Science-Based Design of Experiments and Pyomo.DoE

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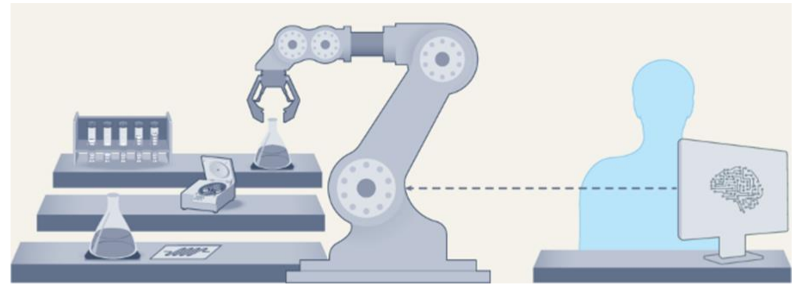
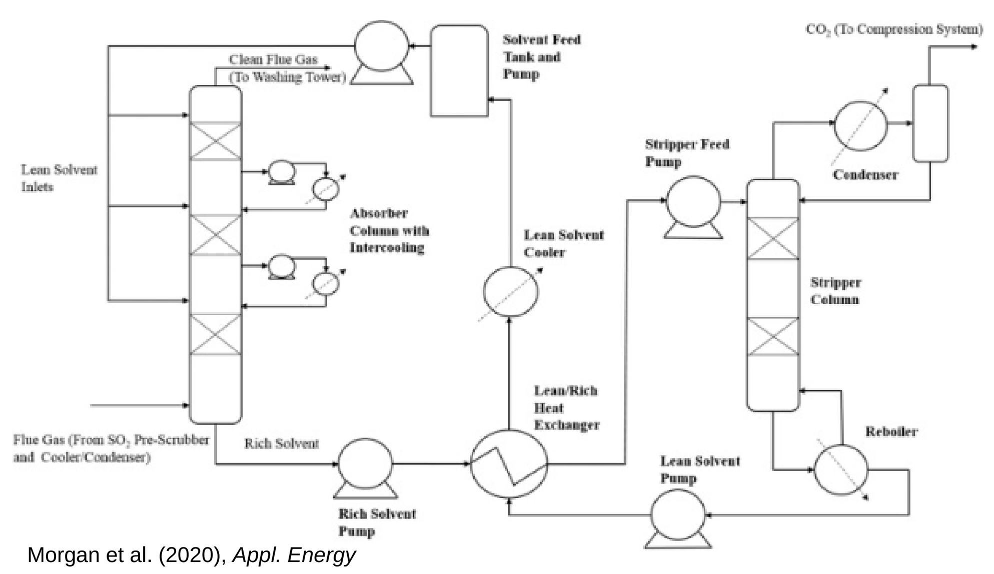
Advances in Design of Experiments[1,2,3]



