An Overview of CCSI2 Capabilities for Accelerating Technology Commercialization

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Technical Project Lead - CCSI²

Carbon Management Review Meeting, Pittsburgh PA

August 29th, 2023

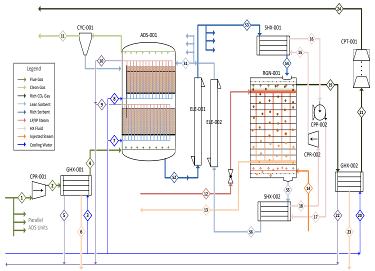
CCSI^2 – Modeling, Optimization and Technical Risk Reduction

CCSI^2
Carbon Capture Simulation for Industry Impact

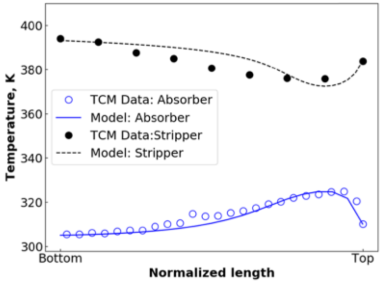
Multi-lab modeling initiative to support carbon capture technology development

NATIONAL ENERGY TECHNOLOGY LABORATORY · BERKELEY LAB · Lawrence Livermore National Laboratory · Los Alamos NATIONAL LABORATORY EST.1943 · Pacific Northwest NATIONAL LABORATORY · OAK RIDGE National Laboratory
Carnegie Mellon · West Virginia University · UNIVERSITY OF NOTRE DAME · THE UNIVERSITY OF TEXAS AT AUSTIN · UT · UNIVERSITY OF PITTSBURGH

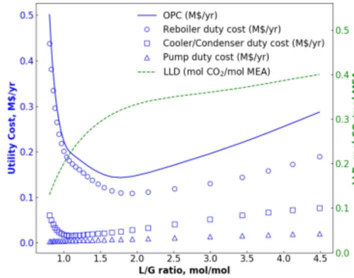
High Fidelity Process Modeling



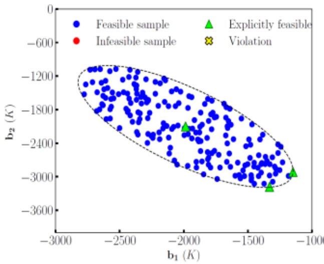
Model Validation



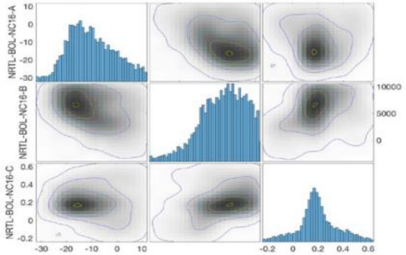
Process Optimization



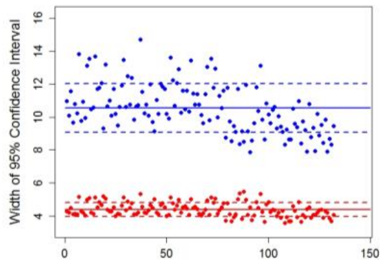
Robust Design

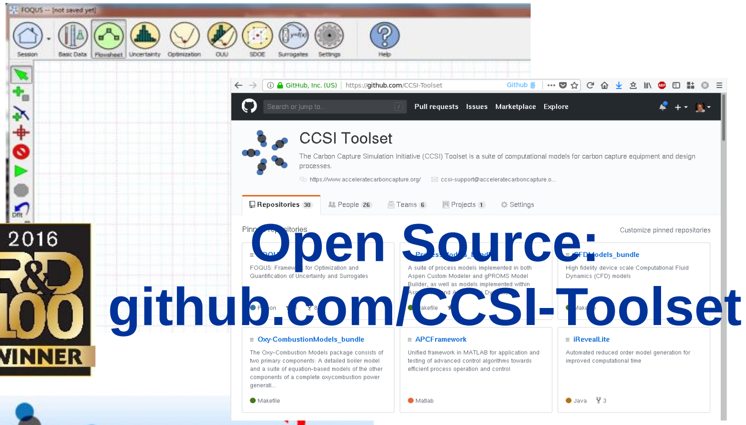


Uncertainty Quantification



Maximizing Learning





2016 R&D 100 WINNER

Open Source: github.com/CCSI-Toolset

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IDAES
Institute for the Design of Advanced Energy Systems

2020 R&D 100 WINNER

Open Source: github.com/IDAES/idaes-pse

Process Modeling Support For DAC and Other CDR Technologies

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

  - ➢ 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

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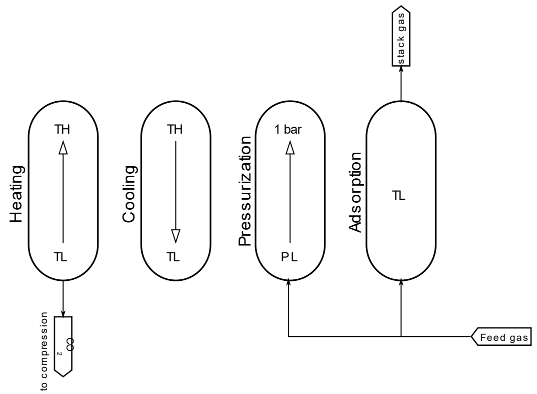
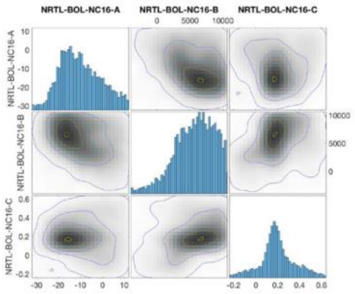
Process Modeling

