RAPID
Transforming Process Industries

Utilizing the MATLAB CAPE-OPEN Unit Operation to Make Real Hydrocarbon Mixture Membrane Separation Predictions

Thursday, Oct. 28th, 2021

Dylan Weber and Dr. Joseph Scott

Georgia Institute of Technology

Georgia Tech College of Engineering
School of Chemical and Biomolecular Engineering

Our Contribution

Present our experience with using AmsterCHEM's MATLAB Unit Operation.

- Specifically, we implemented our novel shooting algorithm for complex hydrocarbon mixture permeation across asymmetric membrane layers[1]

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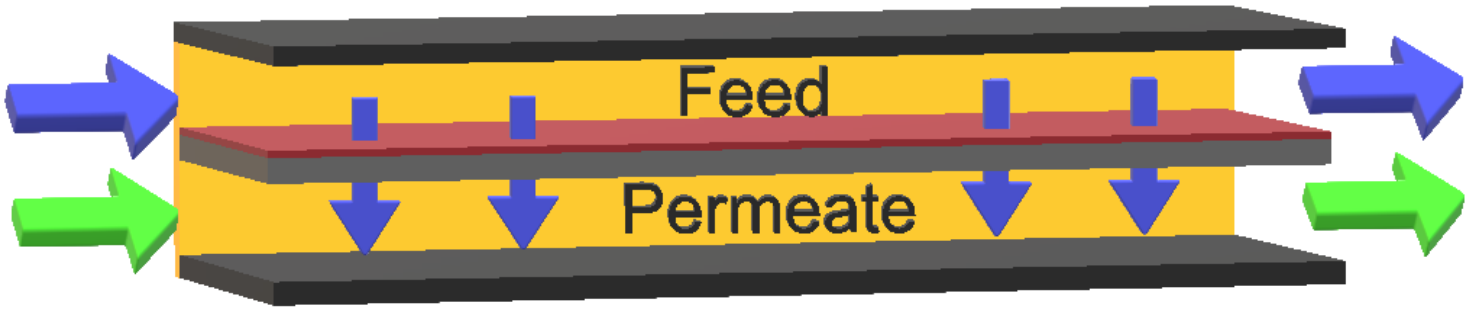

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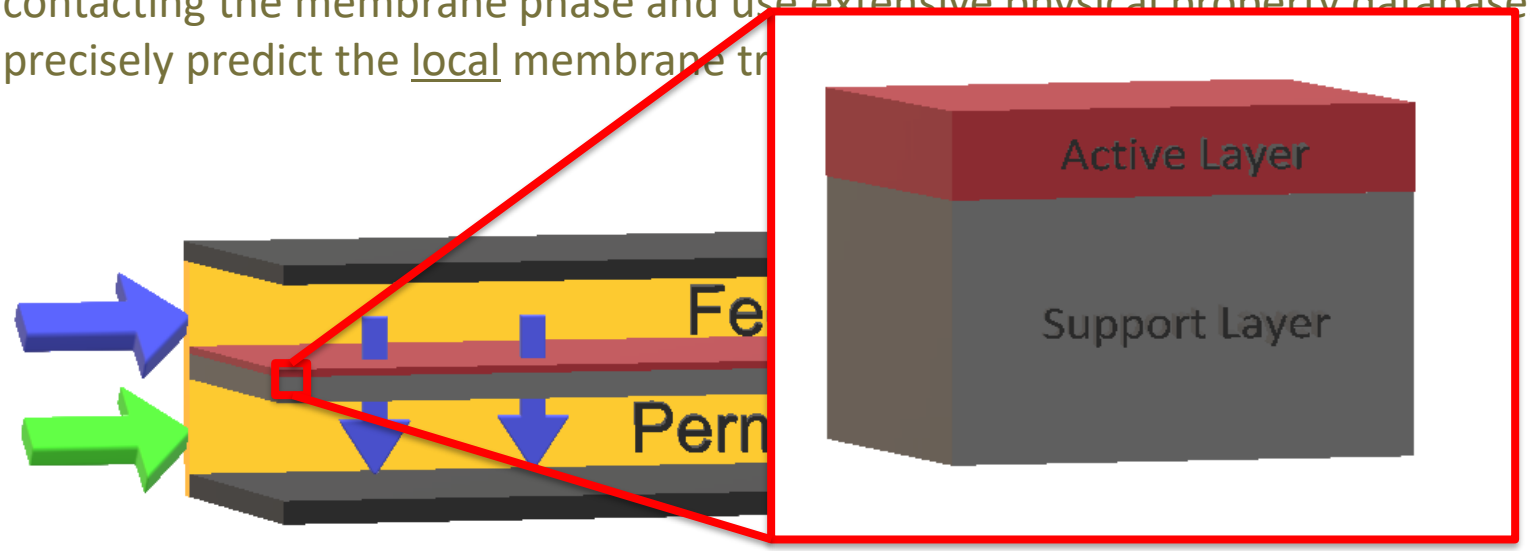

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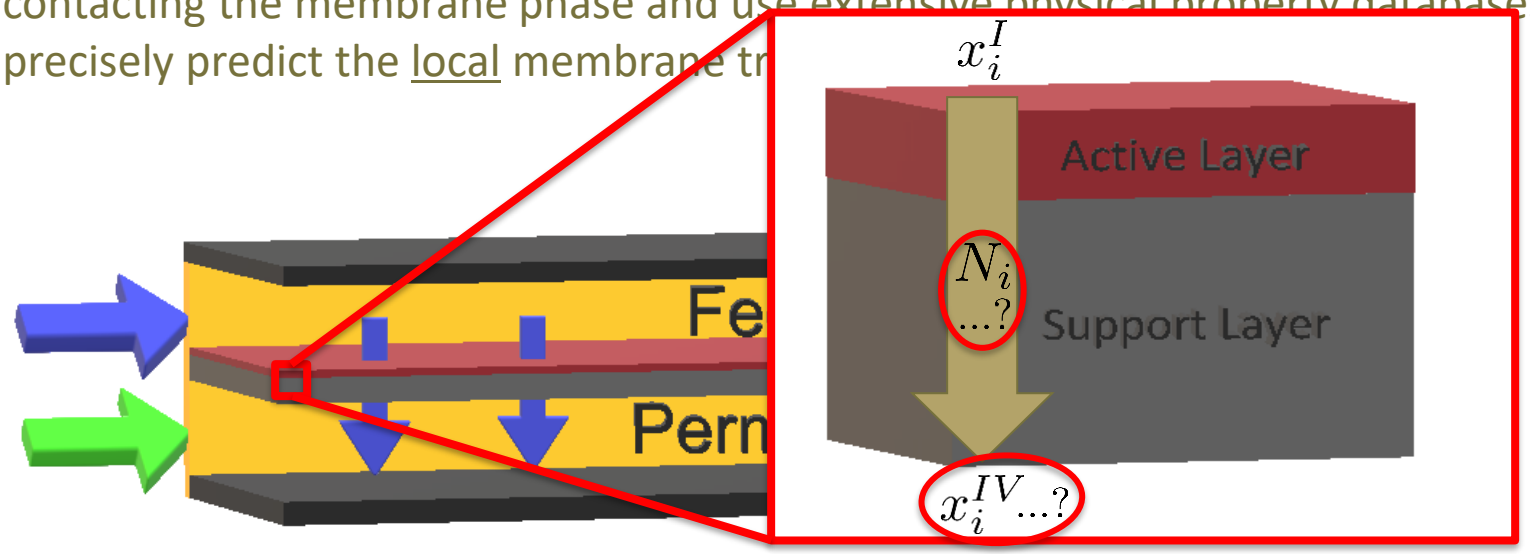

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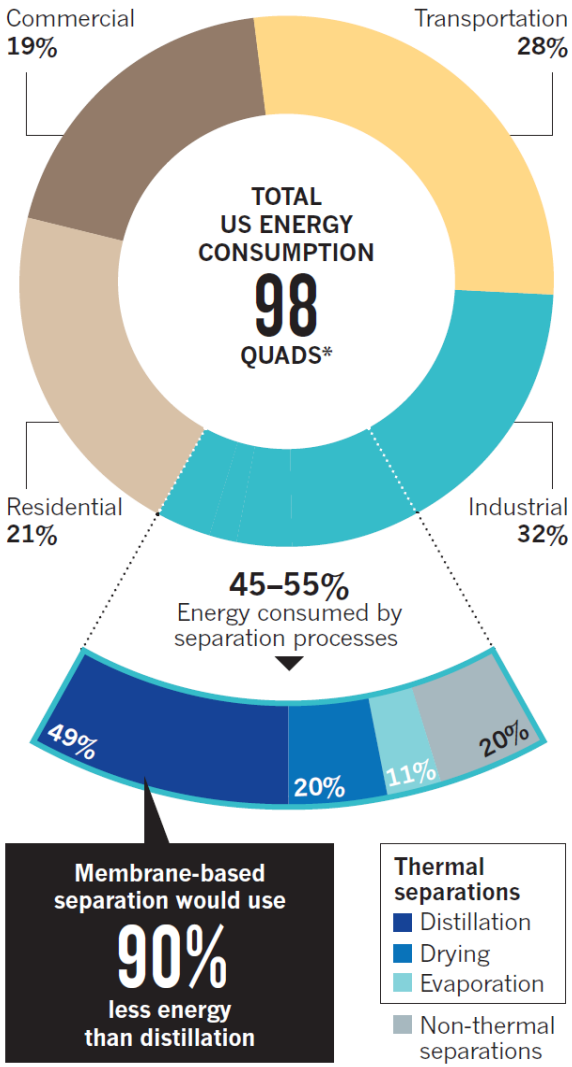
Industrial Membrane Processes



2. Sholl, D. S. and Lively, R. P. (2016). Seven chemical separations to change the world. Nature, 532(7600):435–437.

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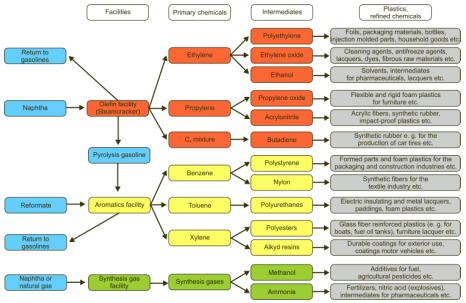
Crude Oil Refining:



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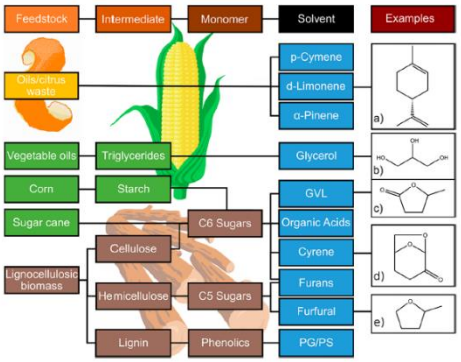
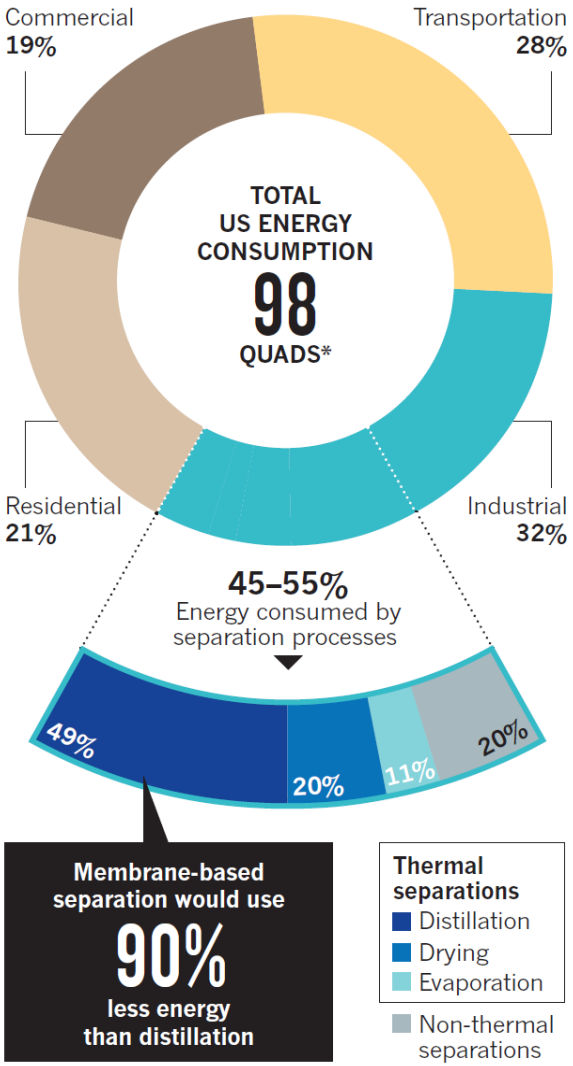
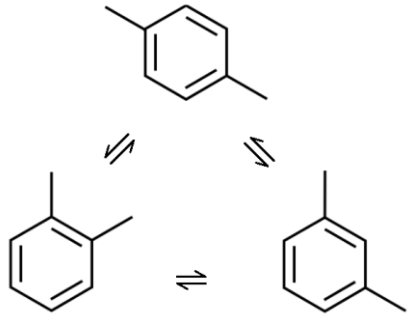




Benzene derivatives:



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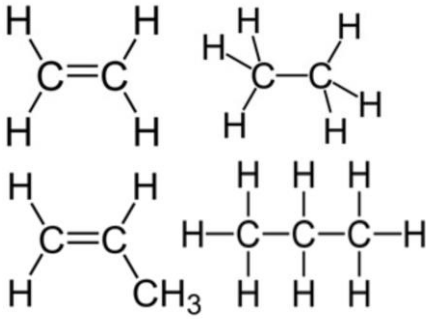

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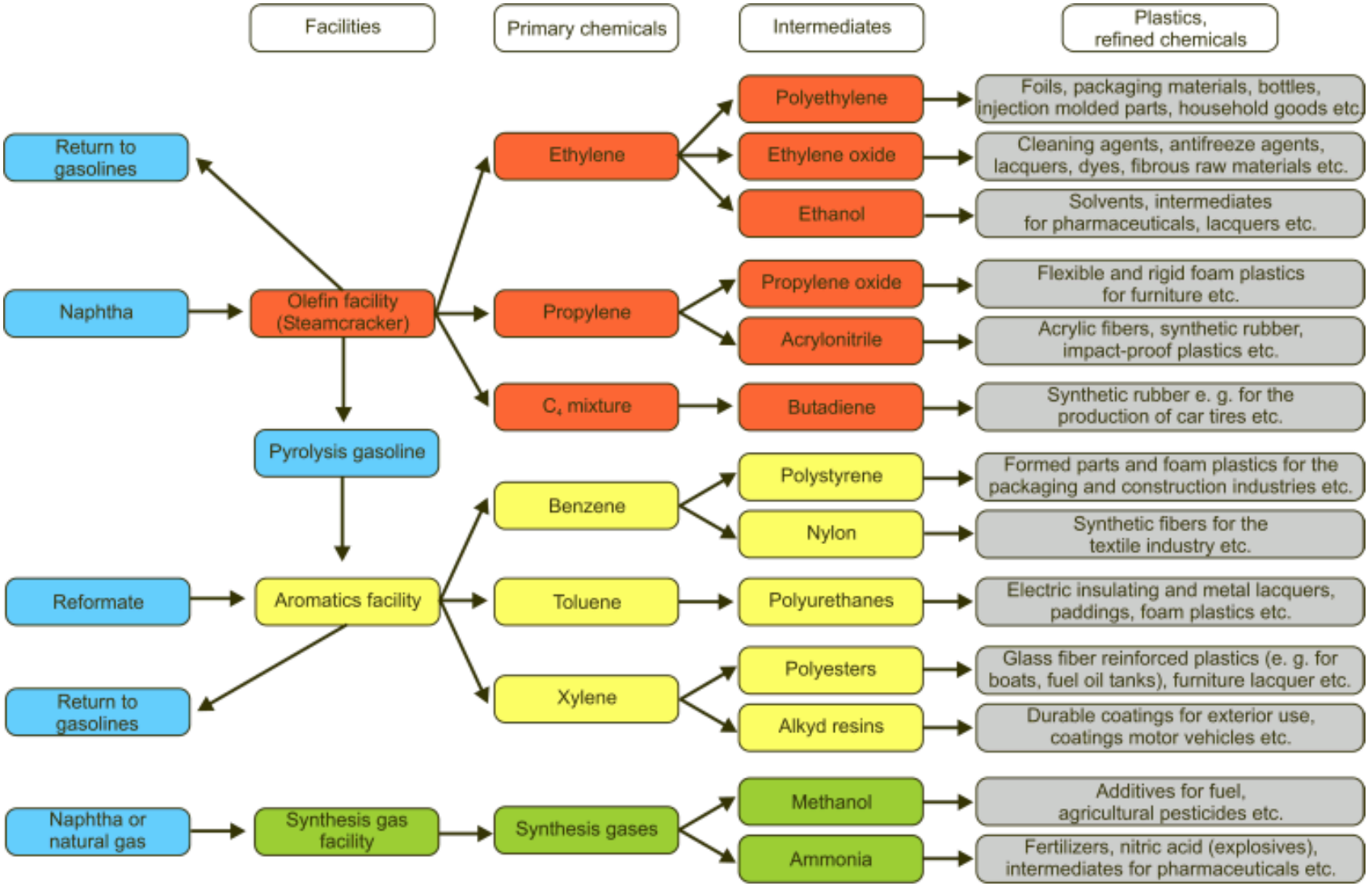

