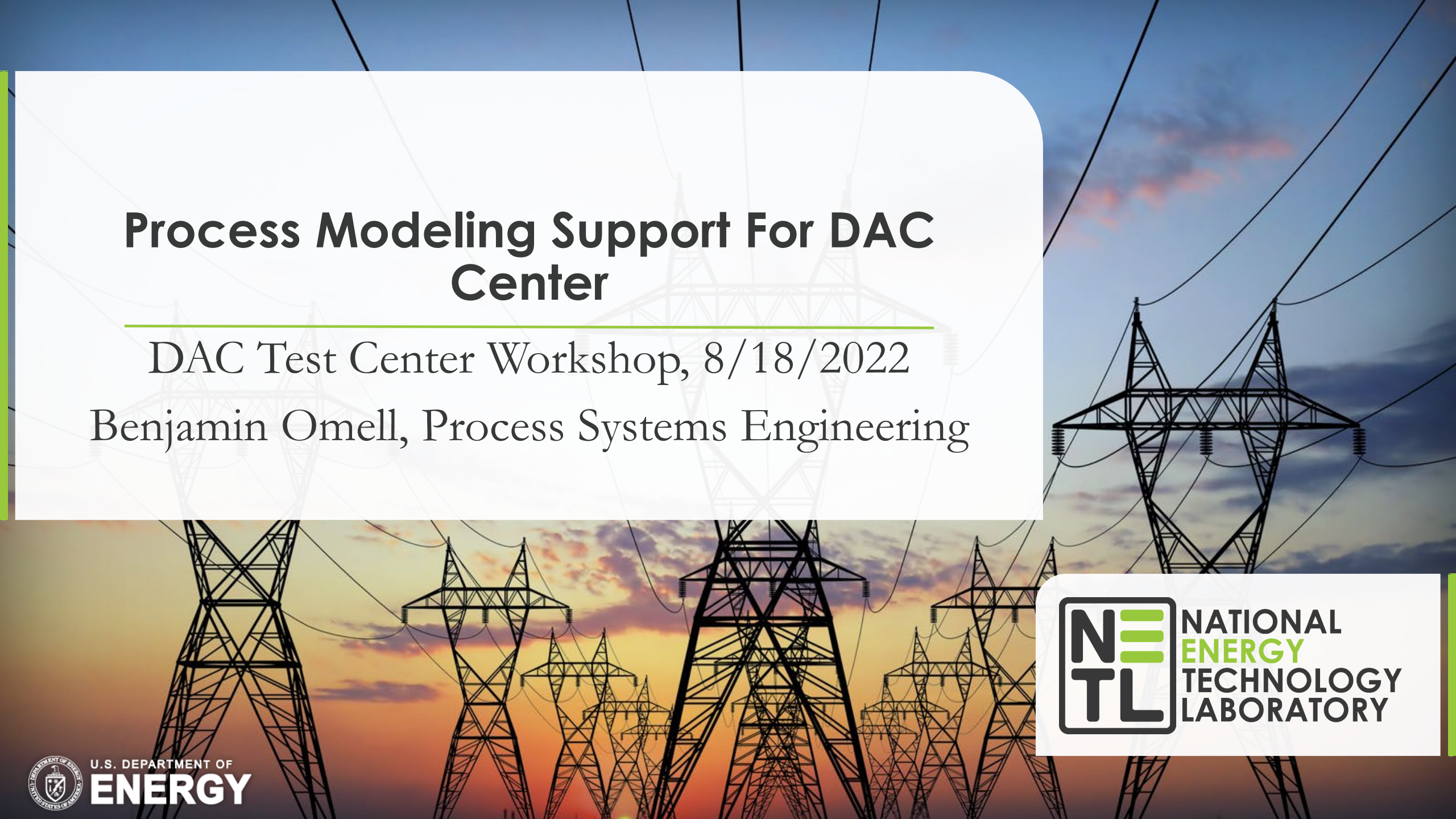
Process Modeling Support For DAC Center

DAC Test Center Workshop, 8/18/2022

Benjamin Omell, Process Systems Engineering



U.S. DEPARTMENT OF ENERGY

NATIONAL ENERGY TECHNOLOGY LABORATORY

Process Modeling Support For DAC Center

Using advanced modeling tools to drive material development for optimal process performance