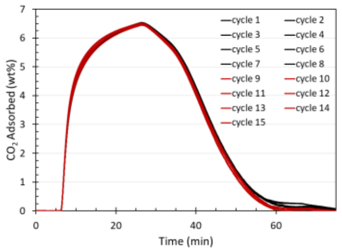


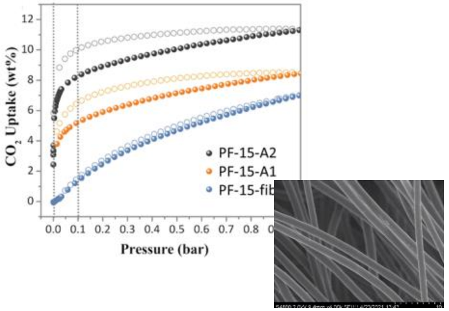
Uncertainty Quantification



Impact on KPIs

Improved Data Collection





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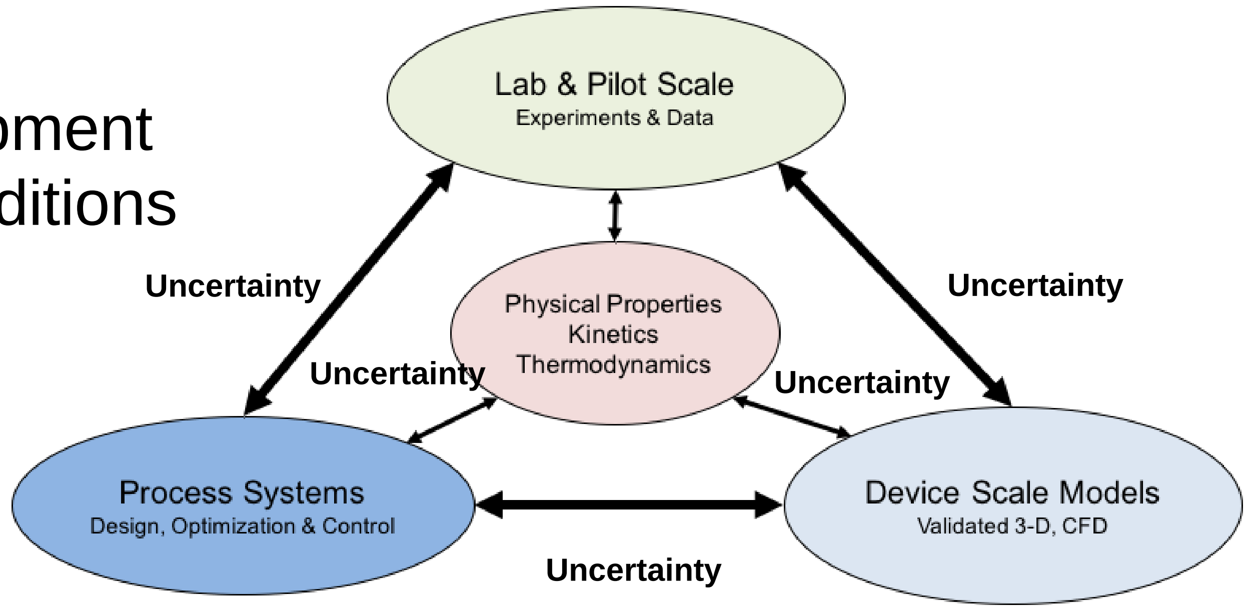
Technology Scale-up: Data Collection and Modeling

Maximize the learning at each stage of technology development

And integrate development stages

- **Early stage R&D**
  - Screening concepts
  - Identify conditions to focus development
  - Prioritize data collection & test conditions
- **Pilot scale**
  - Ensure the right data is collected
  - Support scale-up design
- **Demo scale**
  - Design the right process
  - Support deployment with reduced risk



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Complete CCSI Toolset Publically Available