3. [Flowchart of crude oil products]. (n.d.). https://tinyurl.com/4ujk69pw

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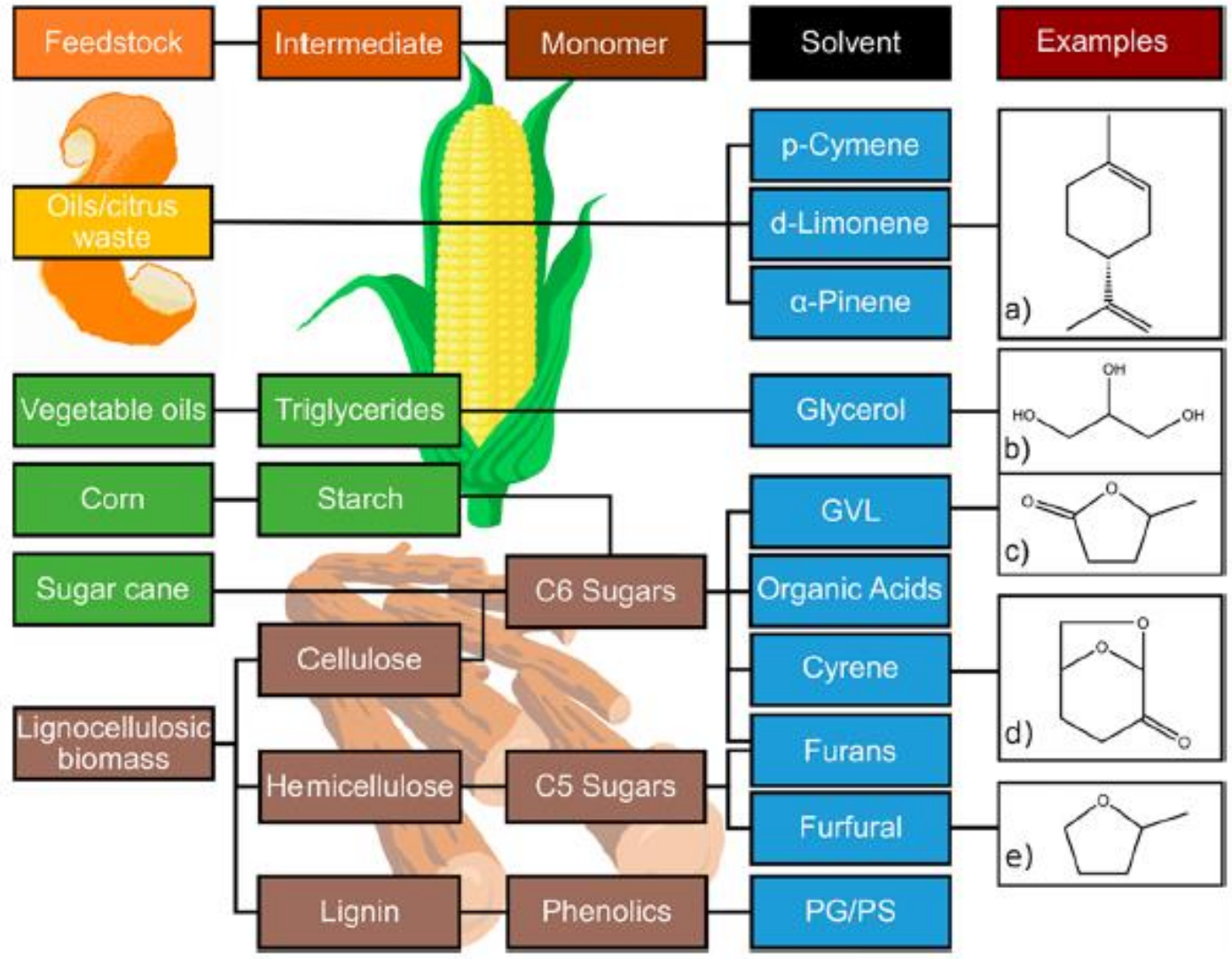

4. Sheldon, R. A. (2005). Green solvents for sustainable organic synthesis: state of the art. Green Chem., 7:267–278.

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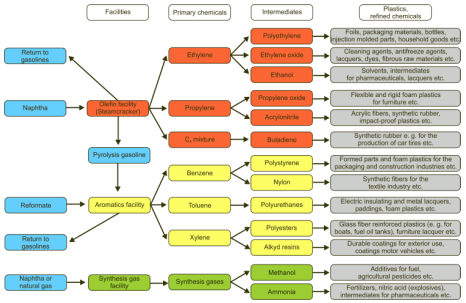

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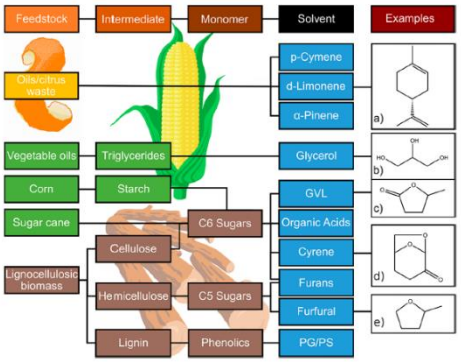

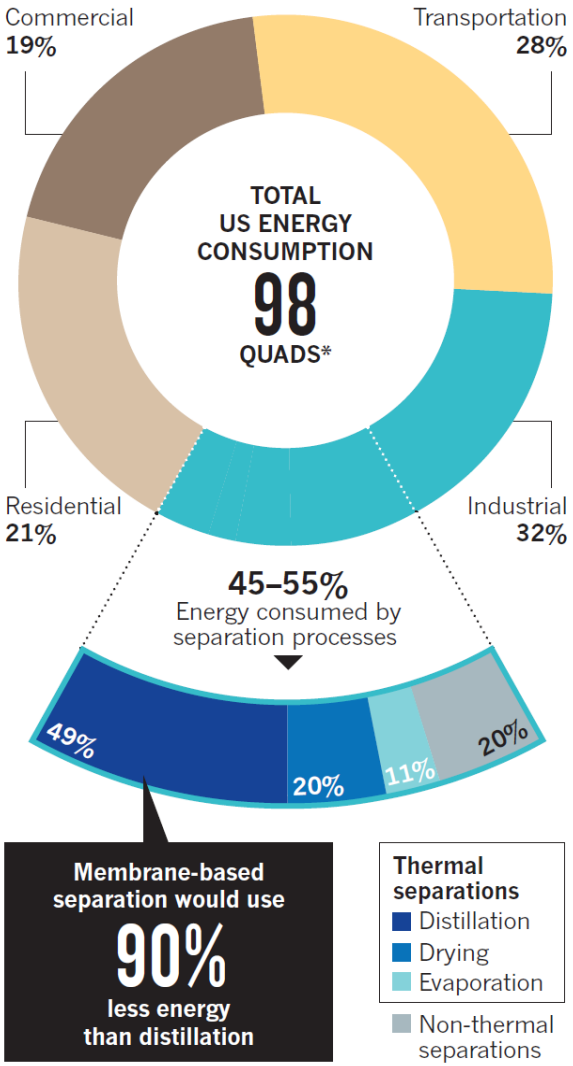

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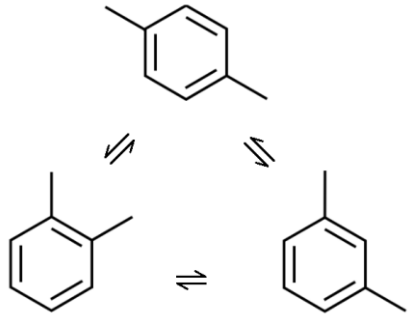

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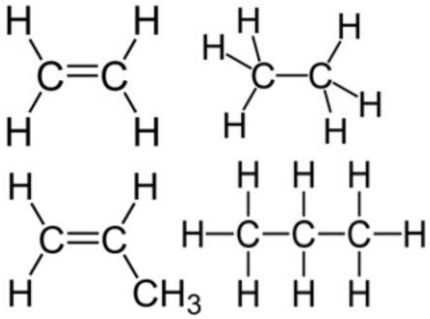

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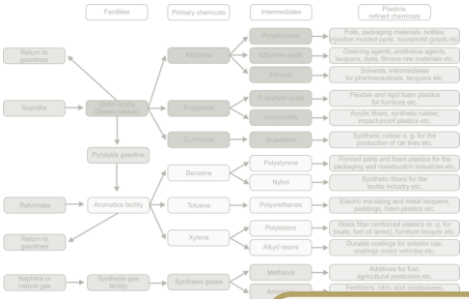

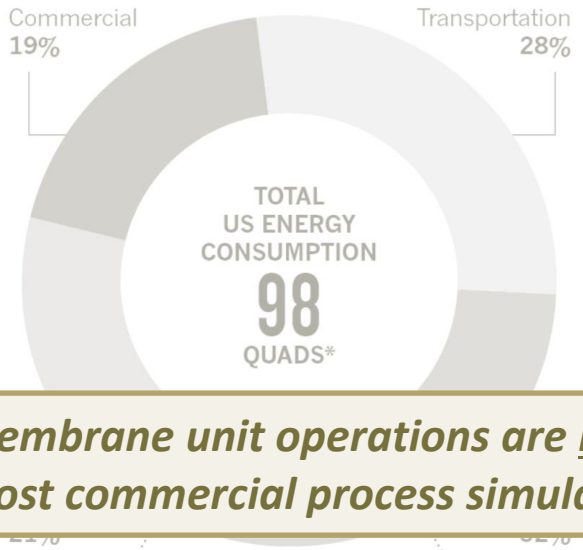

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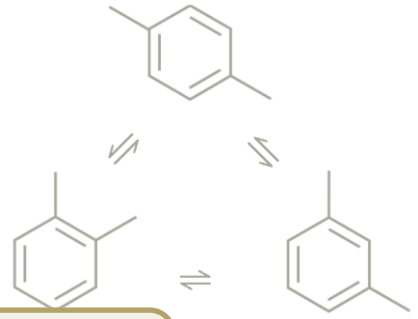

Industrial membrane unit operations are <u>non-existent</u> in most commercial process simulators

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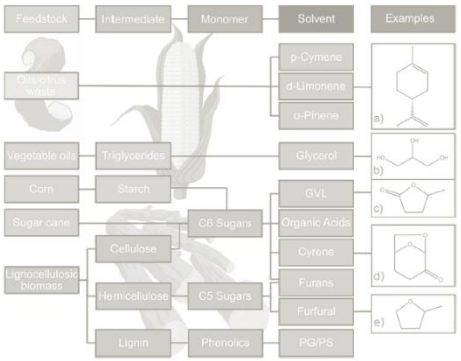

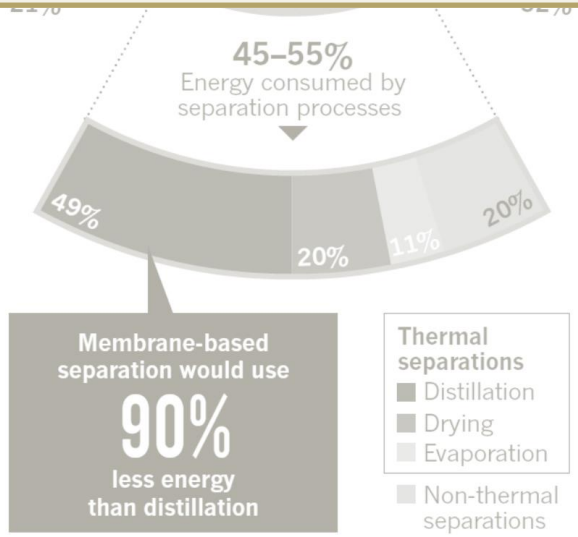

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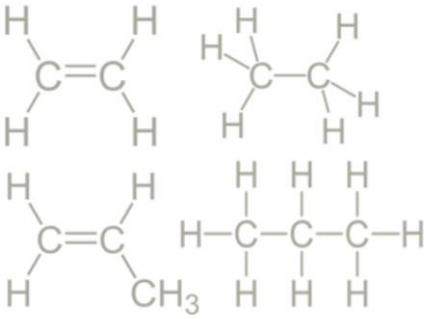
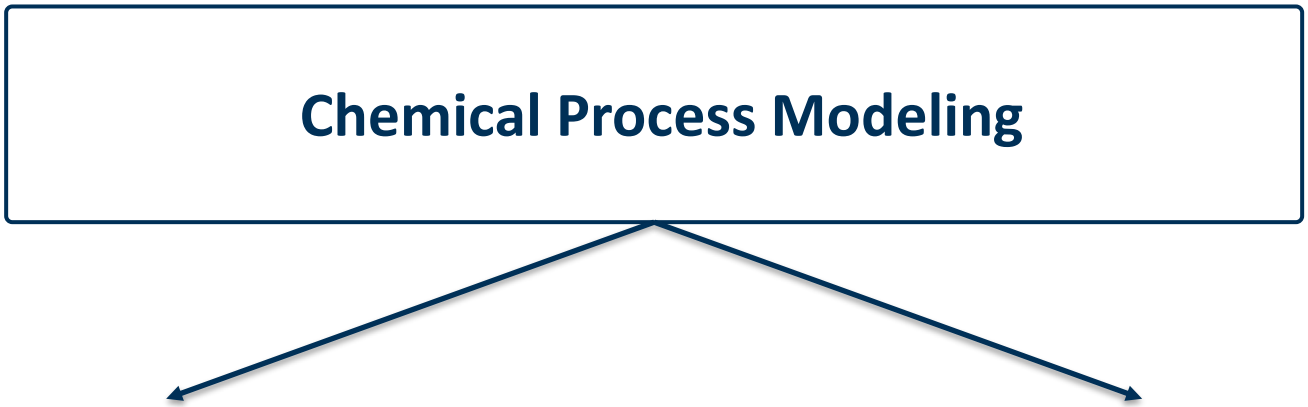


Standardized Interoperability – CAPE-OPEN



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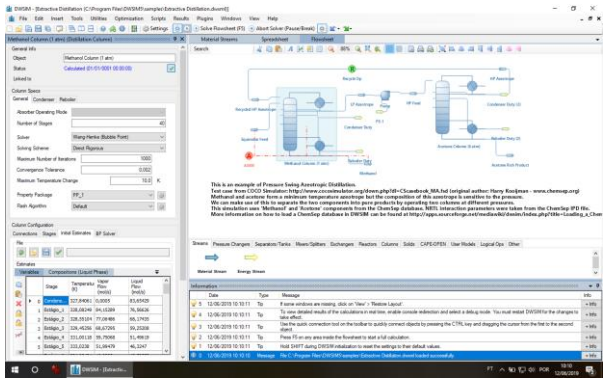
Chemical Process Modeling

Process Modeling Environment (PME)



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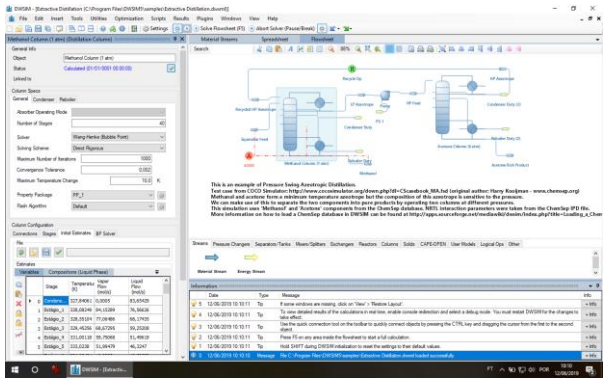
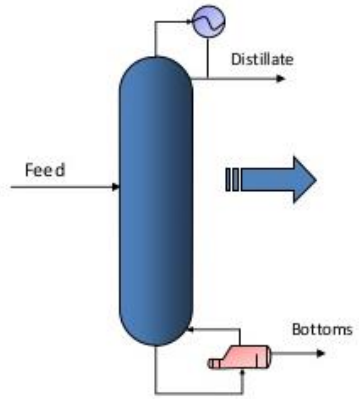
Chemical Process Modeling

Process Modeling Environment (PME)

Process Modeling Component (PMC)





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CO-LaN

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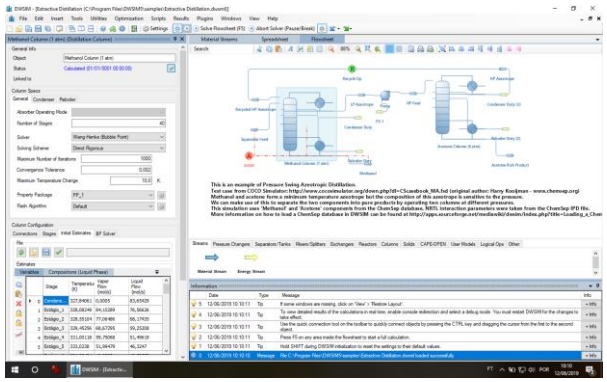
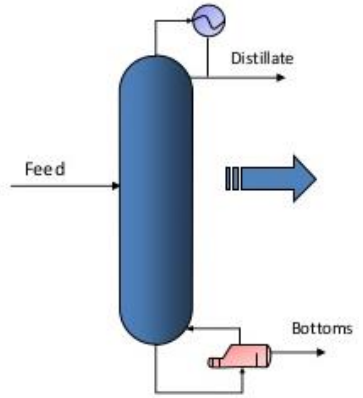
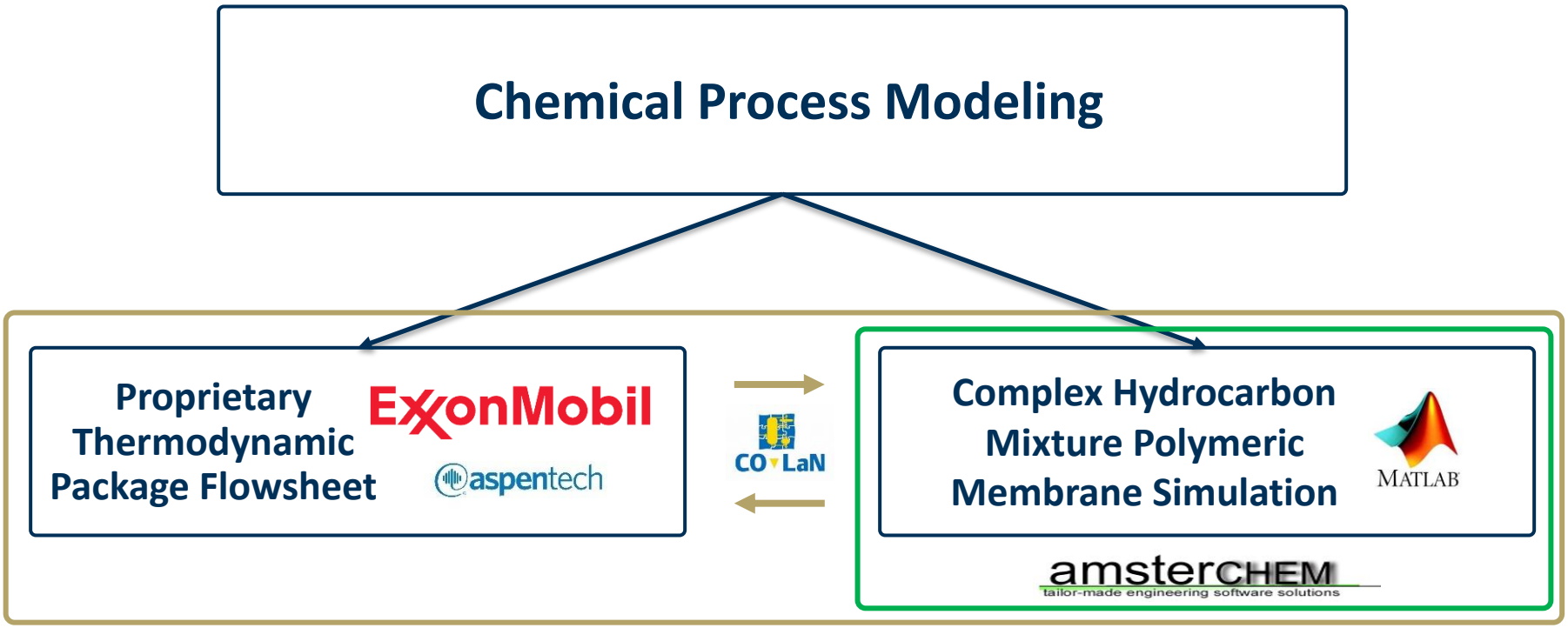