Abolhasani & Kumacheva (2023), *Nature Syn*

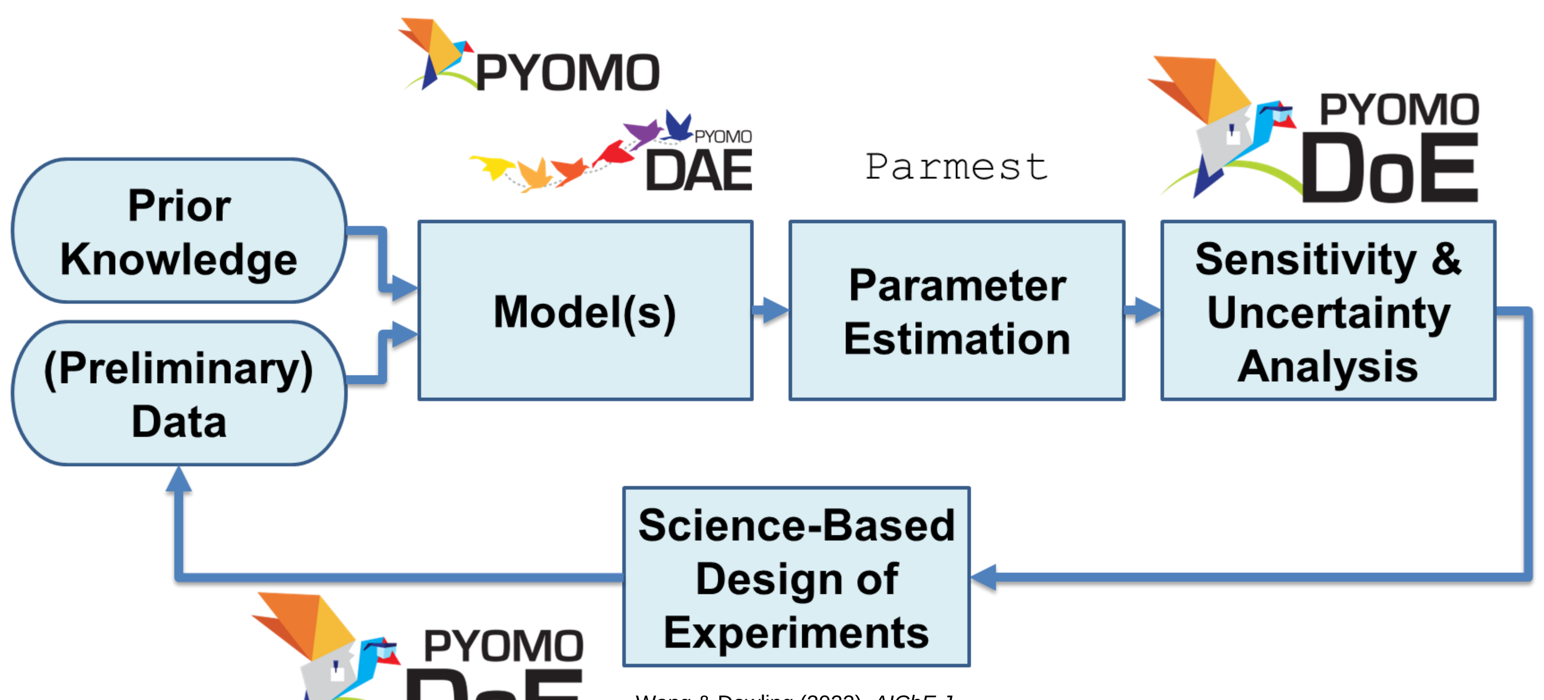
Self-driving laboratories select the next best experimental conditions for maximizing material properties information.

Scaling up CO_2 capture technologies with sequential design of experiments framework reduces model uncertainty.



Morgan et al. (2020), *Appl. Energy*

Science-Based Modeling Workflow[4,5]



Wang & Dowling (2022), *AIChE J.*

What are the most informative data to reduce uncertainty (θ) and derisk technology optimization and scale-up?