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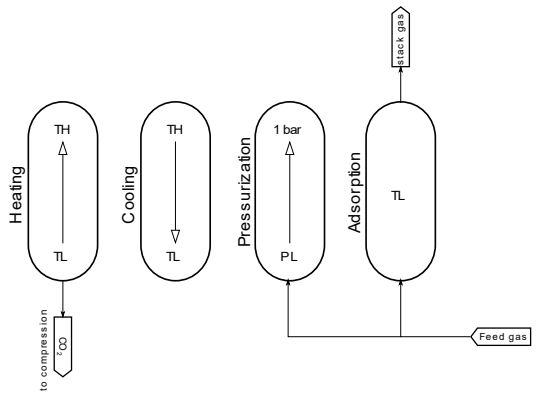
- Develop and apply rigorous models to predict DAC performance and cost
- Understand impacts of uncertainty on Key Performance Indicators (KPIs)
- Guide collection of additional data to further reduce uncertainty and reduce technical risk in scale-up
- Refinement of models through optimal design of experiments

Advanced Modeling tools

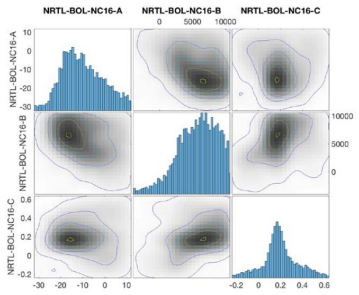
CCSI² Carbon Capture Simulation for Industry Impact

IDAES Institute for the Design of Advanced Energy Systems

Process Modeling

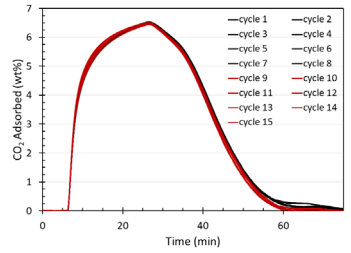


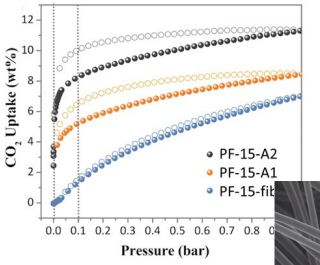
Uncertainty Quantification

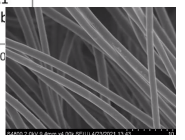


Impact on KPIs

Improved Data Collection







NETL Process Systems Engineering Capabilities

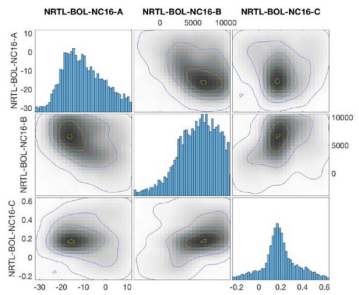
Advanced Process Modeling Tools to enhance data collection, estimate and optimize Performance