Our Use Case


Chemical Process Modeling
Proprietary Thermodynamic Package Flowsheet
ExxonMobil
aspentech
CO-LaN
Complex Hydrocarbon Mixture Polymeric Membrane Simulation
MATLAB
amsterCHEM
tailor-made engineering software solutions

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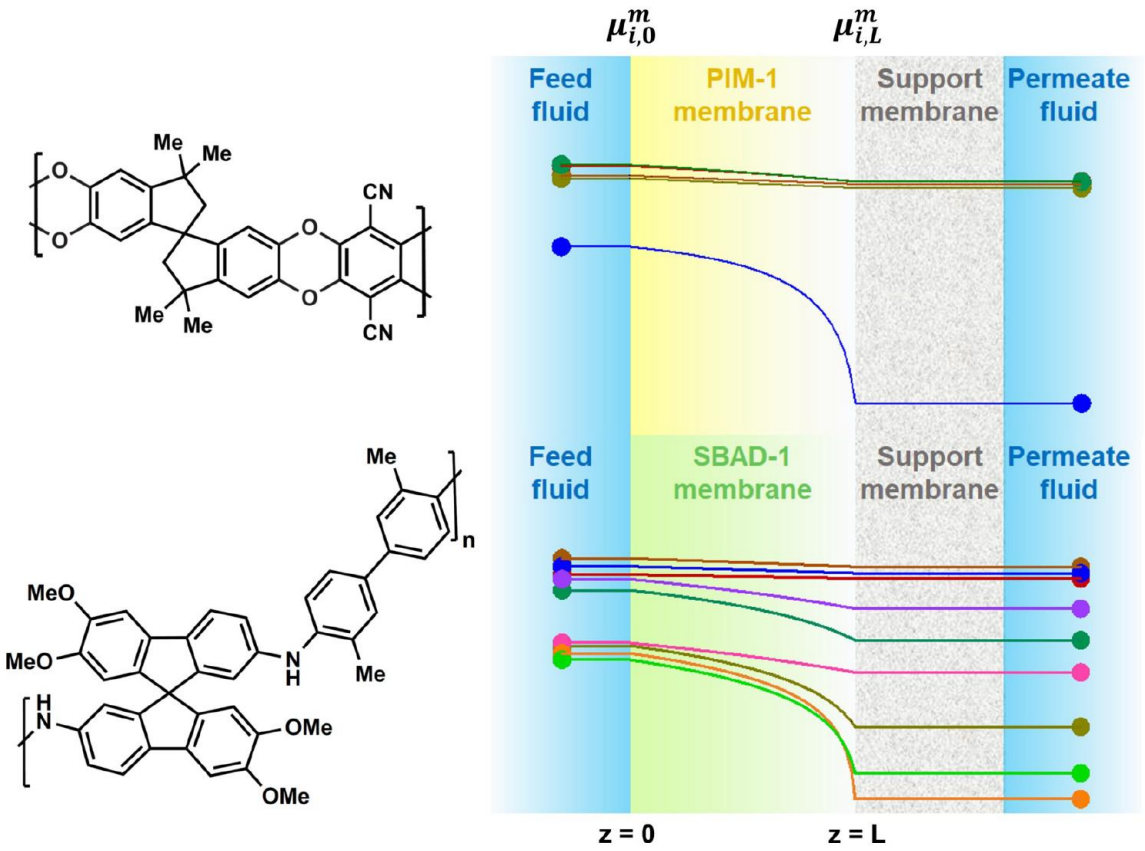

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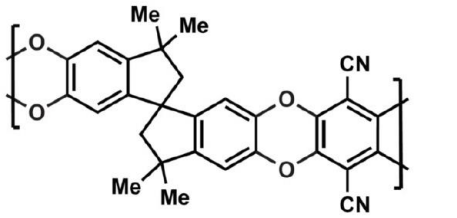

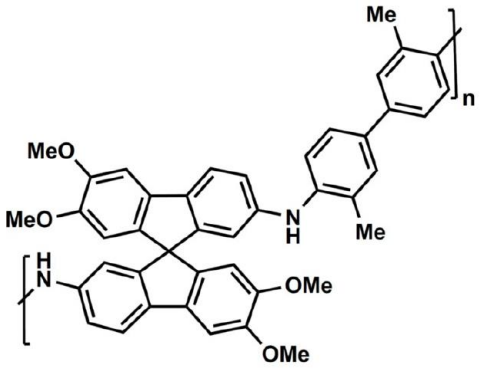

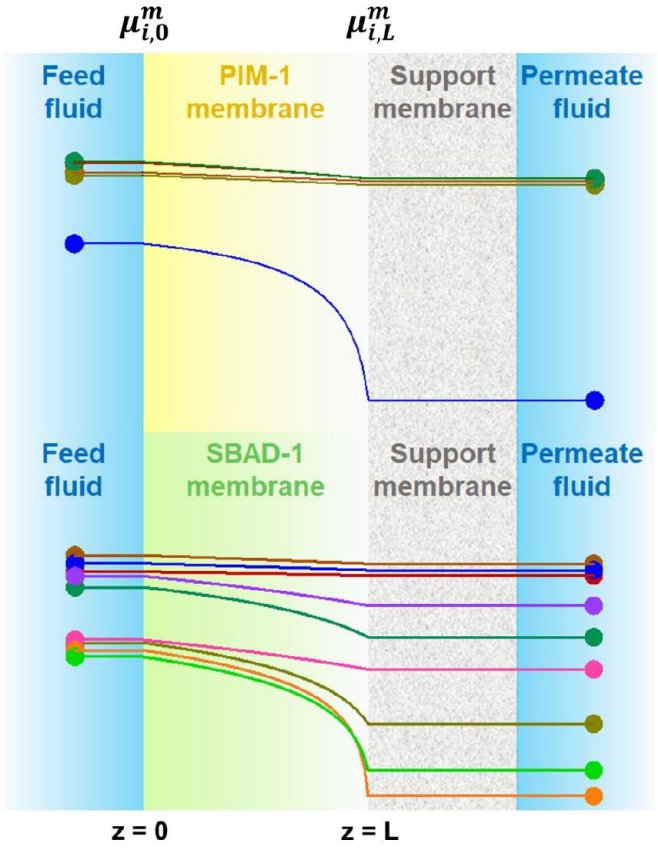

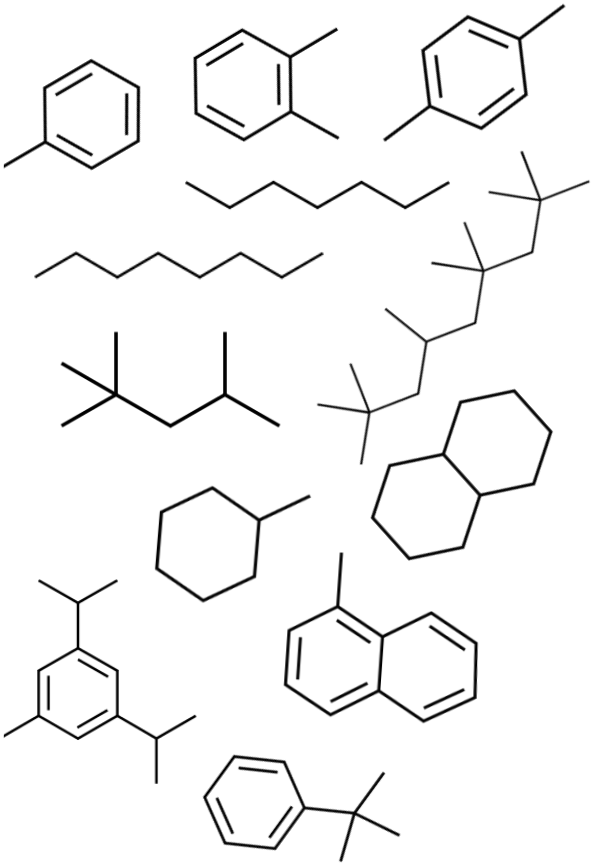

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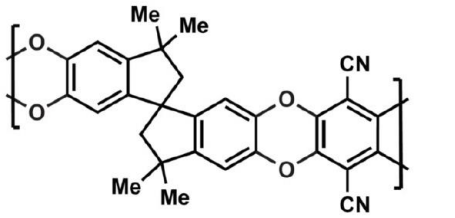

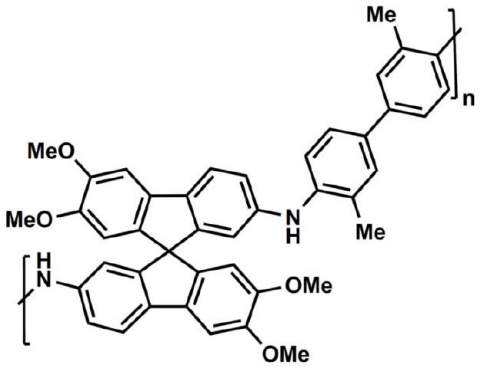

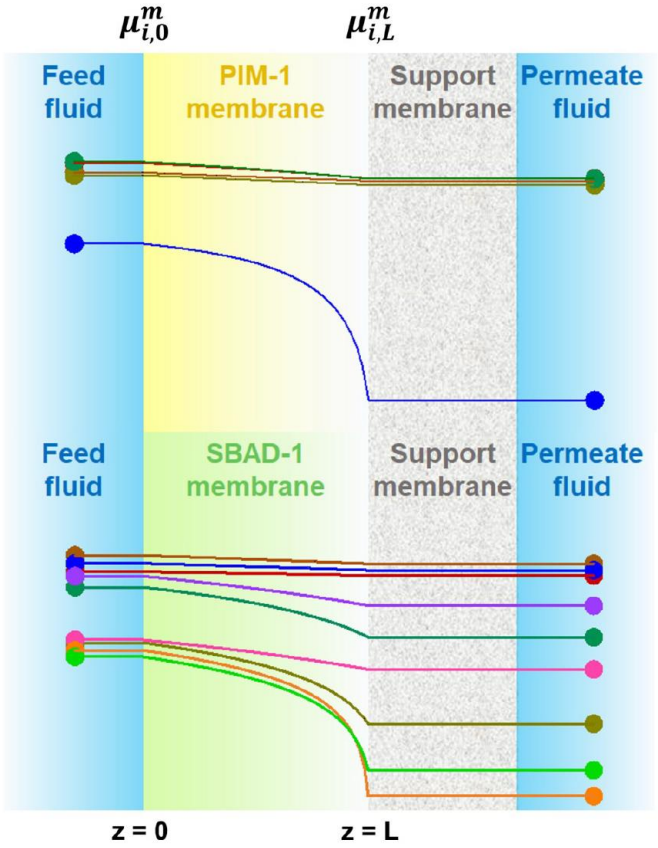

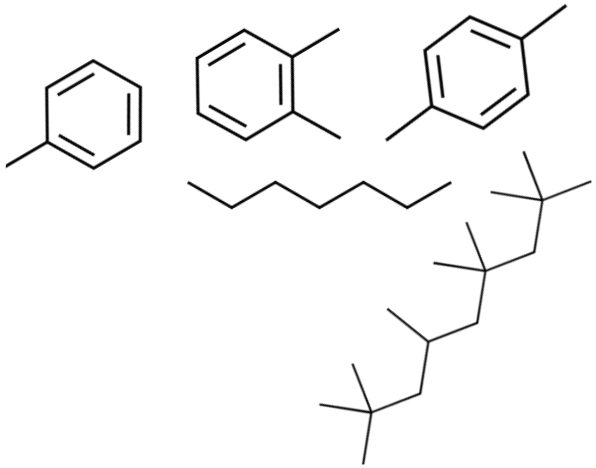

Separation 1 via PIM-1

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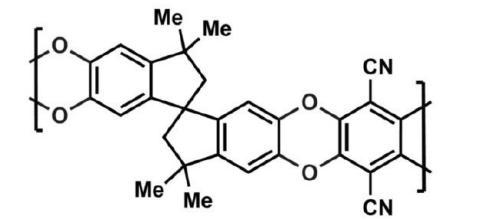

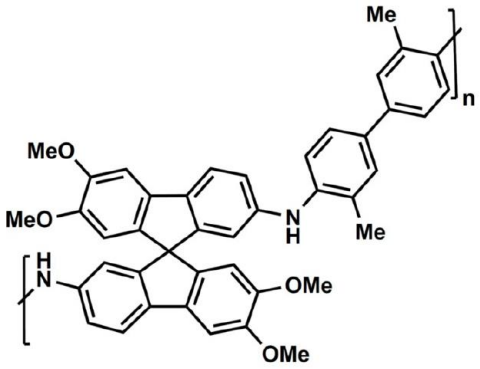

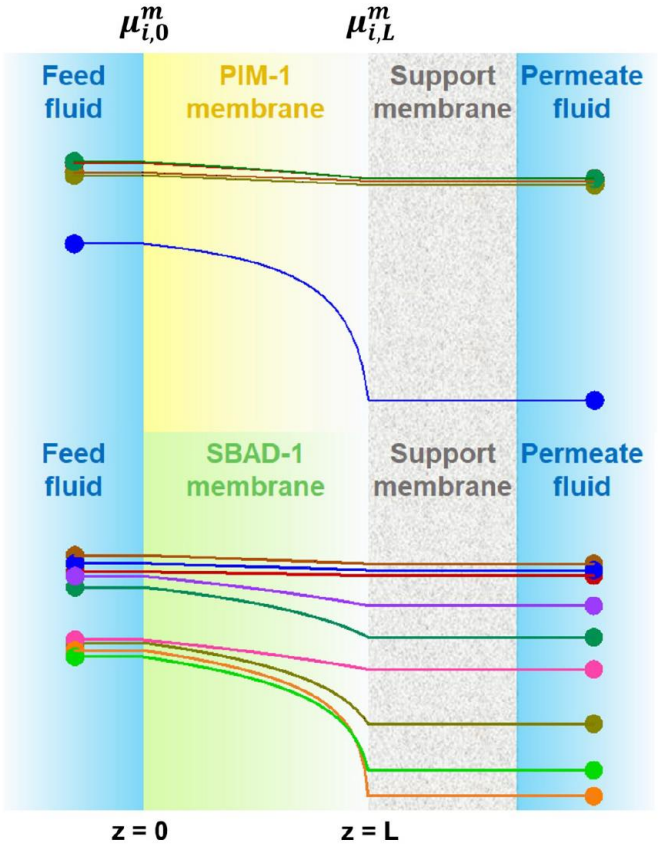

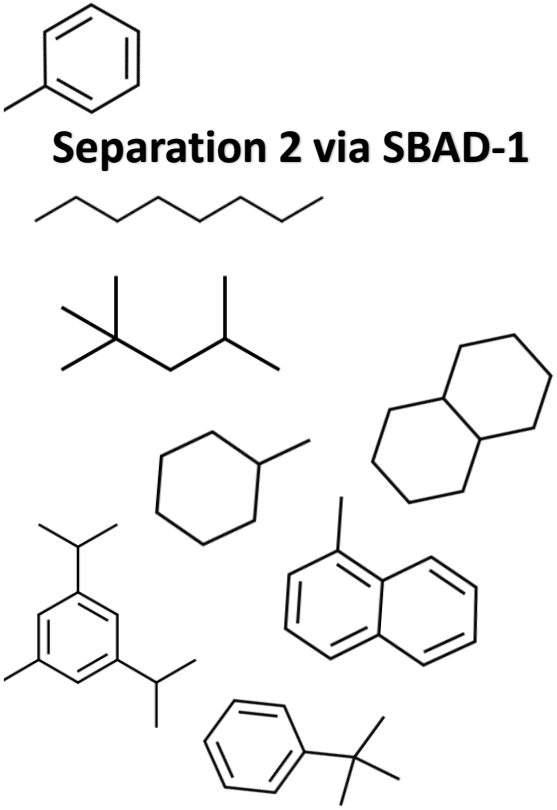

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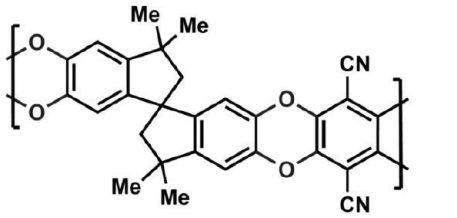