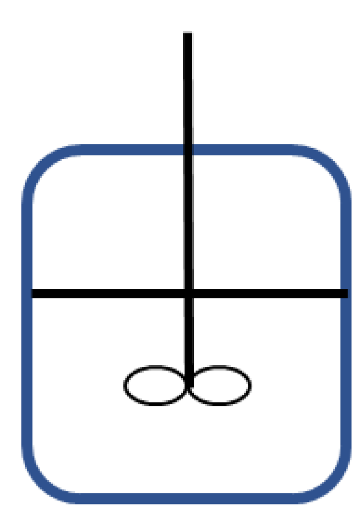
Assumptions and Motivating Example

$$y_i = f(x_i, \theta) + \epsilon_i$$

Model Outputs — Mathematical Model — Decisions — Uncertain Parameters — Error

$$\epsilon \sim \mathcal{N}(0, \Sigma_\epsilon)$$

Error is normally distributed with a multivariate standard deviation Σ_ϵ

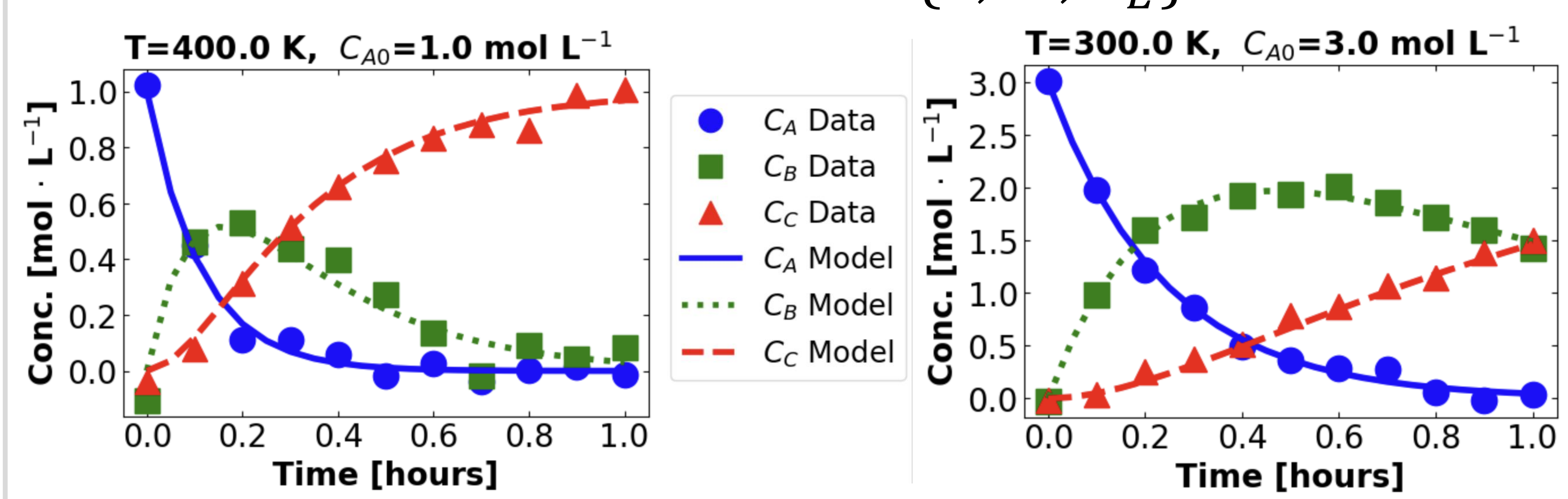


$$\mathrm{A} \xrightarrow{k_1} \mathrm{B} \xrightarrow{k_2} \mathrm{C}$$

Parameter Estimation

Given experimental data (x_i, y_i), how do we find the best fit parameters $\hat{\theta}$ in our mathematical model?

$$\hat{\theta} = \underset{\underline{\theta} \le \theta \le \overline{\theta}}{\mathrm{argmin}}\ \Psi \equiv \sum_{i=1}^{N_E} (f(x_i, \theta) - y_i)^T W_i (f(x_i, \theta) - y_i) \quad \forall i \in \{1, \dots, N_E\}$$



Science-Based Design of Experiments (SBDoE)[4,5]

How do we sequentially choose the experimental conditions (φ) that will maximize information gain?

SBDoE Optimization Problem

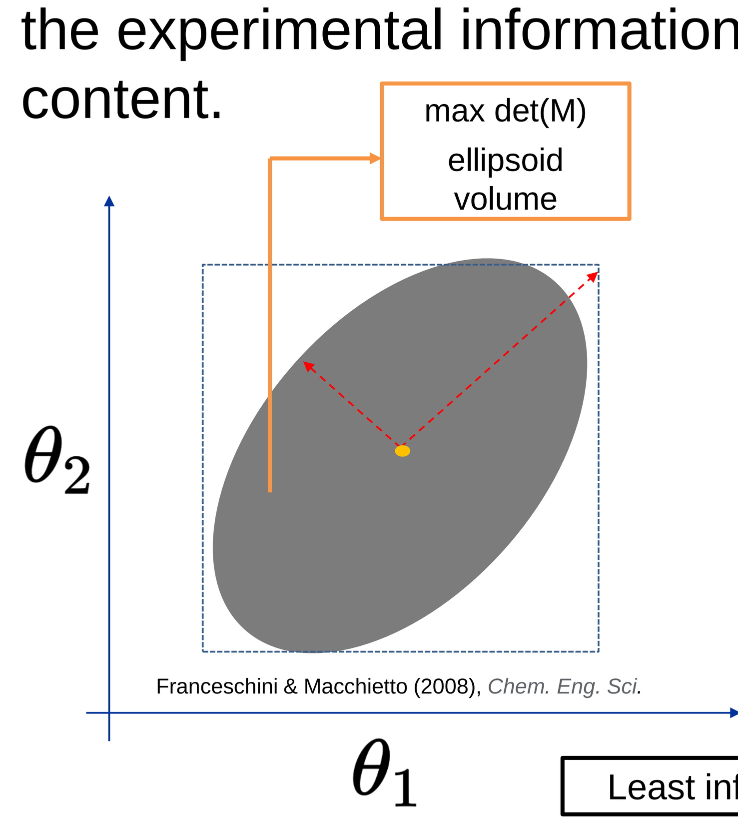
$$\underset{\varphi}{\mathrm{argmax}}\ M(\hat{\theta}, \varphi)$$