CCSI² Carbon Capture Simulation for Industry Impact

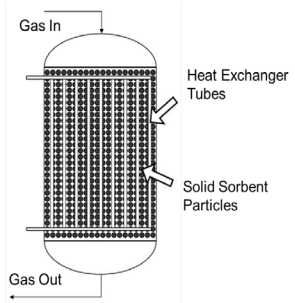
2016 R&D 100 WINNER

IDAES Institute for the Design of Advanced Energy Systems

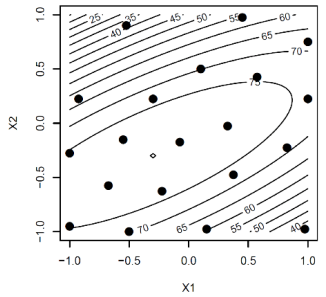
Uncertainty Quantification



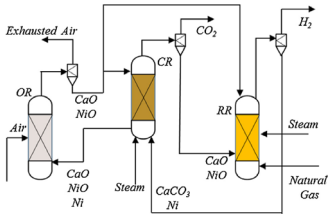
Solid-Gas Contactor models



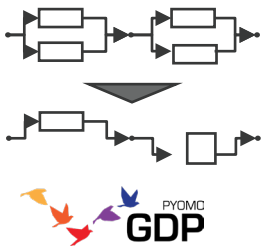
Optimal Design of Experiments



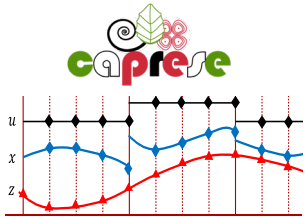
Plant Design Process Optimization



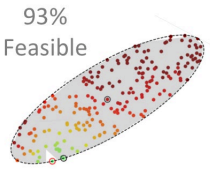
Conceptual Design



Process Operations Dynamics & Control

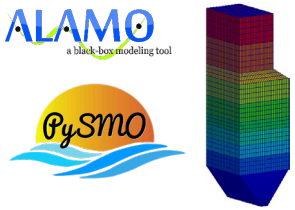


Robust Optimization



PyROS

AI/ML Surrogate Modeling



Open Source: https://github.com/CCSI-Toolset

https://github.com/IDAES/idaes-pse*

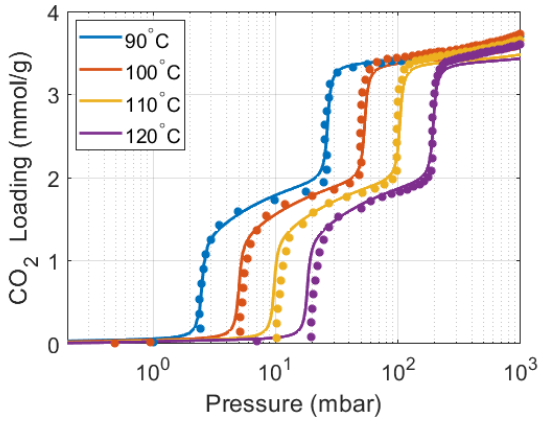
*Lee, et al., *J. of Adv. Manufacturing and Processing* (2021)

Sorbent Models

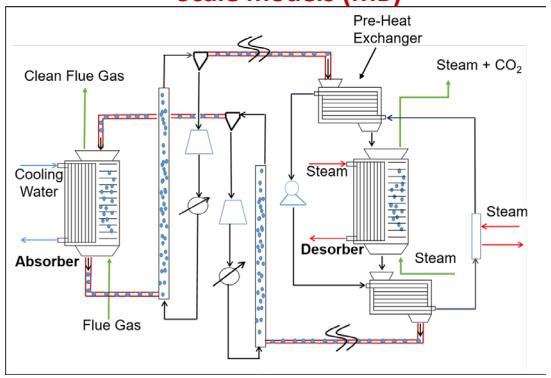
First principal solid-gas contactor models

- **Library of first principle solid –gas contactors**
  - Fixed beds, moving beds, bubbling fluidized beds, rotating packed beds, etc.
  - Support numerous technologies in the capture and DAC space
- **Application in numerous modeling platforms**
  - Aspen, ACM, Python
  - Support for advanced process modeling platforms and optimization
  - Exploration of important inputs
  - Tools for quantification of uncertainty

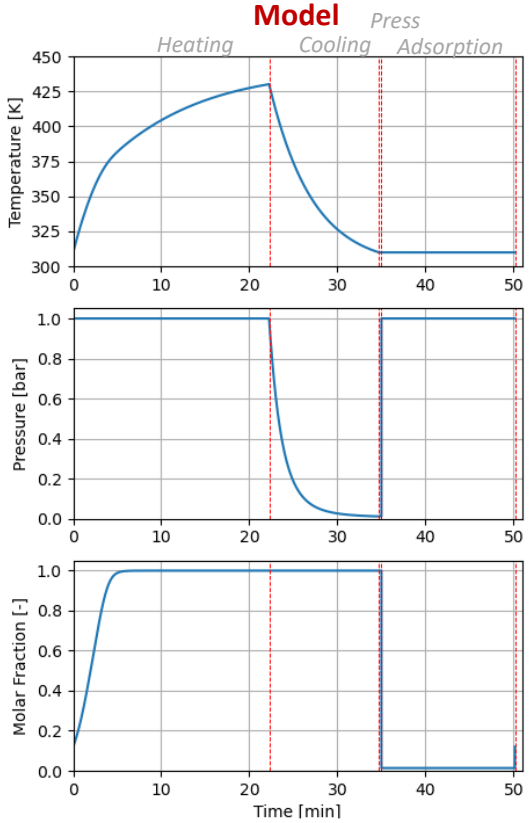
Development of Novel Property Models (Two-step Isotherm of tetraamine-appended MOF[1])