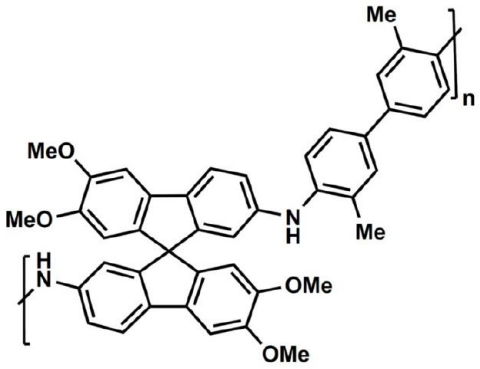

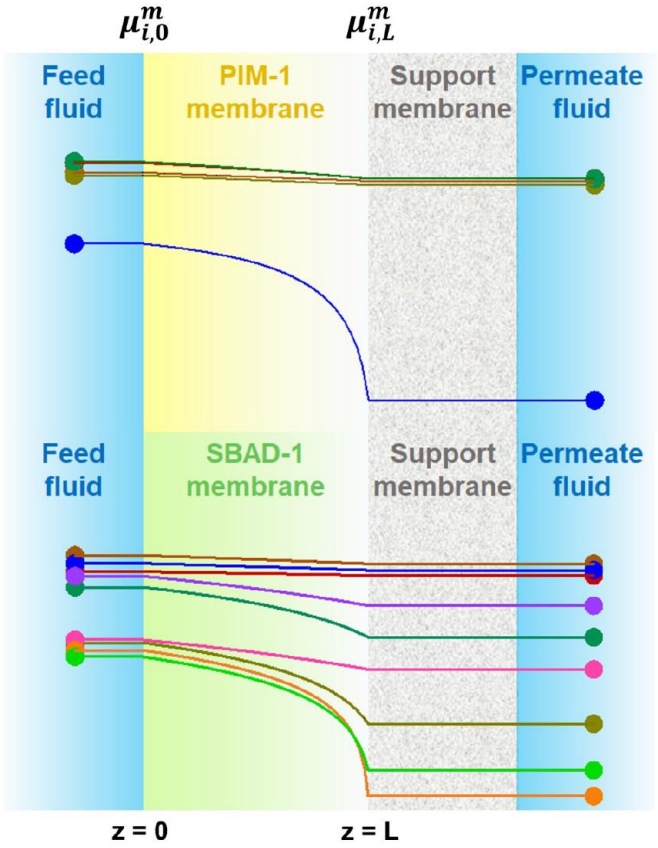

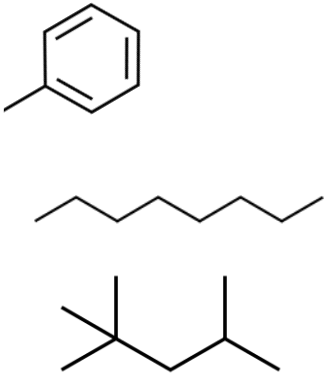

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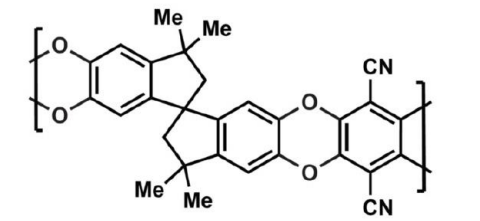

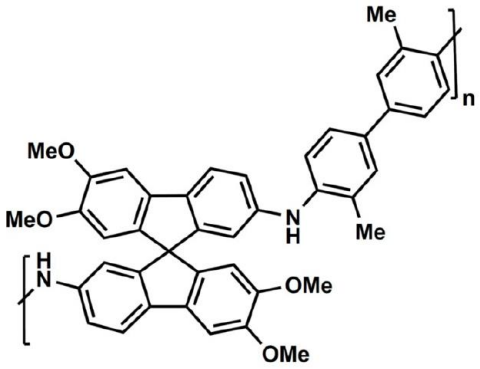

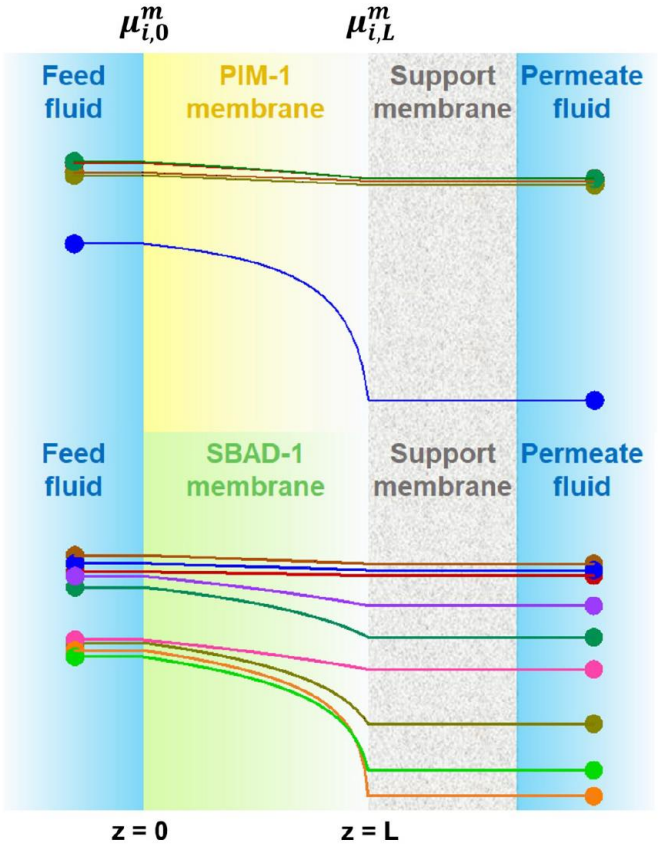

This CAPE-OPEN tool allowed assessment of:
3 different membrane sorption models
5 different diffusion scenarios

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Our Application

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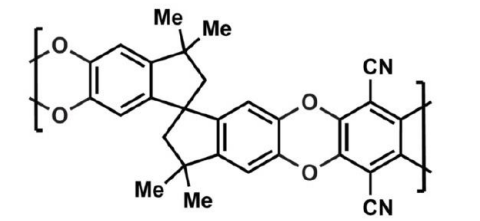

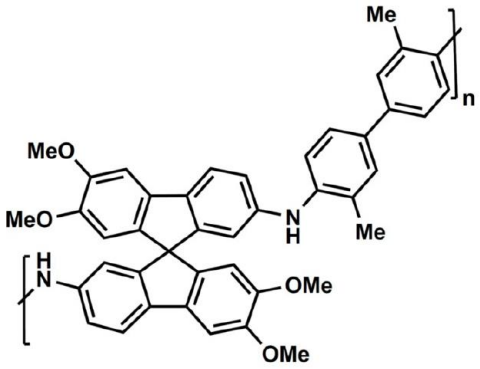

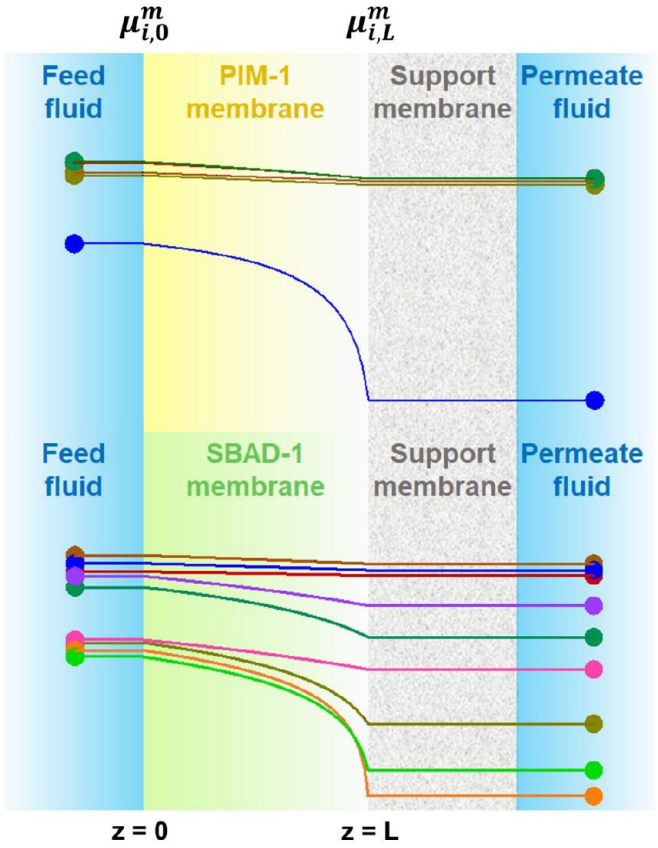

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For glassy polymers we proposed:
1 sorption model
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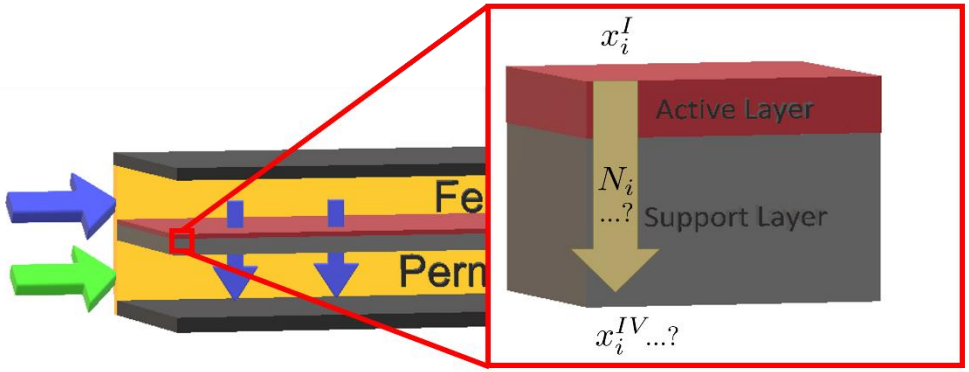
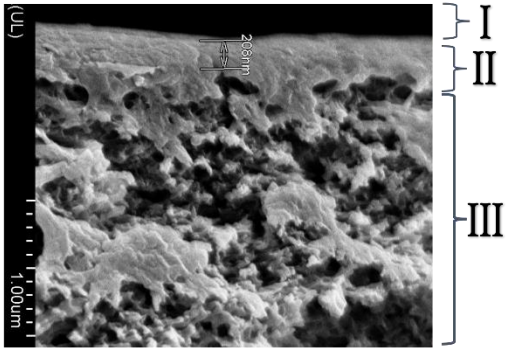
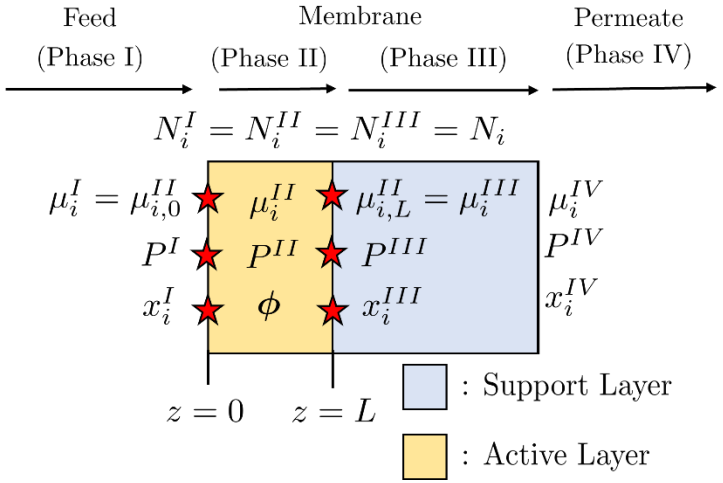
Our Membrane Simulation

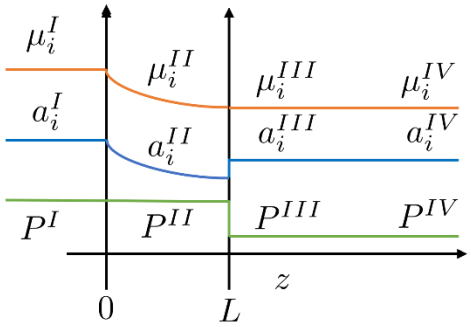
Utilizing this software, we made a custom PMC for industrial membrane modules.

- First, we need to set up the local transport problem through an asymmetric membrane layer[1]









FE-SEM Photo credit Ronita Mathias of Lively Group at GT

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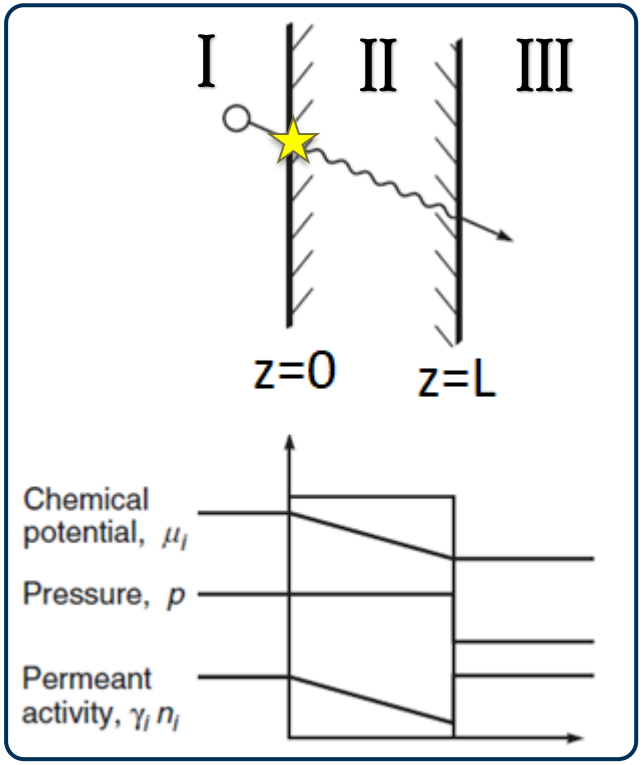

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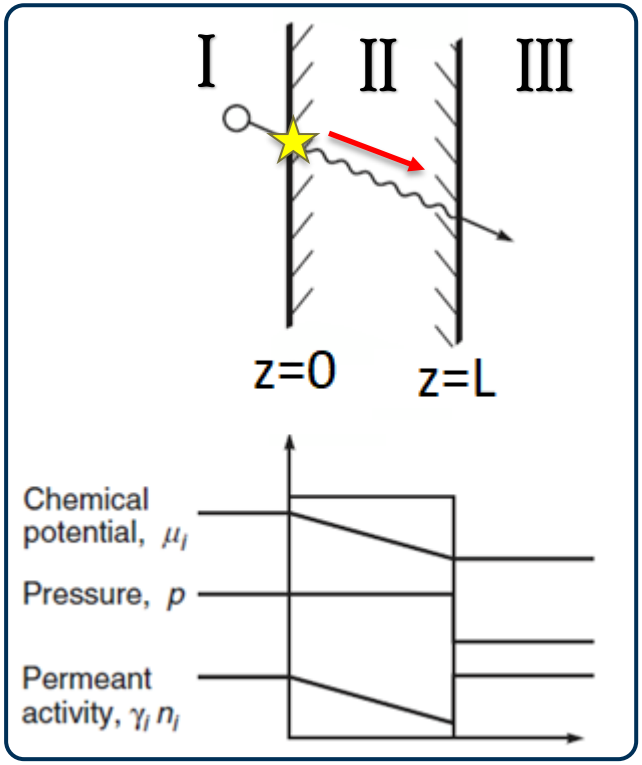

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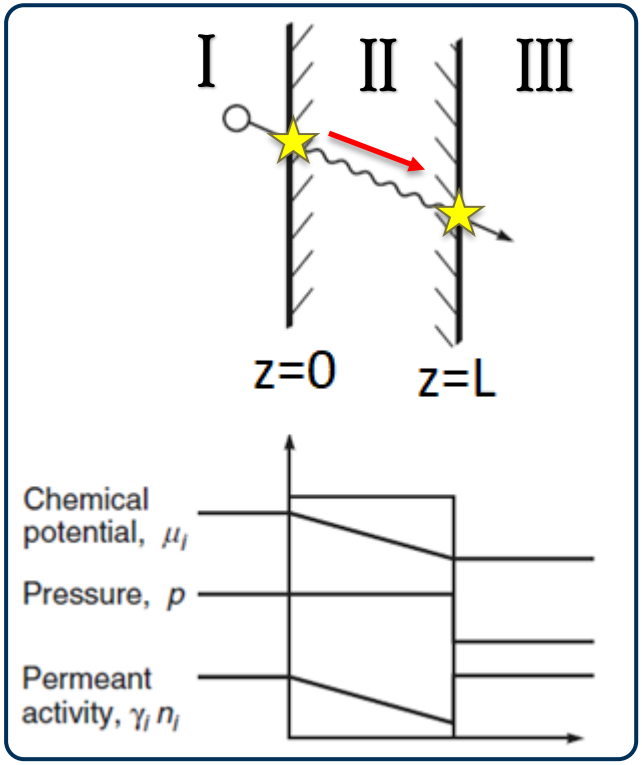

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- Then, we need to picture the full system of equations for the three-step sorption-diffusion model[1]