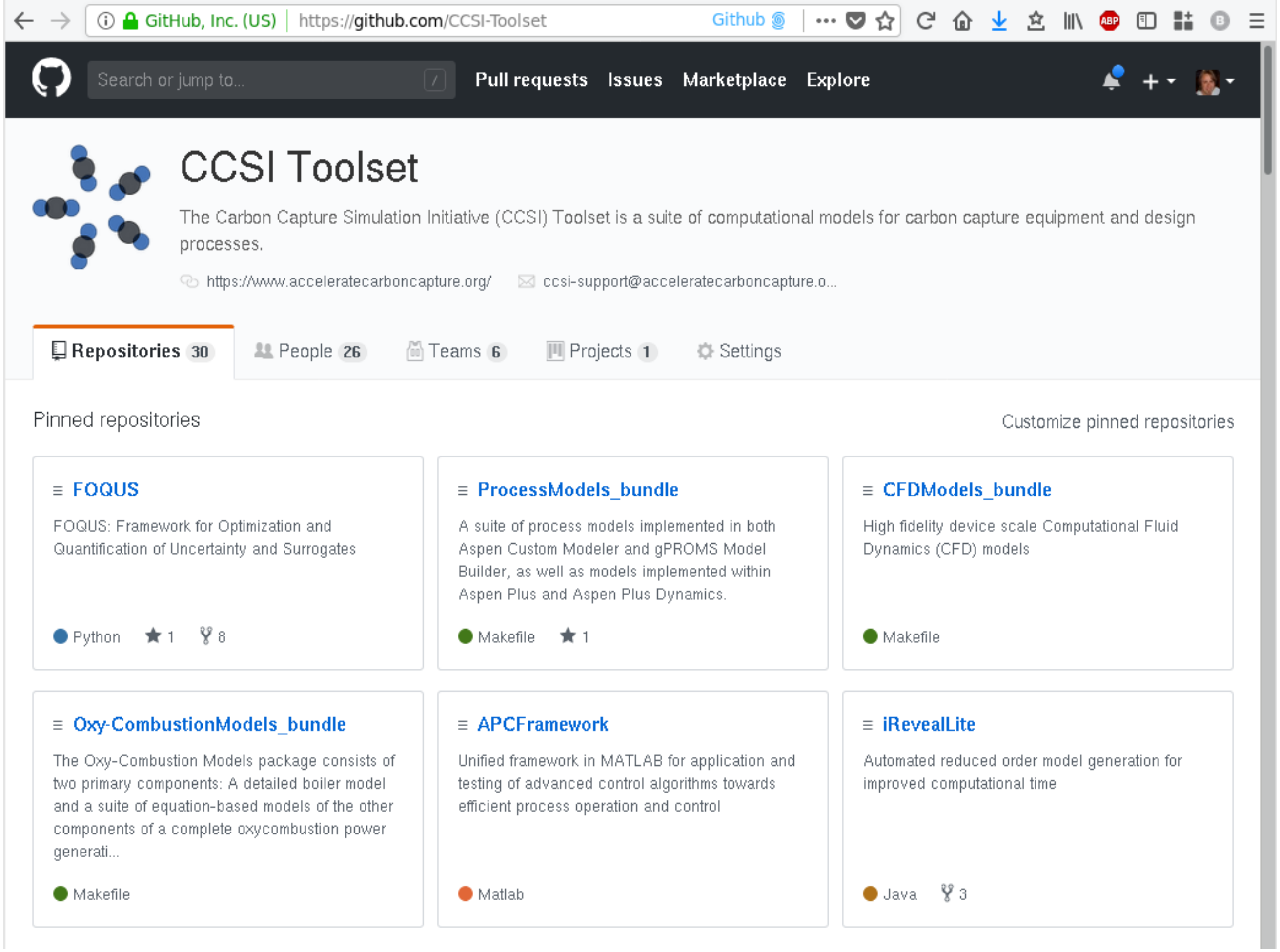
- **2016 R&D 100 Award Winning Software Package**

FOQUS - Framework for Optimization and Quantification of Uncertainty and Surrogates

Full Process Modeling and Optimization Framework -
- Fundamental characterization of material, device and system
- Model library of solvent, solid-gas contactors, and membranes
- Uncertainty quantification
- Optimization (under uncertainty) of process configuration and operation (s.s. and dynamic)

Optimal Design of Experiments - Improves model while optimizing experimental data generation

Surrogate Generation and ML Capabilities – Generate reduced order models for difficult multi-period optimizations, CFD optimizations



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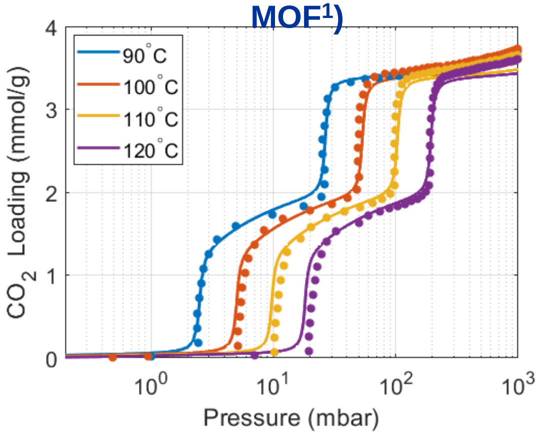
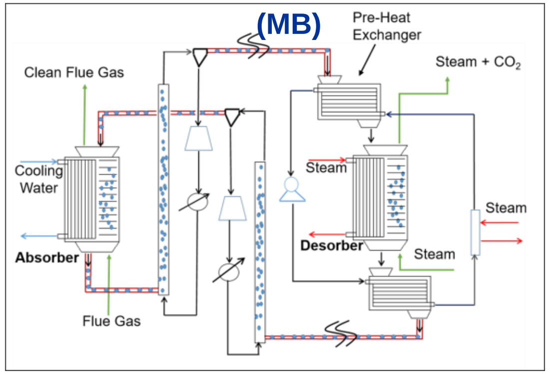
Sorbent Models

- **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/IDAES
  - Support for advanced process modeling platforms and optimization
  - Exploration of important inputs
  - Tools for quantification of uncertainty