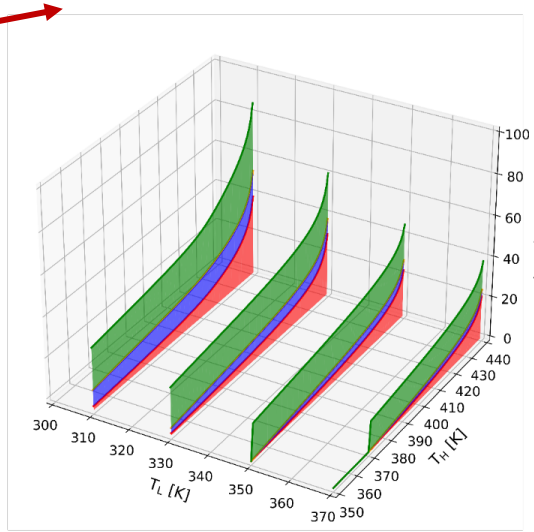
Applications into Process Scale models (MB)



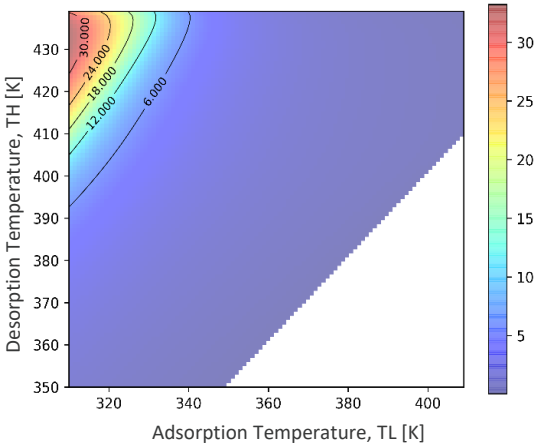
IDAES 0D Screening Model



Effect of T_{ads} and T_{des} on Cycle Times



Productivity [kg CO2/(ton · h)]



1 Kim, E. J., *et al*. *Science* 2020, No. 369, 392–396

Uncertainty Quantification

Quantifying risk for scale-up

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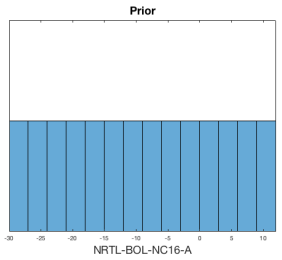
MATERIAL

- **Tools to develop understanding of impacts of uncertain models and data gaps**
- **Provides a "criteria" for experimental testing**
- **Can provide insight into "value" data collection in almost real-time**

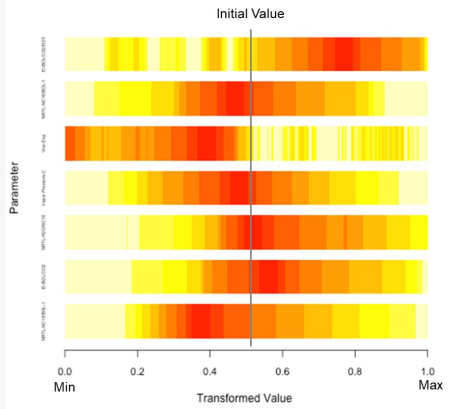
Initial Parameter Range



Gather New Data

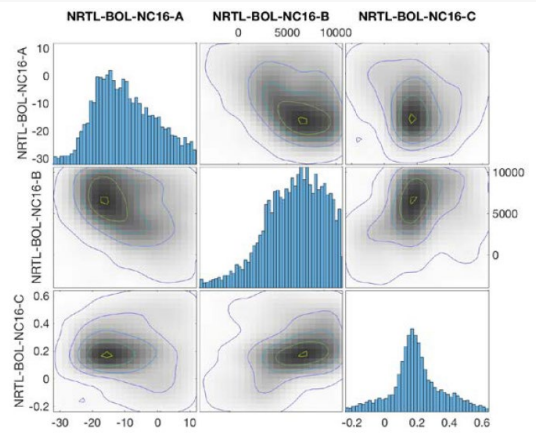
Bayesian Inference to update parameters

Univariate Posterior Distr.



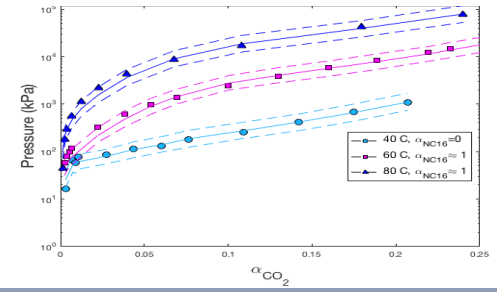
Red = High Likelihood of Parameter Value

Bivariate Posterior Distr.