Sorption-Diffusion Step A

$$0 = g_i^I(\gamma_i^I, \mathbf{x}^I, \mathbf{s}, T, P^I), \ i = 1, 2, \ldots, n$$

$$\hat{f}_{i,0}^{II} = \gamma_{i,0}^I x_i^I f_i^\circ, \ i = 1, 2, \ldots, n$$

$$0 = w_i^{II}(\mathbf{f}^{II}, \phi_0, \mathbf{s}, T, P^{II}), \ i = 1, 2, \ldots, n$$

$$\sum_{j=1}^{n+1} \phi_{j,0} = 1$$

Sorption-Diffusion Step B

$$\frac{d\phi_{1:n}}{dz} = -\mathbf{\Gamma}^{-1}(\phi, \mathbf{f}^{II}, \mathbf{s})\mathbf{B}(\phi)\mathbf{x}^{III} N_{tot}^{V*}$$

$$\frac{d\phi_{n+1}}{dz} = -\sum_{j=1}^{n} \frac{d\phi_j}{dz}$$

$$\mathbf{w}(\phi, \mathbf{f}^{II}) = 0$$

Sorption-Diffusion Step C

$$0 = g_i^{III}(\gamma_i^{III}, \mathbf{x}^{III}, \mathbf{s}, T, P^{III}), \ i = 1, 2, \ldots, n$$

$$\hat{f}_{i,L}^{II} = \gamma_{i,L}^{III} x_i^{III} f_i^\circ \eta, \ i = 1, 2, \ldots, n$$

$$0 = w_i^{II}(\mathbf{f}^{II}, \phi_L, \mathbf{s}, T, P^{II}), \ i = 1, 2, \ldots, n$$

$$\sum_{j=1}^{n} x_j^{III} = 1$$

Known variables:

$$(\mathbf{x}^I, L, T, P^I, P^{II}, P^{III}, \mathbf{s}, \mathbf{Đ})$$

Unknown variables:

$$(\gamma^I, \gamma^{III}, \mathbf{f}_0^{II}, \mathbf{f}_L^{II}, \phi_0, \phi_L, \mathbf{x}^{III}, N_{tot}^{V*})$$

DoF: $4n + 3(n+1)$ equations
$-4n + 3(n+1)$ unknowns
$= \mathbf{0}$ **DoF**

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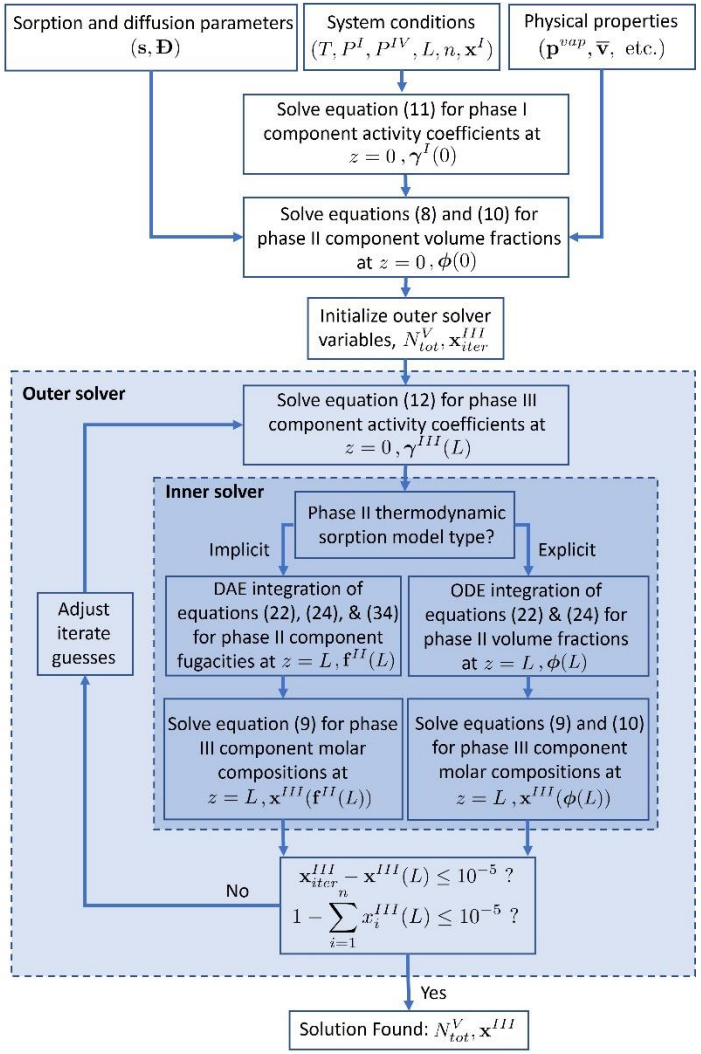
- Finally, we can implement our novel shooting algorithm[1] within this PMC framework



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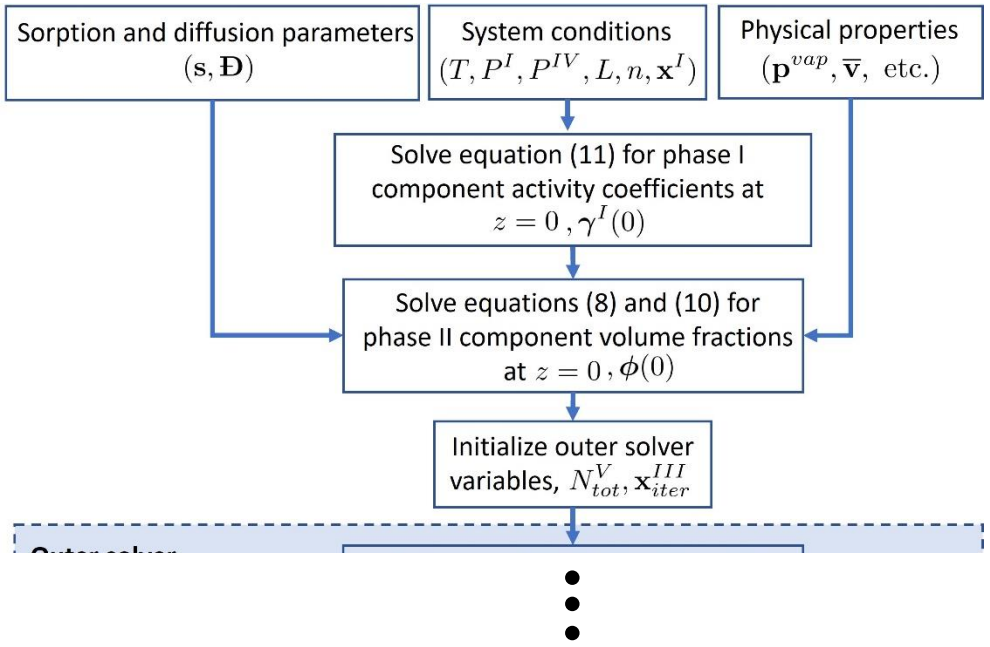

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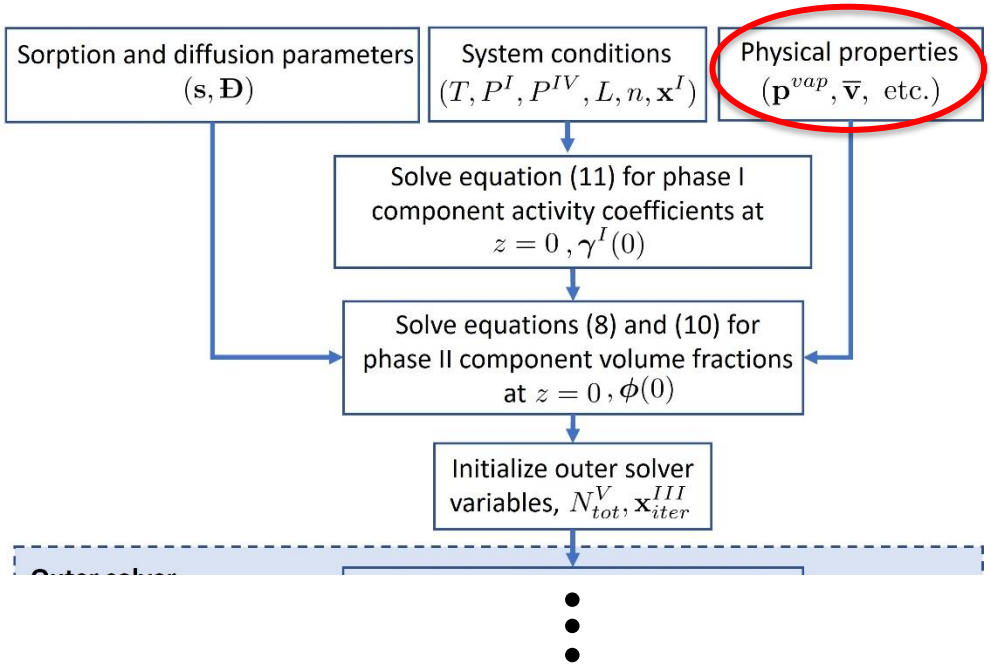
Pure component properties evaluation/lookup for all phases



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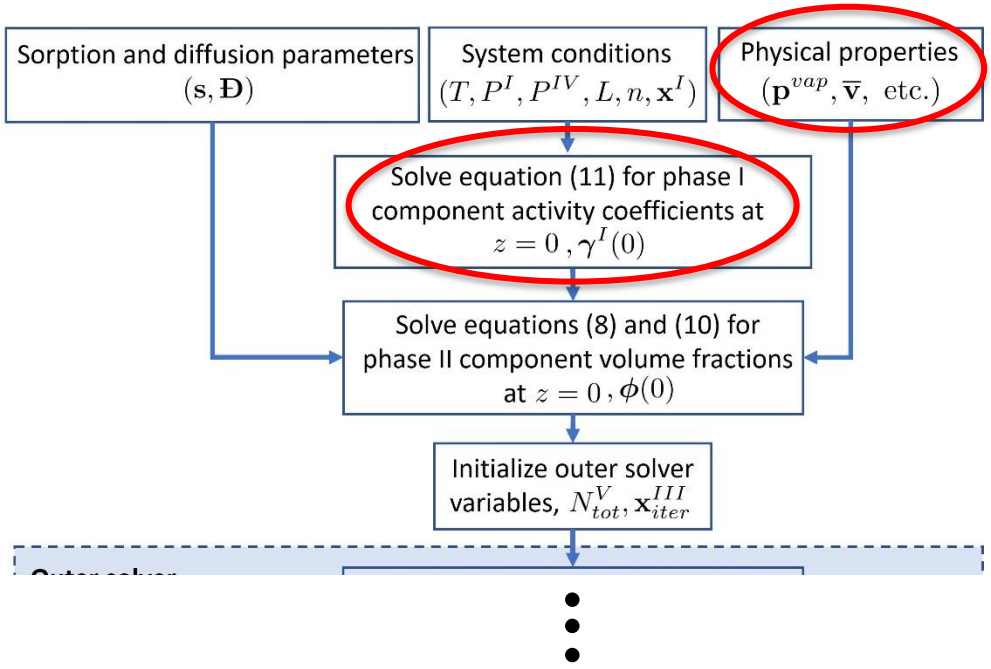

Sorption-Diffusion Step A requires evaluation of activity model for phase I

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getSinglePhaseProperty

getSinglePhaseProperty is used to retrieve single phase mixture properties.

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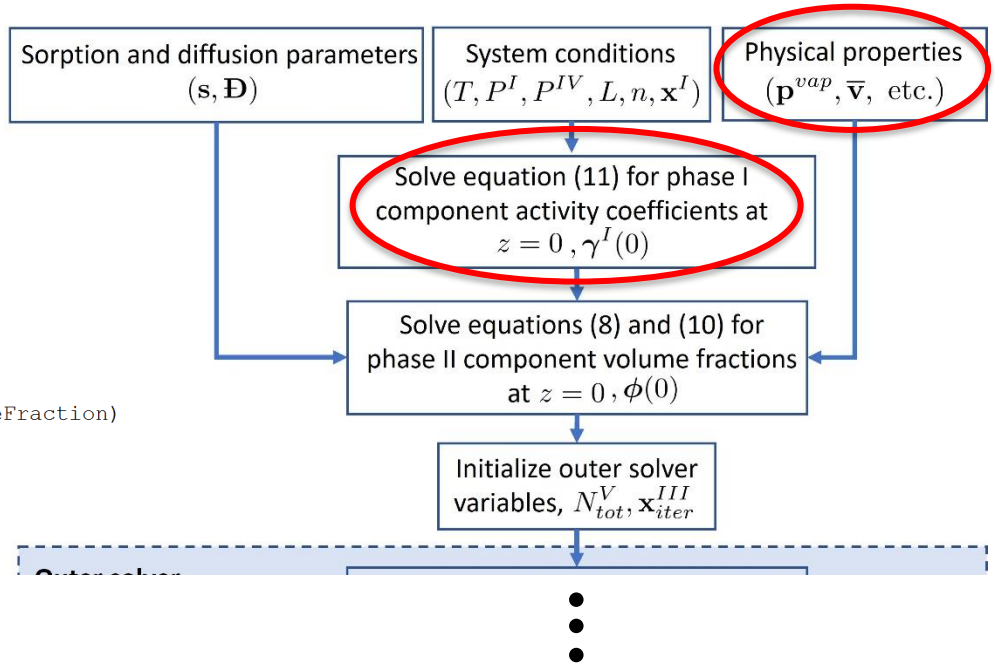

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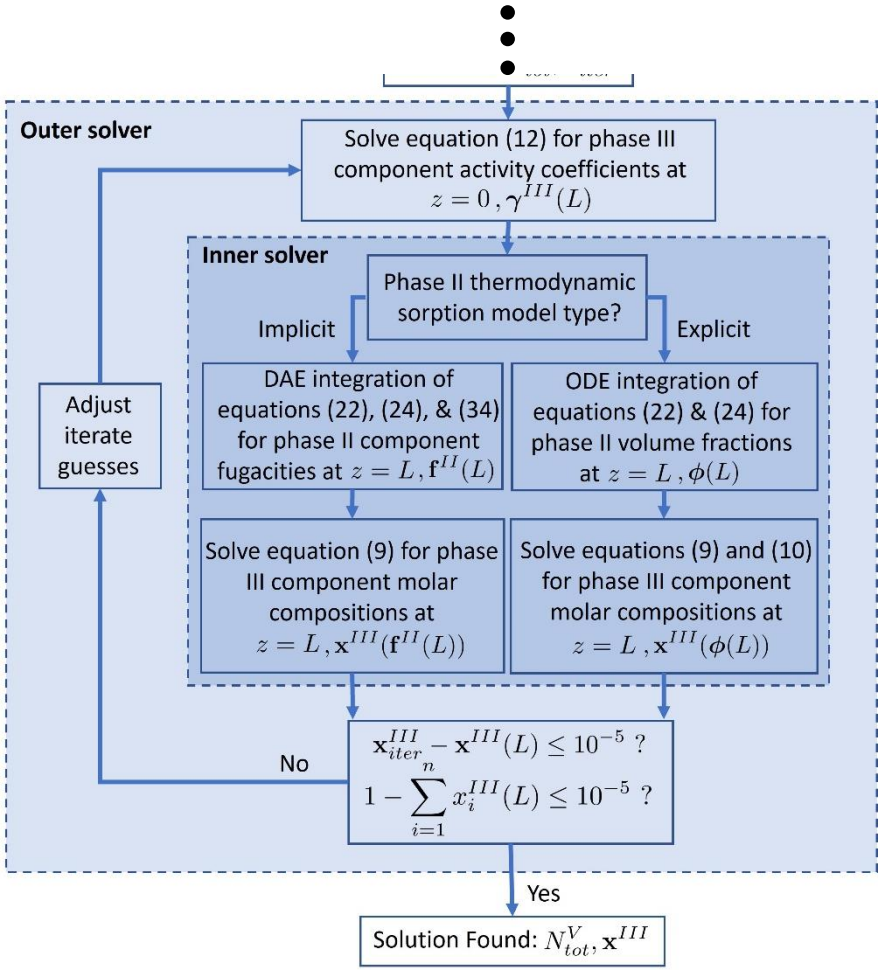

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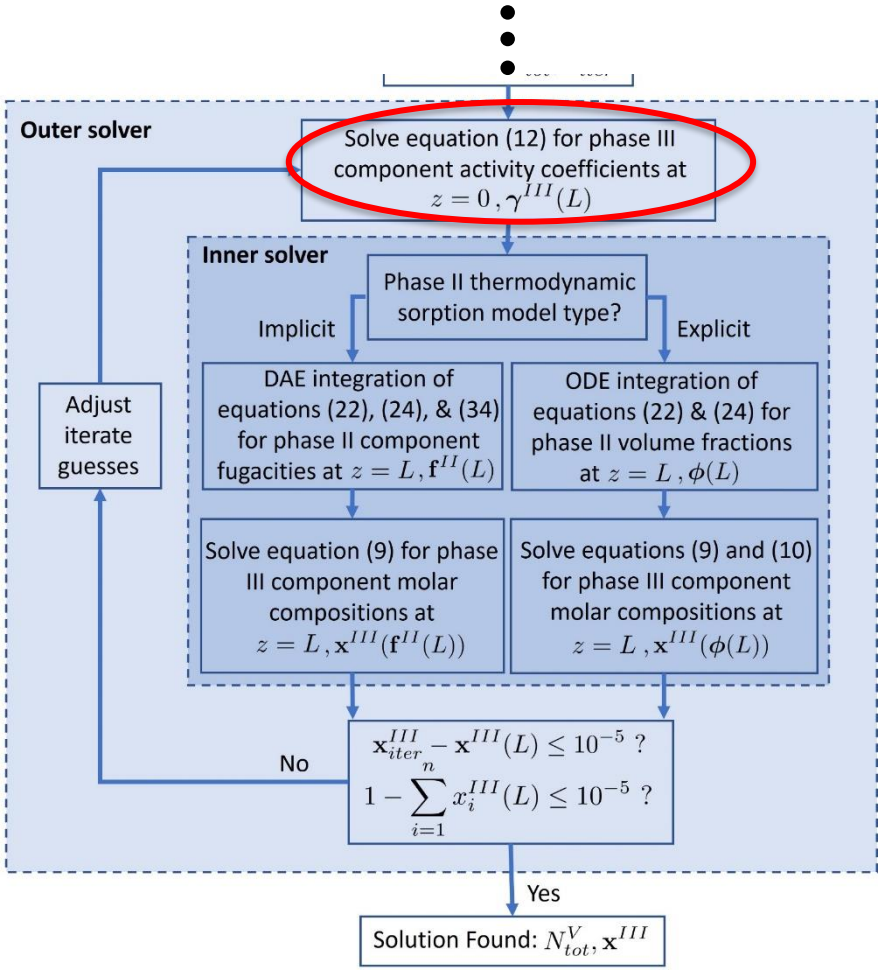