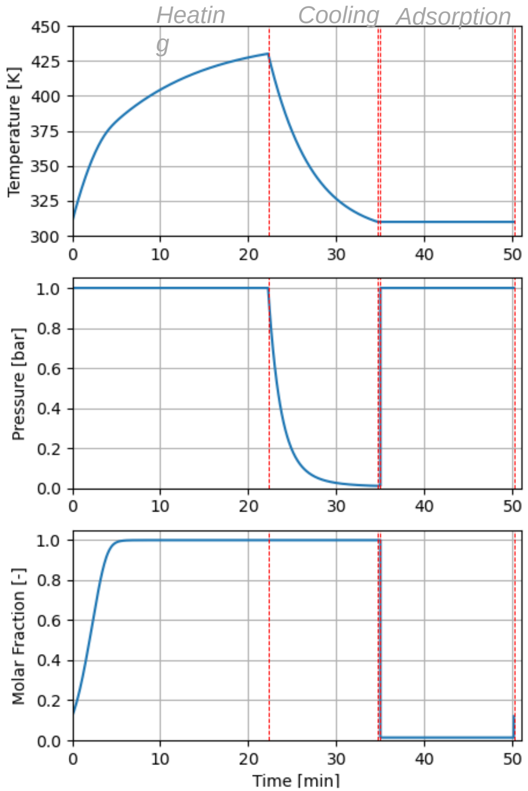
Development of Novel Property Models (Two-step Isotherm of tetraamine-appended MOF[1])



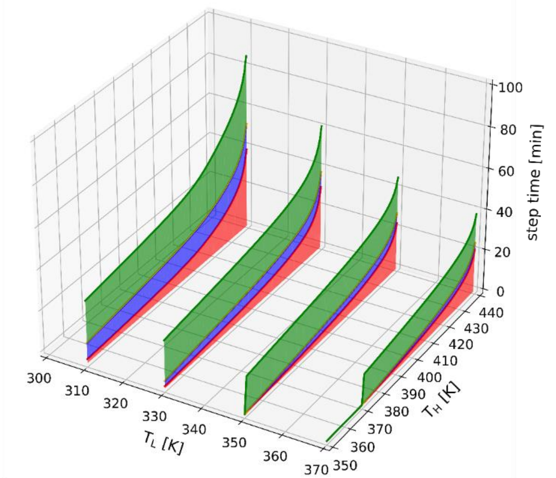
Applications into Process Scale models (MB)