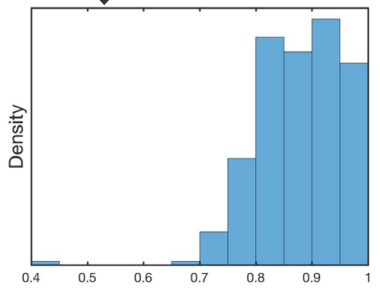


Black = High Likelihood of Parameter Value

Property/Process Sub-models



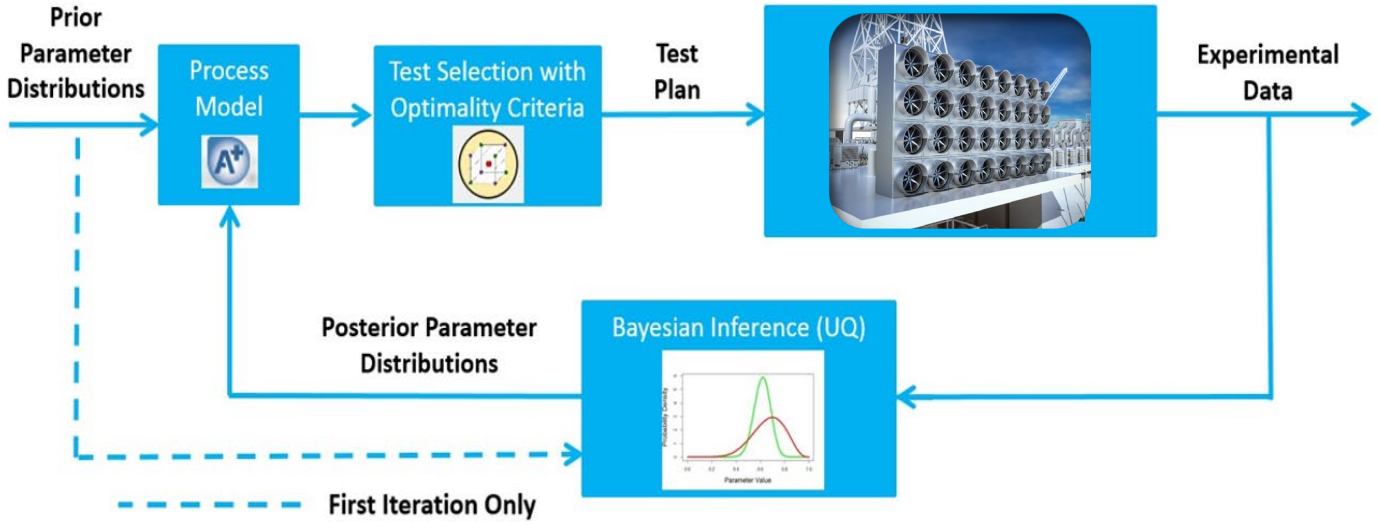
Process Scale



Key Performance Indicators

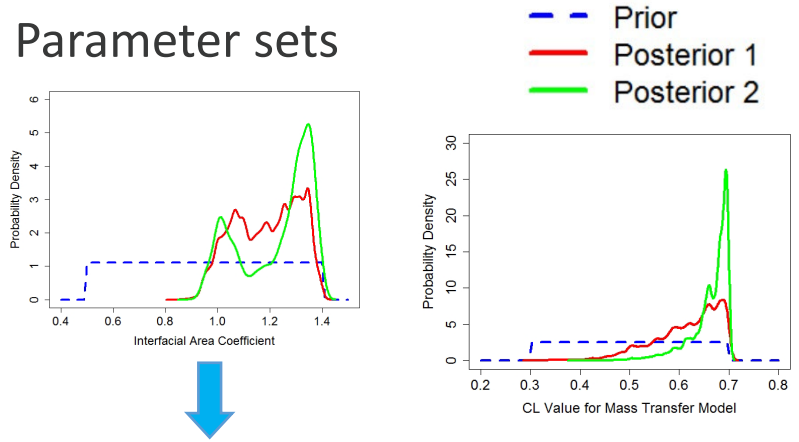
Sequential Design of Experiments

Tools to Maximize Learning for Bench and Pilot Campaigns

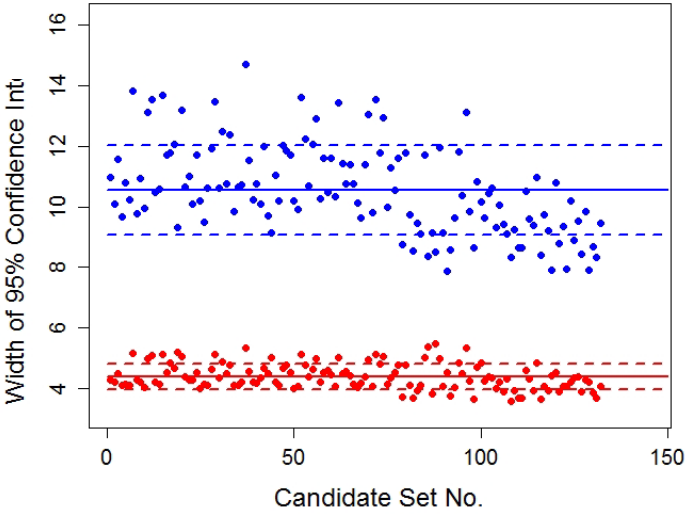


- Bayesian inference is used to refine model parameters via new data
- Experimental runs chosen based on refinement of model (new learning considered)
- Reduction in uncertainty in process model and risk associated with scale-up

Parameter sets



Process Performance Metric

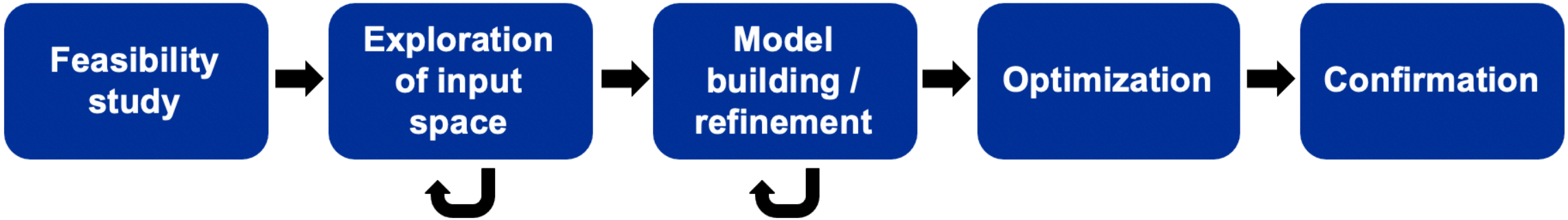


Prior CI Width: (10.5 ± 1.5)%

Posterior: (4.4 ± 0.4)%

Design of Experiment Tool

Flexible testing objectives



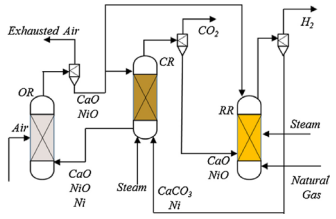
Is it possible to collect quality data? Proof of concept	Understand basic relationship between inputs and responses	Verify that the model captures patterns Add data for better model parameter estimation or prediction	Focus on region of maximum interest Close to most desirable operation conditions	Verify results for production or operational use Ability to duplicate results

Other PSE Tools/Capabilities

- Process development tools providing enhanced optimization capabilities