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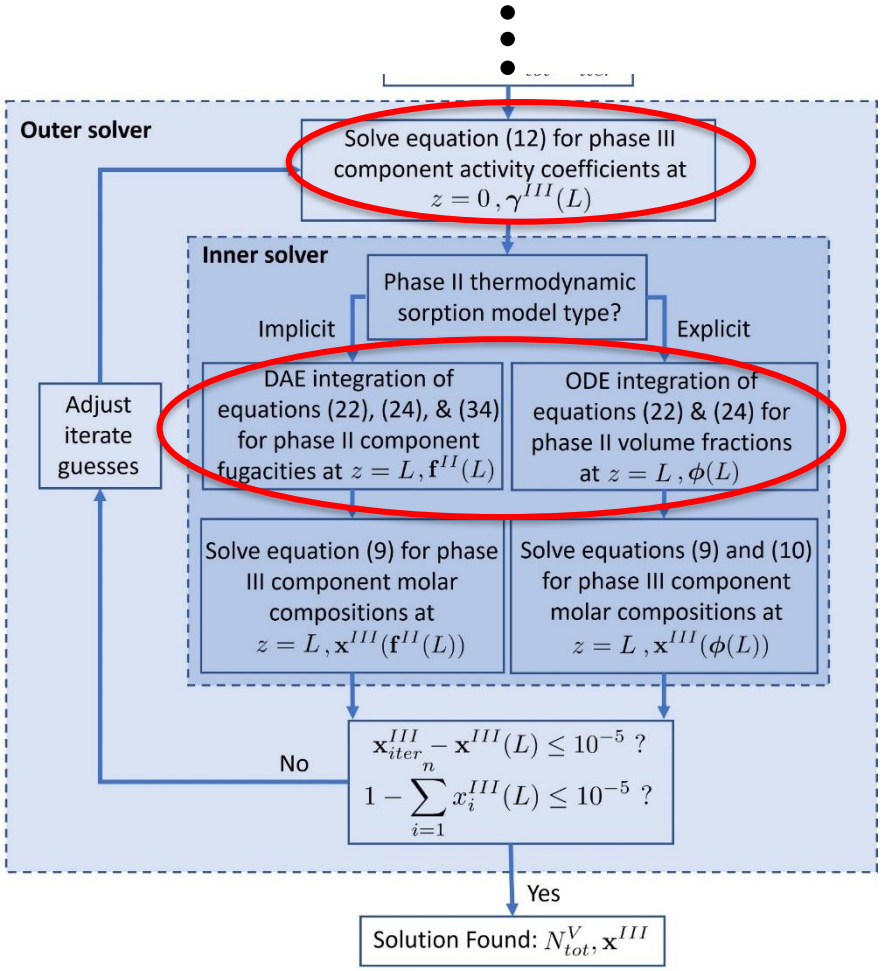
Sorption-Diffusion Step B uses pure component fugacities to evaluate phase II component activities



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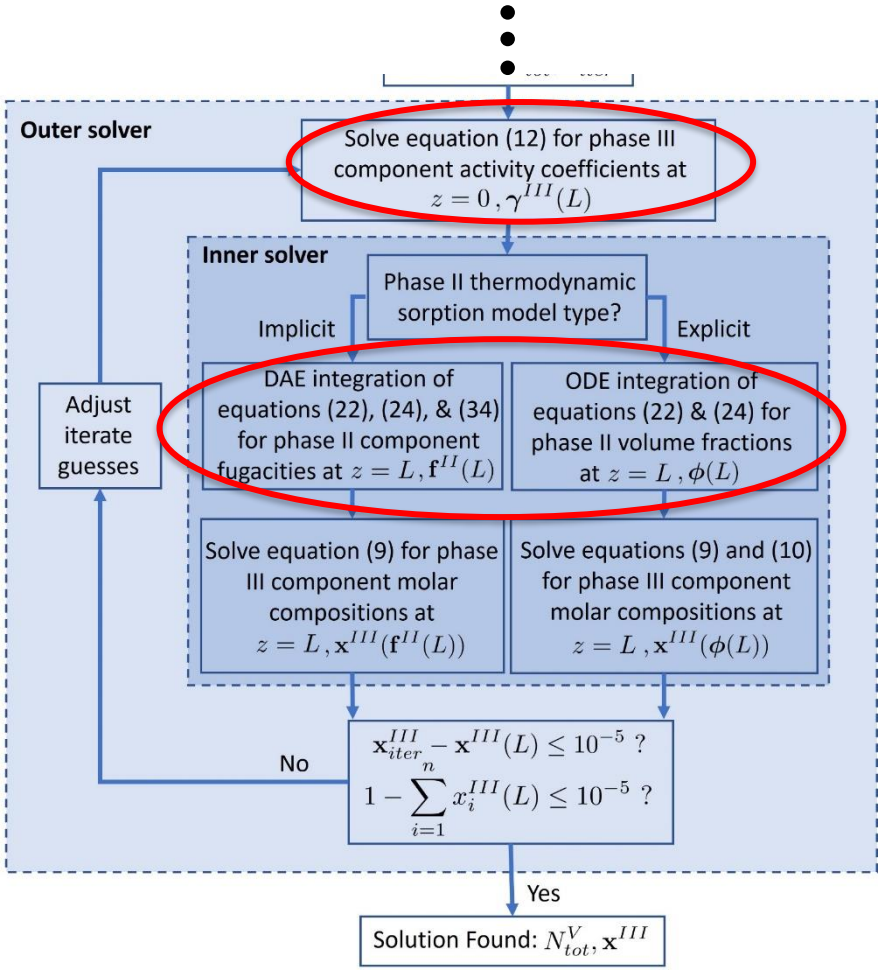

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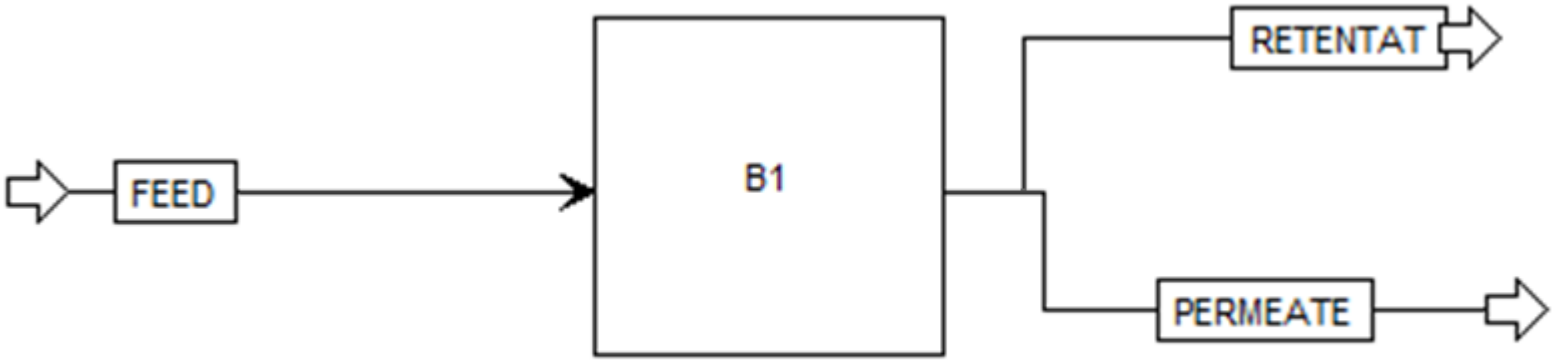

Matlab Unit Operation

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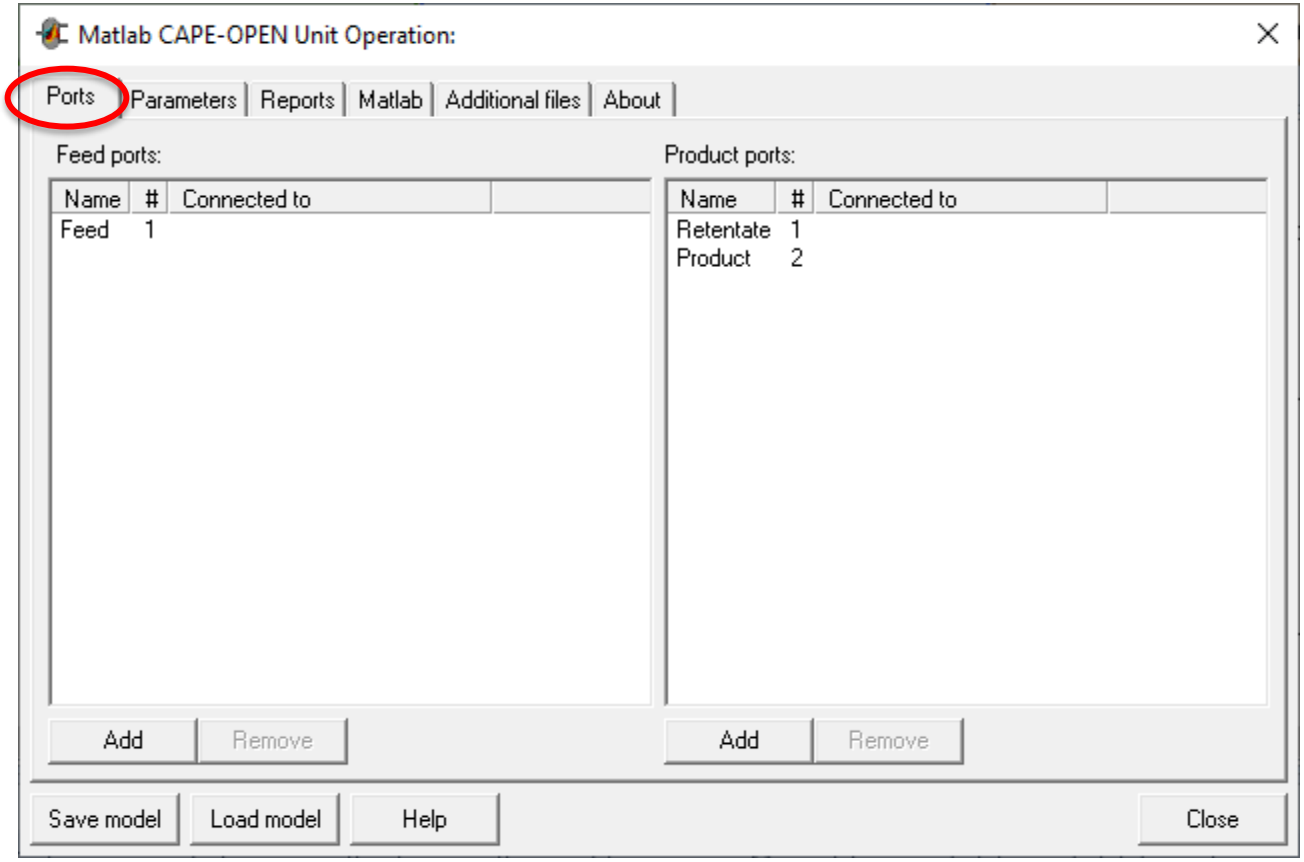

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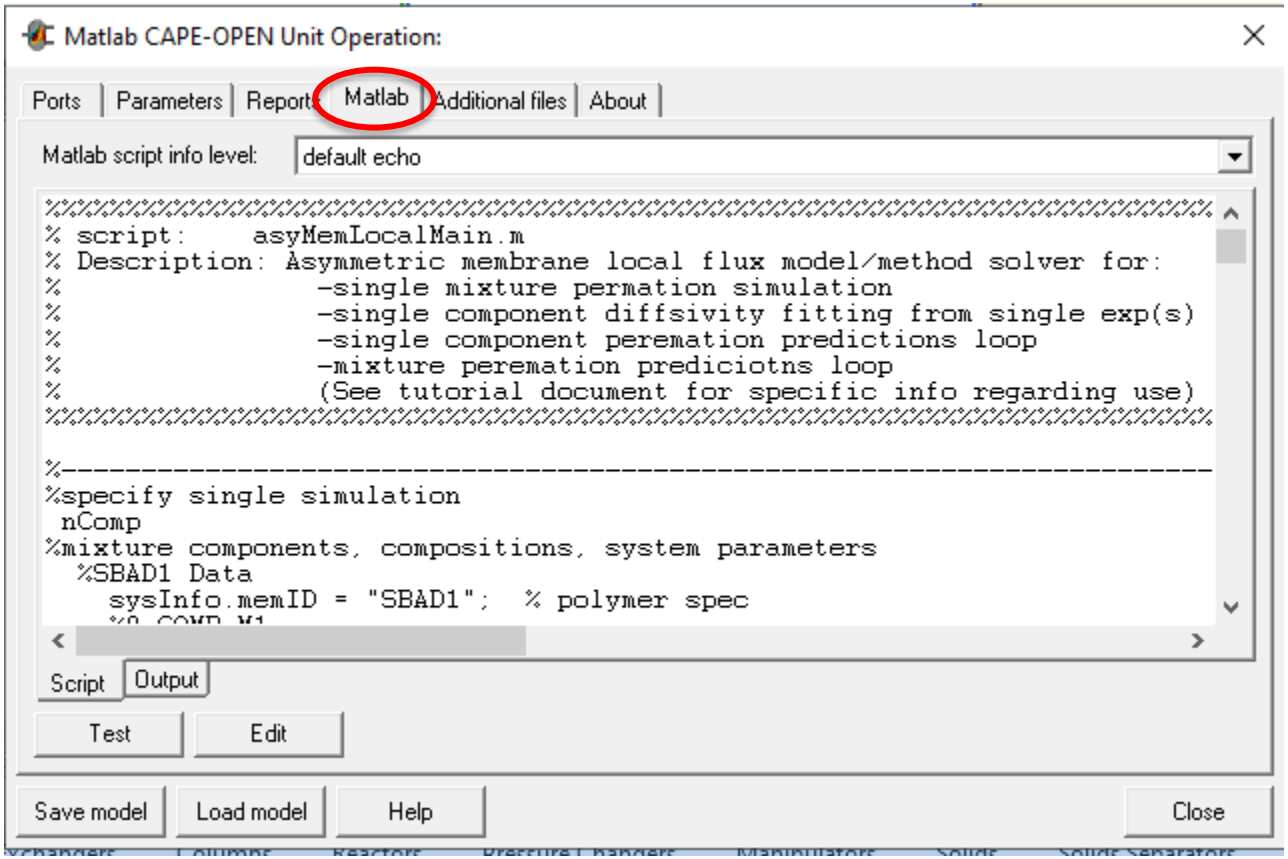

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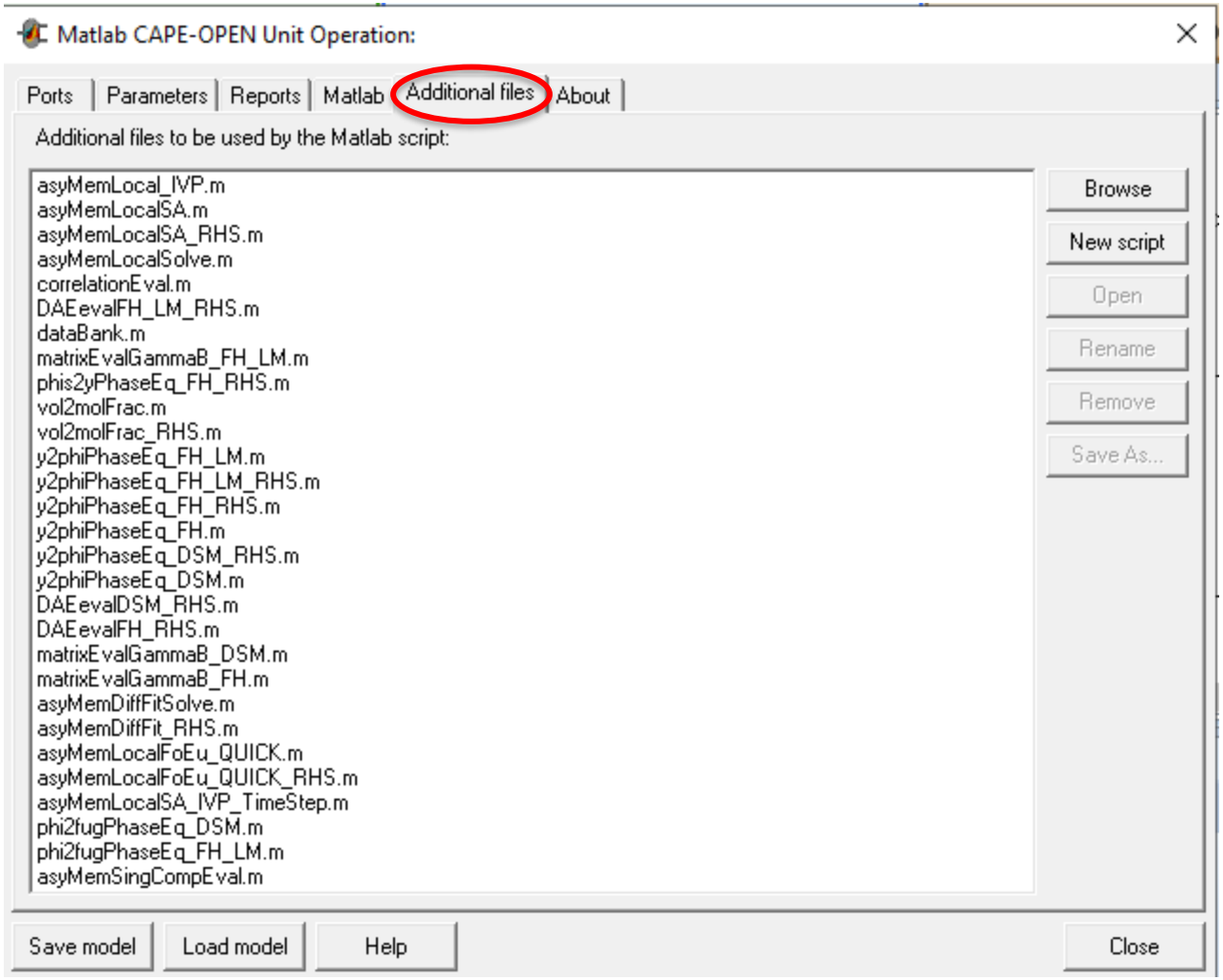

Our Implementation

Custom complex hydrocarbon mixture permeation simulation based on pure component membrane sorption and diffusion properties.