$$\text{s.t.} \quad M = Q^T \Sigma_\epsilon Q$$

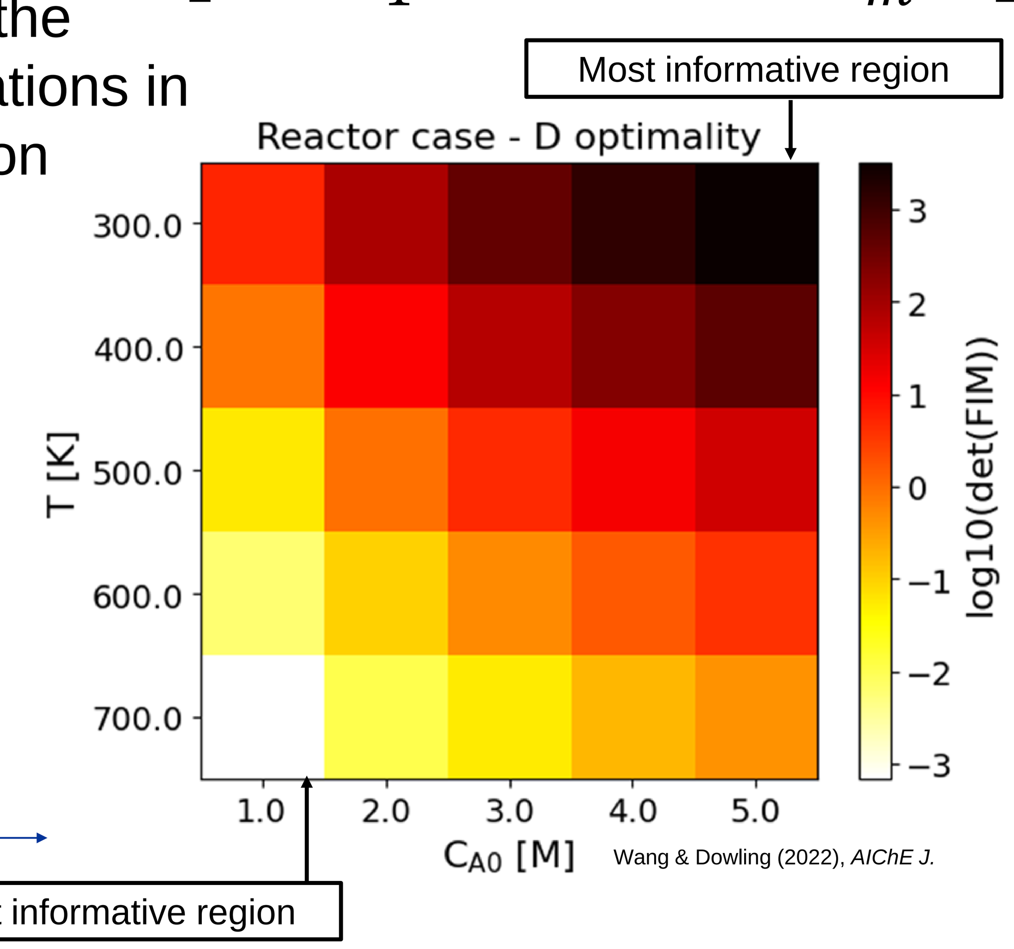
Sensitivity Matrix

$$Q(\theta) = \begin{bmatrix} \frac{\partial f(x_1, \theta)}{\partial \theta_1} & \cdots & \frac{\partial f(x_1, \theta)}{\partial \theta_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(x_n, \theta)}{\partial \theta_1} & \cdots & \frac{\partial f(x_n, \theta)}{\partial \theta_m} \end{bmatrix}$$

Heatmaps show the most informative parameters of the optimal solution from deviations in the experimental information content.