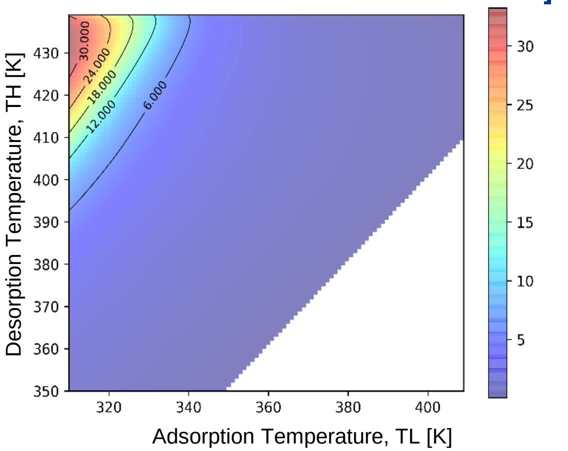
IDAES 0D Screening Model



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

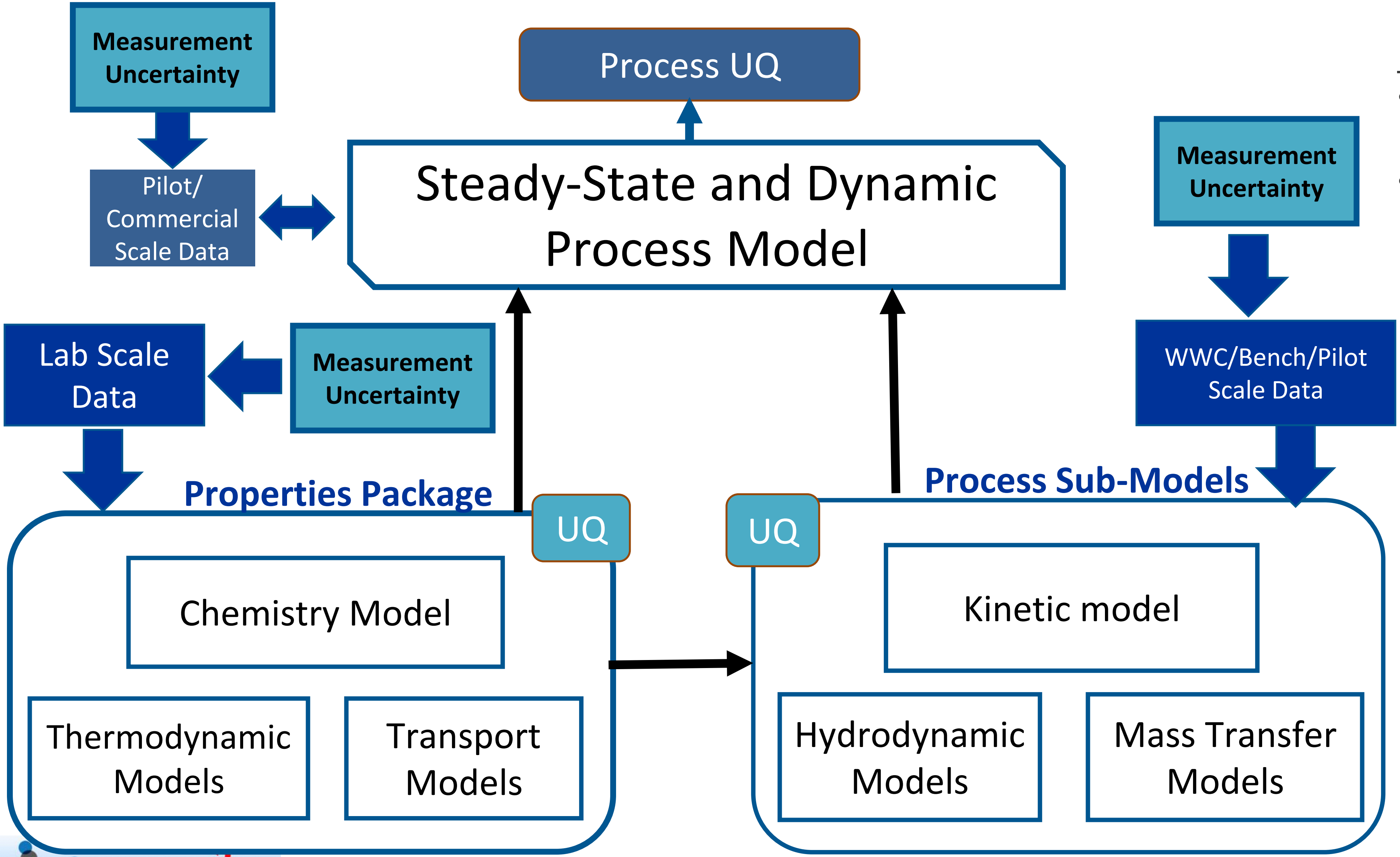


Productivity [kg CO2/(ton · h)]



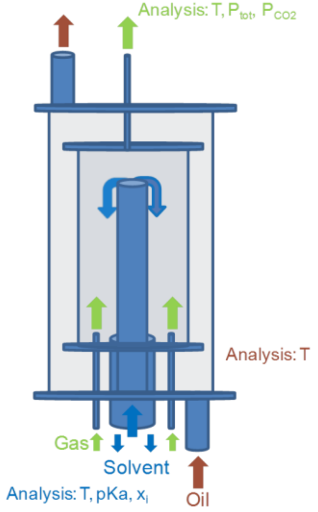
1 Kim, E. J., *et al*. *Science* 2020, No. 369, 392–396

Developing Detailed, Predictive Models of Solvent-Based Capture Processes



<u>Detailed, Rigorous, Modeling</u>

- Integration of multi-scale data
- Inclusion of uncertainty at several scales



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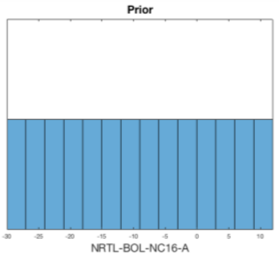
Uncertainty Quantification (UQ)

MATERIAL

- **Quantifying risk for scale-up**
- **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**

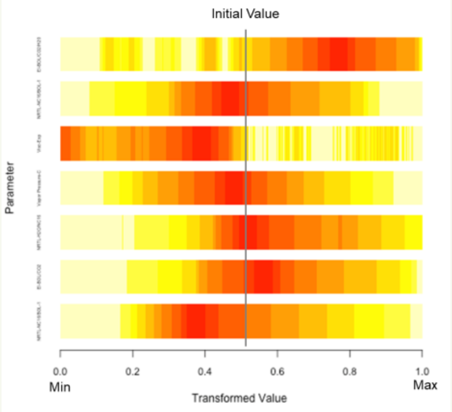
Initial Parameter Range



Gather New Data

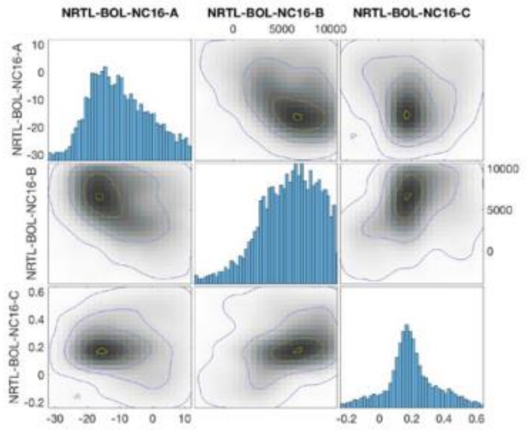
Bayesian Inference to update parameters

Univariate Posterior Distr.



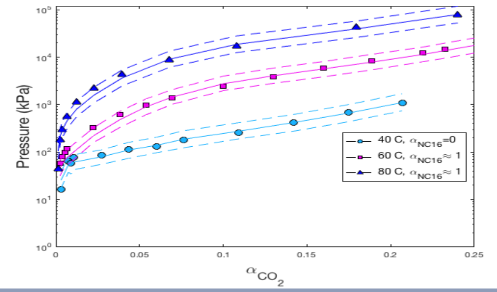
Red = High Likelihood of Parameter Value

Bivariate Posterior Distr.