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Input mixture component, membrane and model selection

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Output all parameter matrices required for custom mixture membrane simulation

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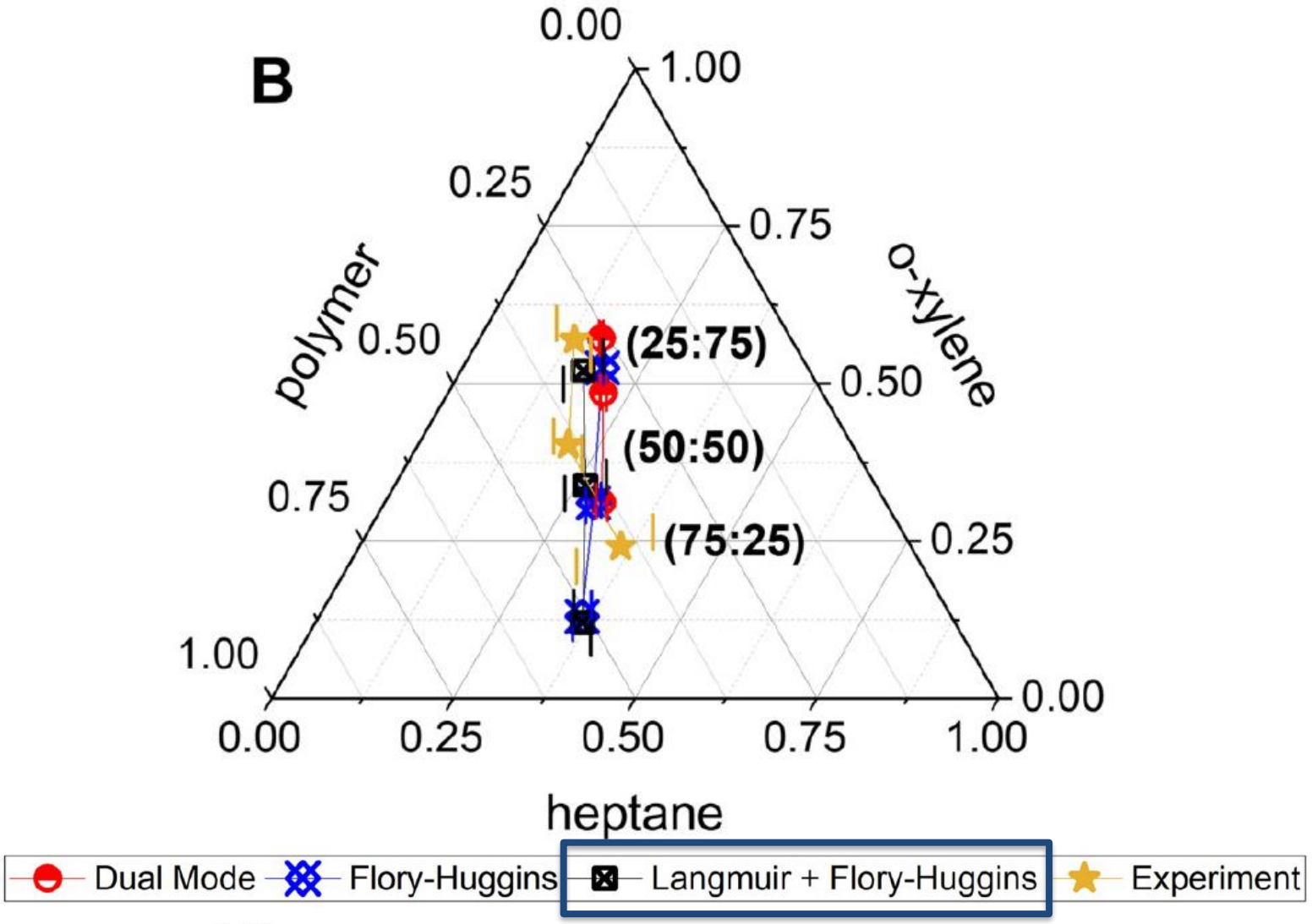
Ability to assess permeation predictions across different sorption/diffusion models and mixtures for validating what simulates a given application best[5].

- **270** mixture permeation simulations across 3 mixtures
- **330** pure component permeation simulations across 12 components
- A handful of multicomponent sorption simulations

Predictions of Complex Mixture Sorption



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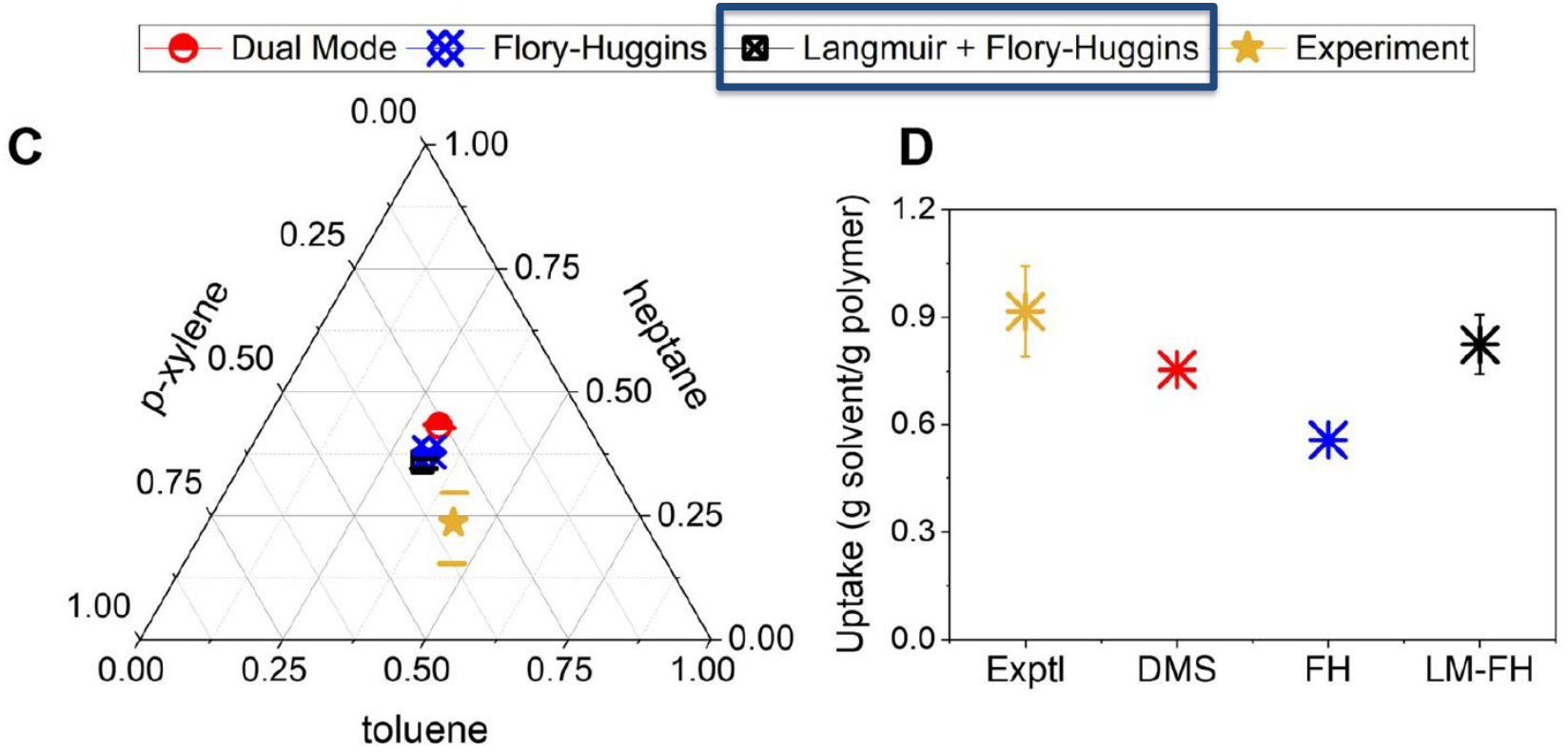

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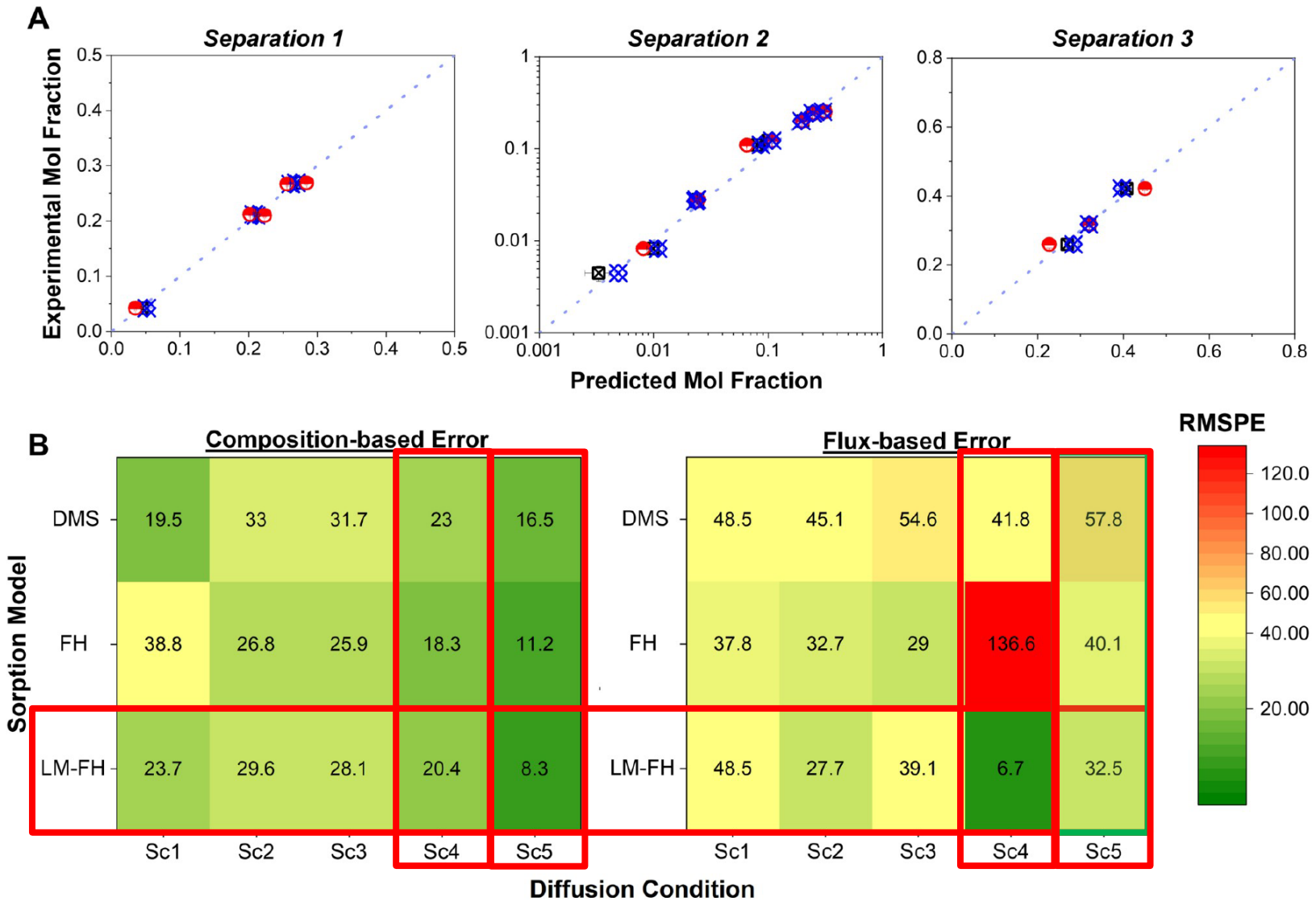
Predictions of Complex Mixture Permeation



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The only other software bug (PME or PMC) encountered was the global variable *nComp* sometimes reading 0 components when in fact there were 14 for the specific flowsheet.

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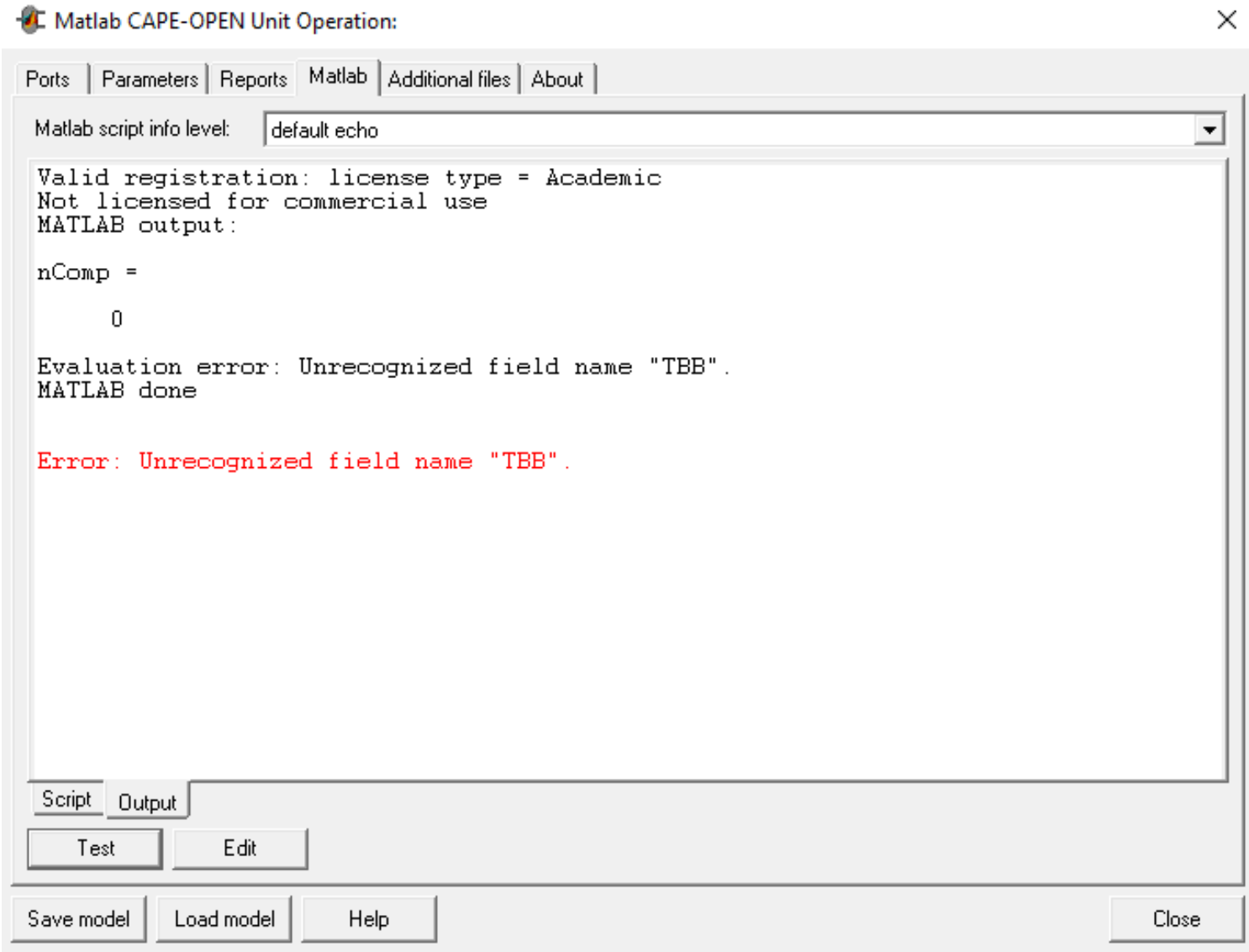

