterns created higher surface areas compared to a flat membrane, leading to a higher nominal flux through the membrane surface in the models.
- The fouling mitigation seen in experiments with nanoscale patterns is likely due to other factors.
- Future studies will incorporate adsorptive fouling.

5: Acknowledgements

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- Computational resources provided by the Palmetto Cluster at Clemson University.

6: Selected References

1: Chan, C. C. V., P. R. Bérubé, and E. R. Hall. "Relationship between types of surface shear stress profiles and membrane fouling." *Water research* 45.19 (2011): 6403-6416.
2: Radu, A. I., et al. "Spacer geometry and particle deposition in spiral wound membrane feed channels." *Water research* 64 (2014): 160-176.
3:Won, Young-June, et al. "Correlation of membrane fouling with topography of patterned membranes for water treatment." *Journal of Membrane Science* 498 (2016): 14-19.