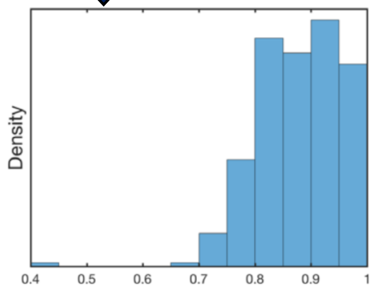


Black = High Likelihood of Parameter Value

Property/Process Sub-models



Process Scale



Key Performance Indicators

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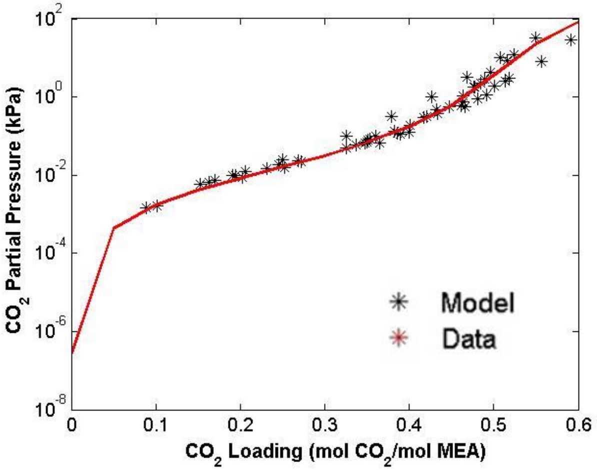
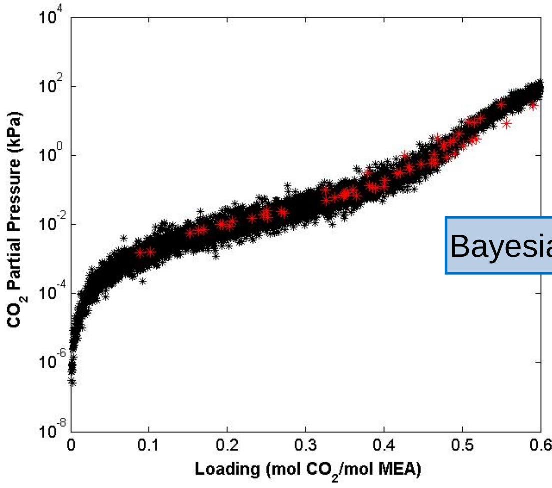
Uncertainty Quantification Bayesian Inference Example: VLE Models