  - Traditional process optimization
  - Conceptual design
  - Robust optimization (accounting for uncertainty)
- Integration with AI/ML tools
- Energy market tools / understand impacts of variable market conditions on NPV and deployability

Advanced Process Design and Optimization

Plant Design
Process Optimization



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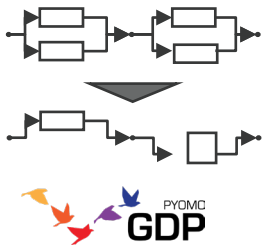
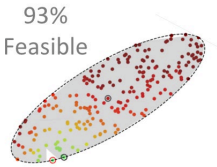


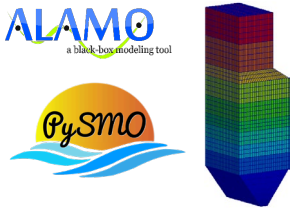
Robust Optimization



PyROS

Enterprise Optimization
Grid & Planning

AI/ML
Surrogate Modeling



Summary

Testing Support at NETL DAC Center

- Develop and apply rigorous models to predict DAC performance and cost
  - Adaptable model library for sorbent contactors in IDAES/CCSI2
- Target maximum value data – refine models that reduce technical risk at scale up
  - Understand impacts of uncertainty on Key Performance Indicators (KPIs)
  - Guide collection of additional data to further reduce uncertainty and reduce technical risk in scale-up
- Framework to develop/ design optimal DAC processes
  - IDAES – Advanced equation-oriented modeling platform
  - CCSI2 - Optimization/ UQ framework that can utilize commercial modeling platforms

Thank you

Benjamin.Omell@netl.doe.gov

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