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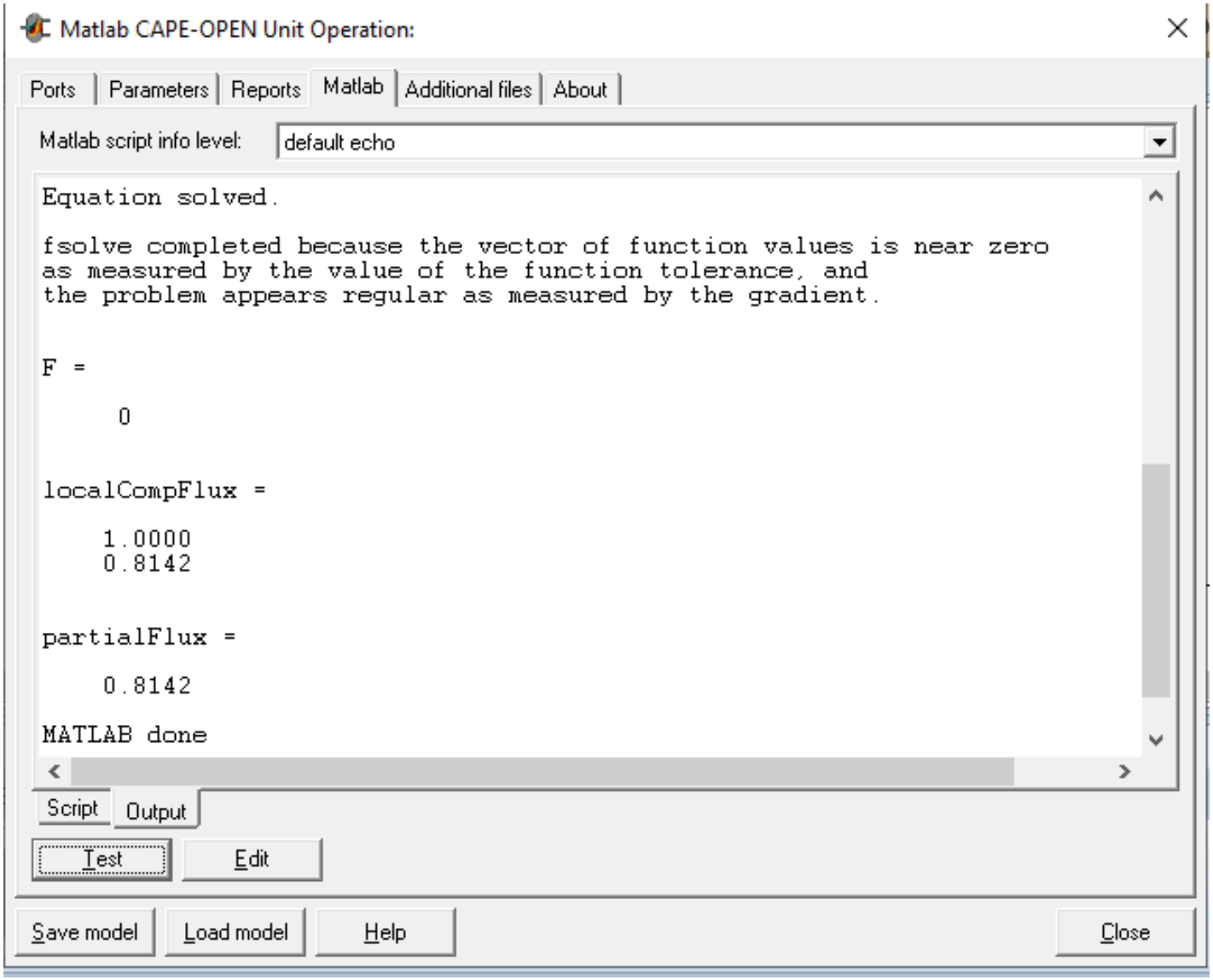

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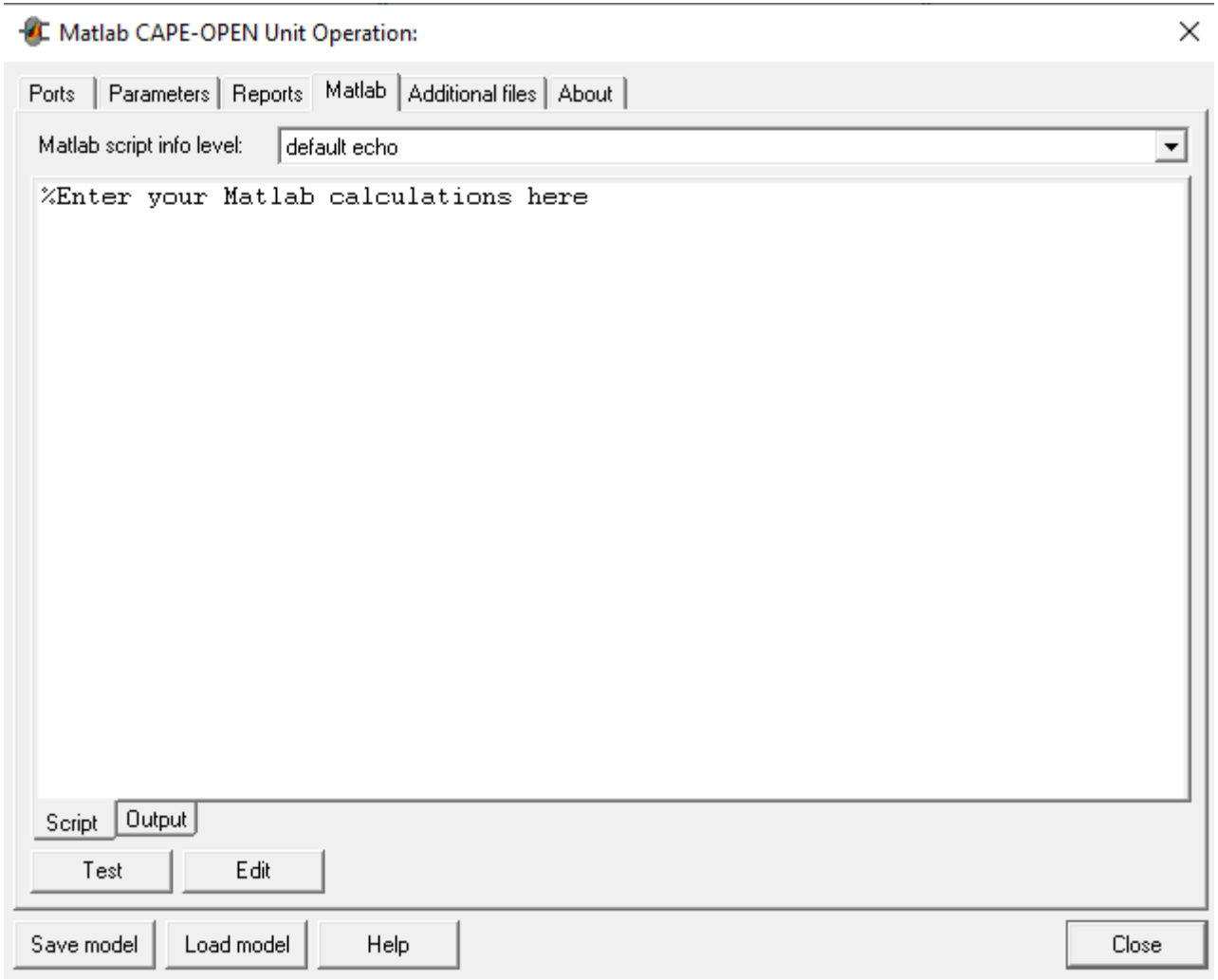

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The ability to save the MATLAB unit-op model is valuable for use between different CAPE-OPEN compliant PMEs.

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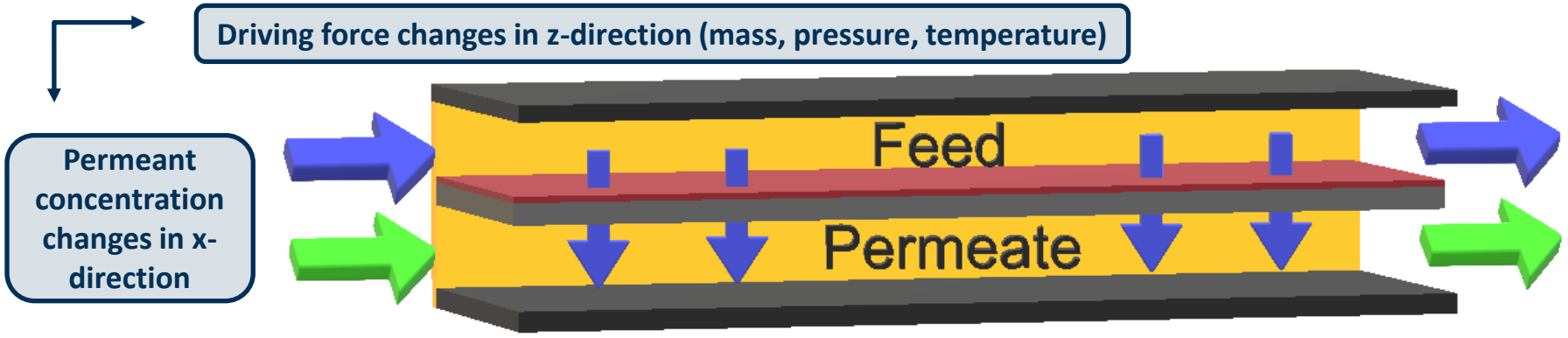

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Future work:

- Extend rigorous local membrane transport simulation to global module transport simulation and interface with overall process flowsheet
- Release our CAPE-OPEN unit-op (standalone MATLAB implementation available, please contact for .zip download)

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Academic Institutions

TEXAS TECH UNIVERSITY

Dr. Chau-Chyun Chen

Savannah River National Laboratory®
OPERATED BY SAVANNAH RIVER NUCLEAR SOLUTIONS

Dr. Maximilian B. Gorensek

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Thank you for your attention!

Questions?

Direct Contact:

Dylan Weber
Email: djweber@gatech.edu
Phone: +1.864.202.2298


Georgia
Tech

Supplemental Slides

Our Specific Application

Separation 1 via PIM-1 at a transmembrane pressure of 30 bar			
Permeate flux ($L/m^2/h$) =	6.33 ± 3.96		
	Feed Conc. mole fraction	**Permeate Conc. mole fraction**	**Permeate Conc. Error %**
Toluene	0.257	0.267	0.37
Heptane	0.216	0.210	0.95
p-xylene	0.205	0.212	0.47
o-xylene	0.264	0.269	0.74
iso-cetane	0.058	0.042	4.8

5. Mathias, R.[†],**Weber, D.[†],** Thompson, K., Marshall, B., Finn, M., Scott, J., and Lively, R. (2021). A framework for predicting the fractionation of complex liquid feeds via polymer membranes. Journal of Membrane Science, 640:119767

Our Specific Application

Separation 2 via SBAD-1 at a transmembrane pressure of 40 bar

Permeate flux ($L/m^2/h$) 0.88 ± 0.52

=

	Feed Conc. mole fraction	Permeate Conc. mole fraction	Permeate Conc. Error %
Toluene	0.171	0.201	1.5
methylcyclohexane	0.281	0.253	0.79
1-methylnaphthalene	0.020	0.028	3.6
Decalin	0.107	0.110	0.91
n-octane	0.221	0.245	2.0
iso-octane	0.150	0.123	6.5
tert-butylbenzene	0.022	0.027	3.7
1,3,5-triisopropylbenzene	0.016	8.2×10^{-3}	12
iso-cetane	0.013	4.5×10^{-3}	22

5. Mathias, R.[†], **Weber, D.[†],** Thompson, K., Marshall, B., Finn, M., Scott, J., and Lively, R. (2021). A framework for predicting the fractionation of complex liquid feeds via polymer membranes. Journal of Membrane Science, 640:119767

Our Specific Application

Separation 3 via SBAD-1 at a transmembrane pressure of 30 bar

Permeate flux ($L/m^2/h$) = 0.40 ± 0.12

	Feed Conc. mole fraction	Permeate Conc. mole fraction	Permeate Conc. Error %
Toluene	0.284	0.318	1.9
iso-octane	0.388	0.422	1.4
iso-cetane	0.328	0.260	4.2

5. Mathias, R.[†], **Weber, D.[†],** Thompson, K., Marshall, B., Finn, M., Scott, J., and Lively, R. (2021). A framework for predicting the fractionation of complex liquid feeds via polymer membranes. Journal of Membrane Science, 640:119767

Ideal Solution vs. Real Mixture Predictions

Comparing ideal solution (IS) and real mixture (RM) predictions for the most complex 9 component permeation simulation:

RM

Full MS, no diff coupling, Vignes avg FH-LM	
Molar Comp	Partial Flux (LMH)
0.1995	0.1708
0.3158	0.3252
0.0239	0.0269
0.0789	0.0995
0.2469	0.3243
0.0977	0.1299
0.0227	0.0284
0.0103	0.0198
0.0043	0.0102
1.1350	Total Flux (LMH)

TOL
MCH
MNP
DEC
NOC
IOC
TBB
TIPB
ICE

IS

Full MS, no diff coupling, Vignes avg FH-LM	
Molar Comp	Partial Flux (LMH)
0.2002	0.1700
0.3136	0.3203
0.0242	0.0270
0.0804	0.1006
0.2457	0.3201
0.0995	0.1313
0.0231	0.0287
0.0099	0.0190
0.0033	0.0078
1.1249	Total Flux (LMH)

All mixture composition and total flux predictions get marginally better (~3%)

Ideal Solution vs. Real Mixture Predictions

After looking into the details, the feed and permeate activity coefficients are almost identical and this acts to "cancel out" the nonideality on both sides.

Feed-side (phase I) activity coefficients		Permeate-side (phase III) activity coefficients
1.4445	TOL	1.4413
1.0969	MCH	1.1111
2.1656	MNP	2.0411
1.0138	DEC	0.991
0.9678	NOC	0.969
1.1228	IOC	1.1317
1.0836	TBB	1.051
0.9311	TIPB	0.9001
0.7949	ICE	0.7895

After arbitrarily setting the activity coefficients for phase III to be different, IS vs RM predictions were vastly different (50-100%). Generally, the use of real mixture predictions is needed.

Process Flowsheet Modeling and Membrane Unit-Ops

The advantages of including industrial membrane unit operation models within overall process flowsheet simulations include[7]:

7. Kancherla, R., Nazia, S., Kalyani, S., and Sridhar, S. (2021). Modeling and simulation for design and analysis of membrane-based separation processes. Computers Chemical Engineering, 148:107258.

Process Flowsheet Modeling and Membrane Unit-Ops

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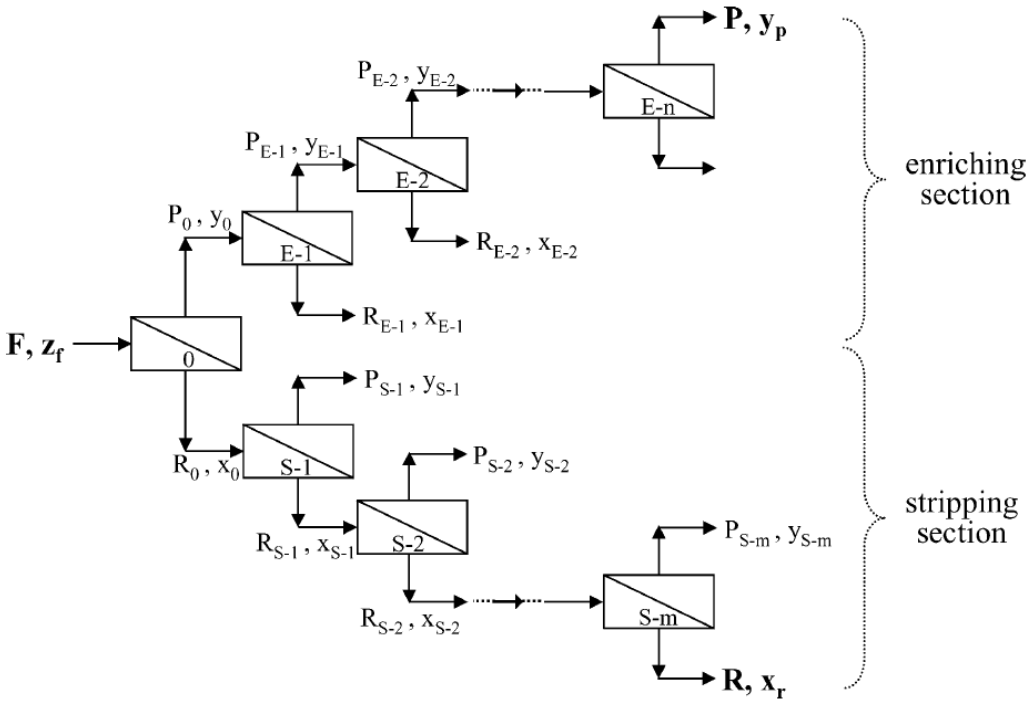
- Test membrane cascades in series or parallel arrangements with (or without) recycle loops



8. Avgidou, M. et. al. (2004). DOI:10.1016/j.memsci.2003.12.007

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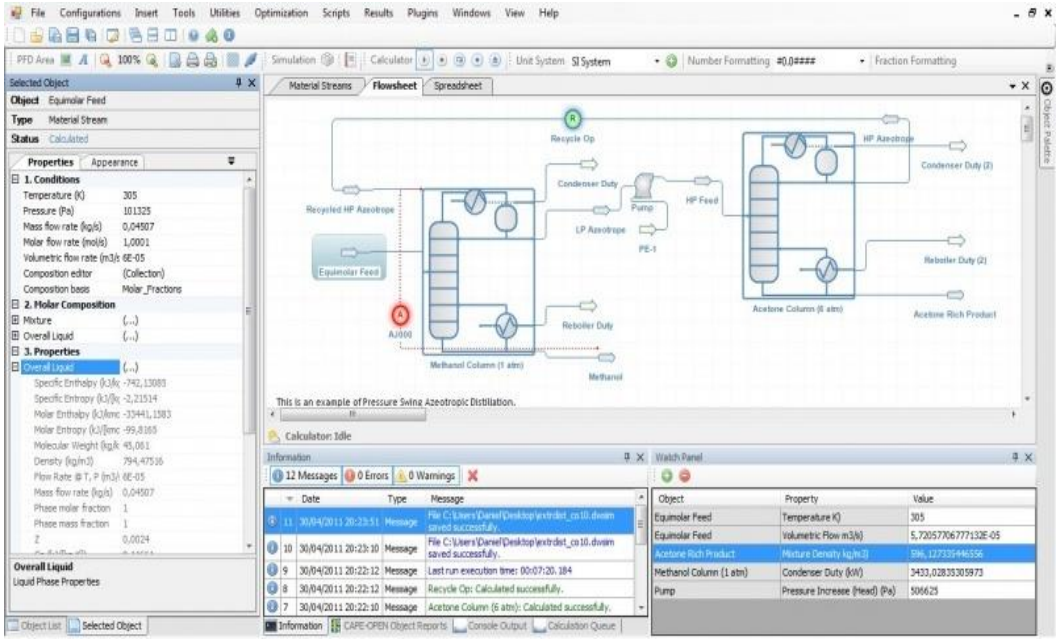

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- Use powerful thermodynamic models and component property databases
- Predict process sustainability and techno-economic (TEA) competitiveness versus energy intensive separation methods

Process Flowsheet Modeling and Membrane Unit-Ops

Realistically, this work will be a step forward towards widespread industrial adoption of membrane processes involving complex mixtures