VLE Data/Model Comparison at 40°C

Deterministic sub-model

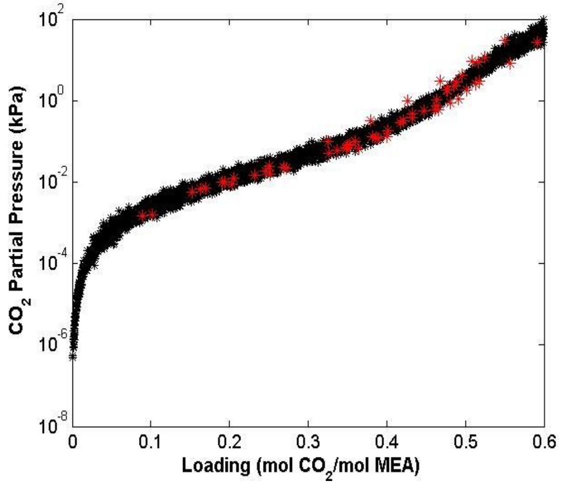


Best initial guess of parameter set



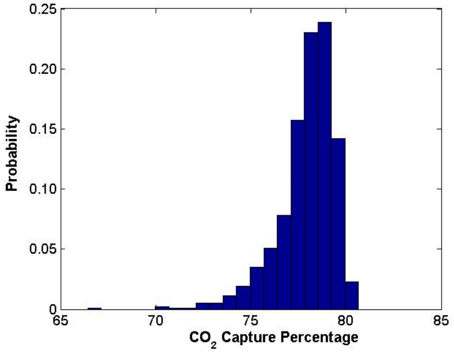
Bayesian inference

Refined parameter set

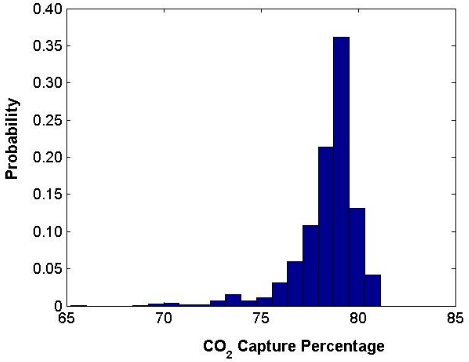


Process Model

Process Model



high uncertainty



reduced uncertainty

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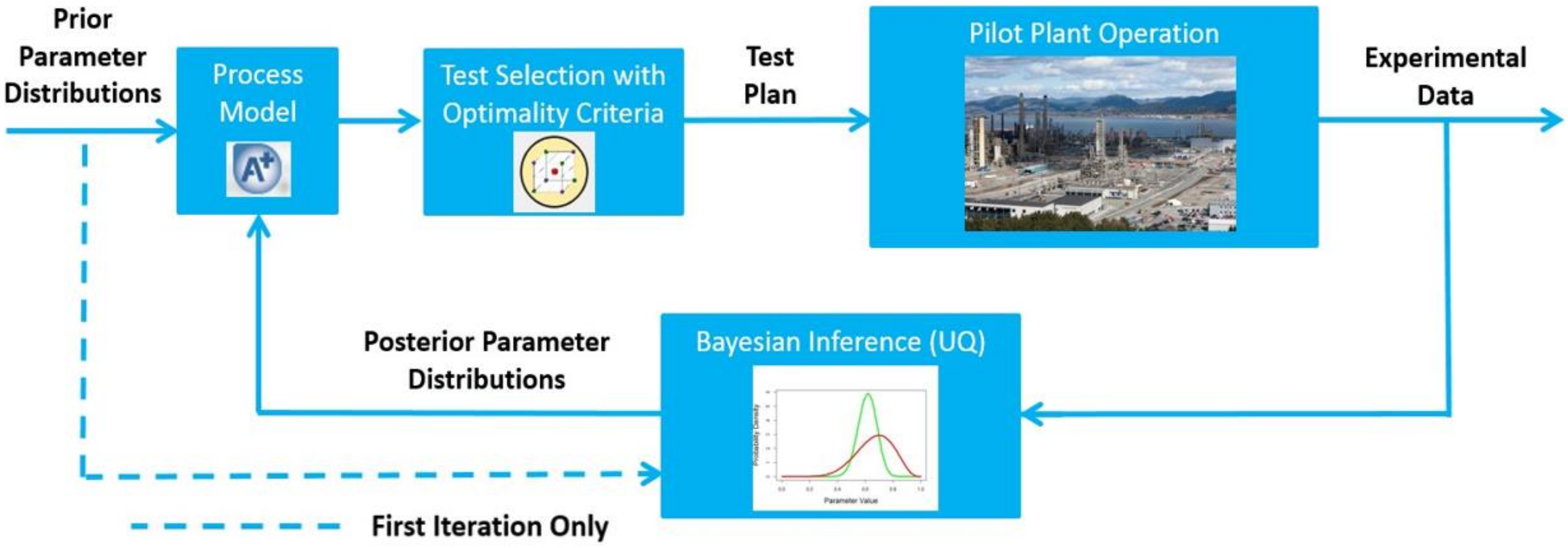
Sequential Design of Experiments

- Develop systematic approach to conducting pilot plant testing, regardless of scale, process configuration, technology type, etc.
- Ensure right data is collected
- Maximize value of data collected

Schematic of Sequential Design of Experiments



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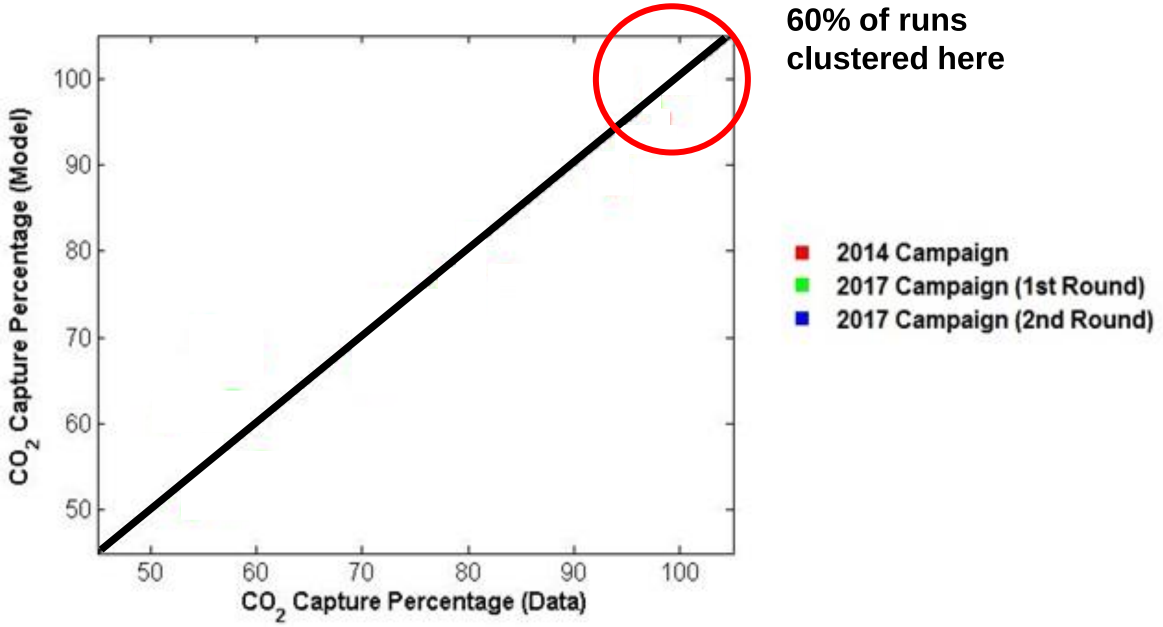
NCCC Model Improvement after SDoE

Three Beds with Intercooling Cases



2014 Campaign (Before SDoE)

- Conventional test plan caused “clustering”
- Not ideal for complete understanding
- Used data to refine model

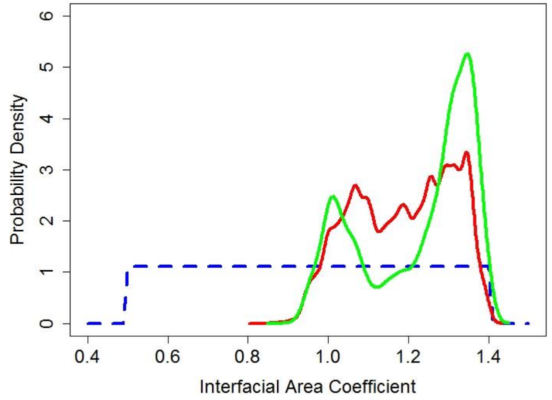
Wait 3 years….