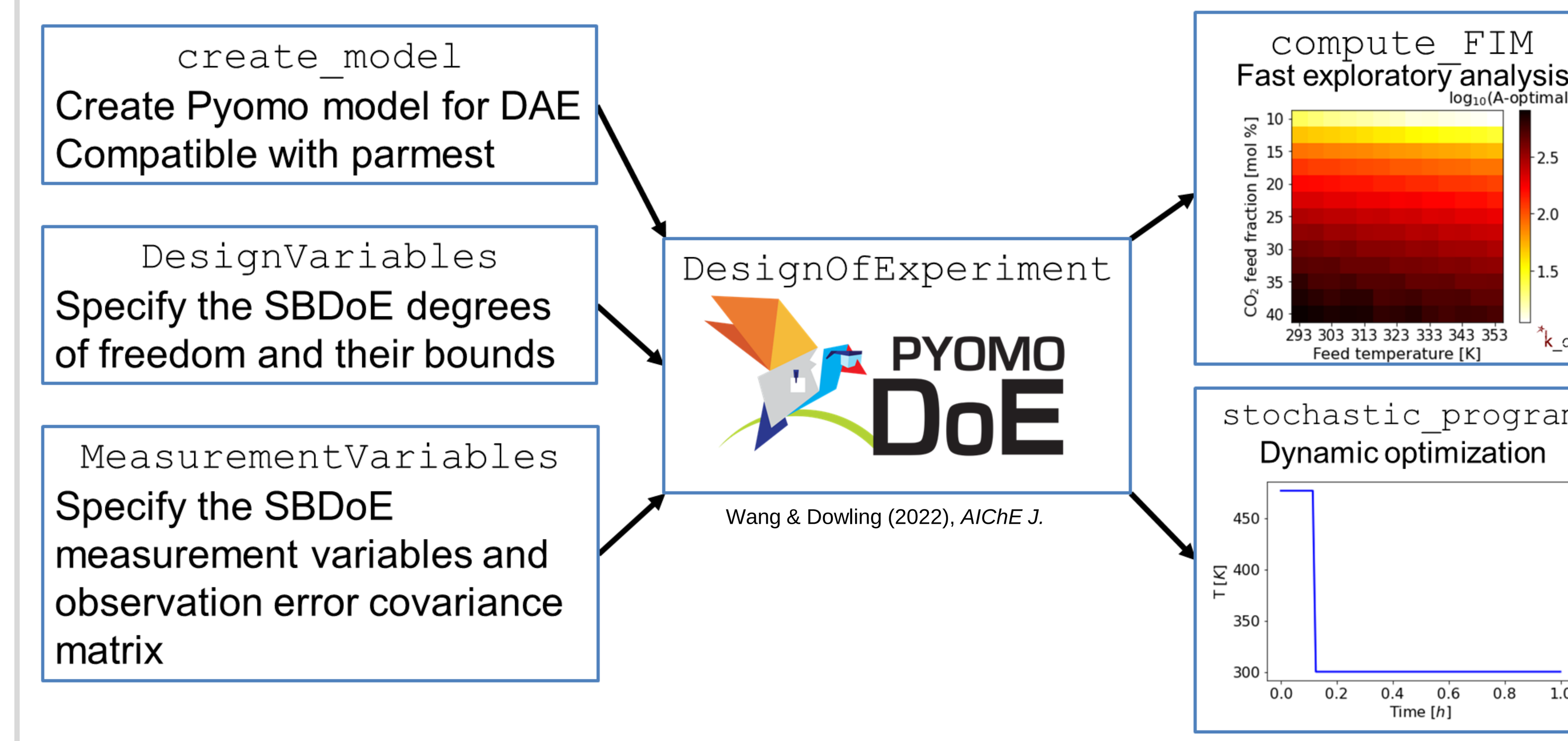


Franceschini & Macchietto (2008), *Chem. Eng. Sci.*



Wang & Dowling (2022), *AIChE J.*

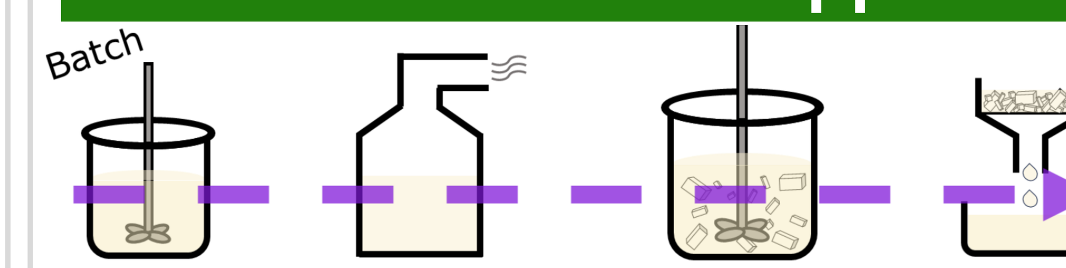
Pyomo.DoE Interface[4]



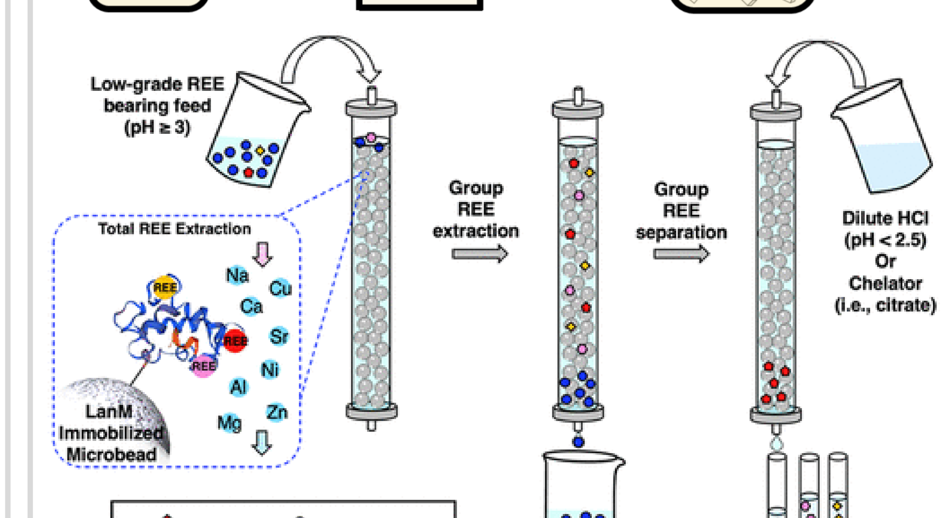
Wang & Dowling (2022), *AIChE J.*

Pyomo.DoE supports SBDoE for parameter precision which reduces uncertainty and leads to faster and derisked decision-making.

PrOMMiS Opportunities[6]



Integrated SBDoE framework for batch crystallization.



Dong et al. (2021), *ACS Cent. Sci*

Dynamic membrane modeling calibration using SBDoE for critical materials and rare earth elements.

Acknowledgements

This effort was funded by the U.S. Department of Energy's Process Optimization and Modeling for Minerals Sustainability (PrOMMiS) Initiative, supported by the Office of Fossil Energy and Carbon Management's Office of Resource Sustainability.

For more information, please reach out to Thomas Tarka, PrOMMiS Technical Director (Thomas.Tarka@netl.doe.gov)

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[1] Abolhasani, Milad, and Eugenia Kumacheva, Nature Synthesis (2023): 1-10.
[2] Langner, Stefan, et al. Advanced Materials 32, no. 14 (2020): 1907801.
[3] Morgan, Joshua C., et al. Applied Energy 262 (2020): 114533.
[4] Wang, Jialu, and Alexander W. Dowling. AIChE Journal (2022): e17813.
[5] Franceschini, Gaia, and Sandro Macchietto. Chemical Engineering Science 63, no. 19 (2008): 4846-4872.
[6] Dong, Ziye, et al. *ACS Central Science* 7.11 (2021): 1798-1808.