2017 Campaign (Using SDoE)

- Much more distributed output
- Much more complete understanding
- *In manner of weeks*, further reduced uncertainty in capture rate by 60%

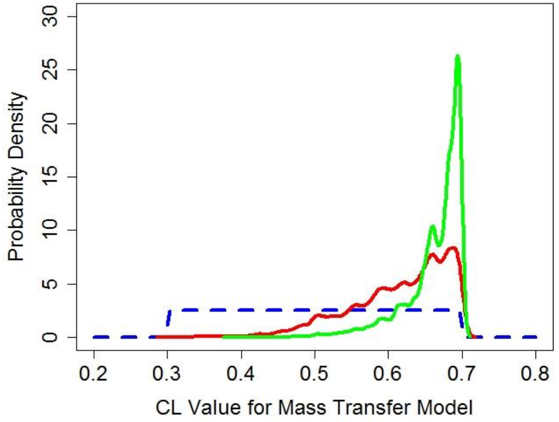
TCM Model Improvement after SDoE

Update in Parameter Distributions for Absorber Packing

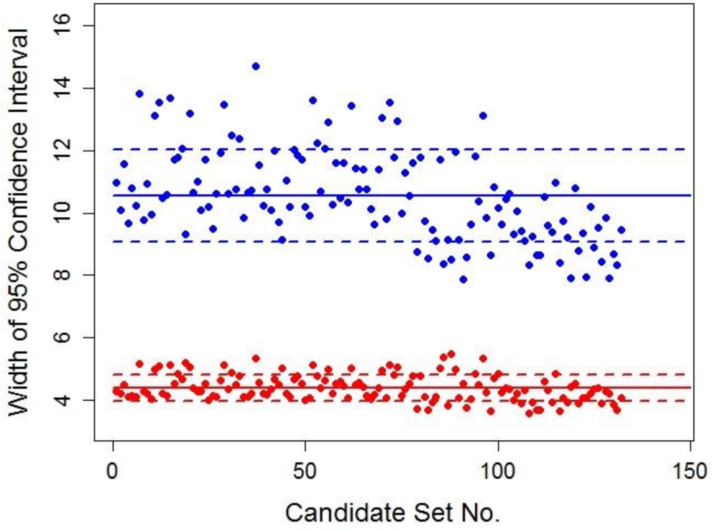


Mass transfer and interfacial area parameters are packing-dependent, and therefore are assigned uniform prior distributions over wide ranges, indicating assumption of relatively large uncertainty before collection of process data.

Bayesian inference, through process data collected using SDoE, results in refined estimates of parameters, and thus reduction in uncertainty in process model and risk associated with scale-up



Reduction in CO_2 Capture Percentage Prediction Accuracy



Prior CI Width: (10.5 ± 1.5)%

Posterior CI Width: (4.4 ± 0.4)%

Average reduction in uncertainty: 58.0 ± 4.7%

<u>Candidate set includes variation in</u>:

- **Solvent Circulation Rate**
- **Flue Gas flowrate and CO_2 concentration**
- **Reboiler steam flowrate**

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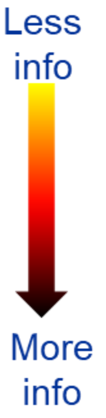
Science Based Design of Experiments

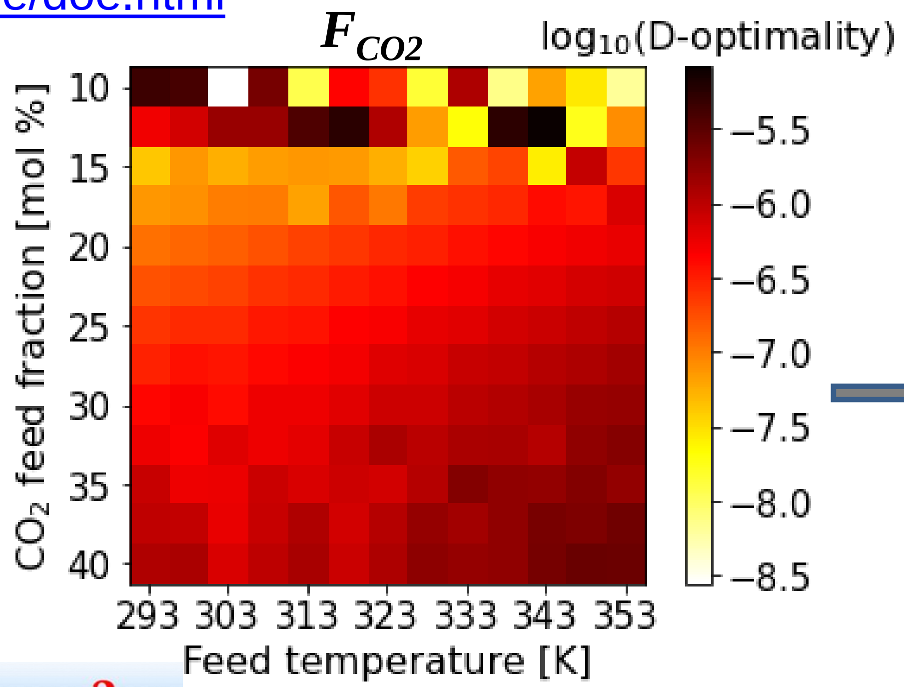
DesignOfExperiment

PYOMO DOE

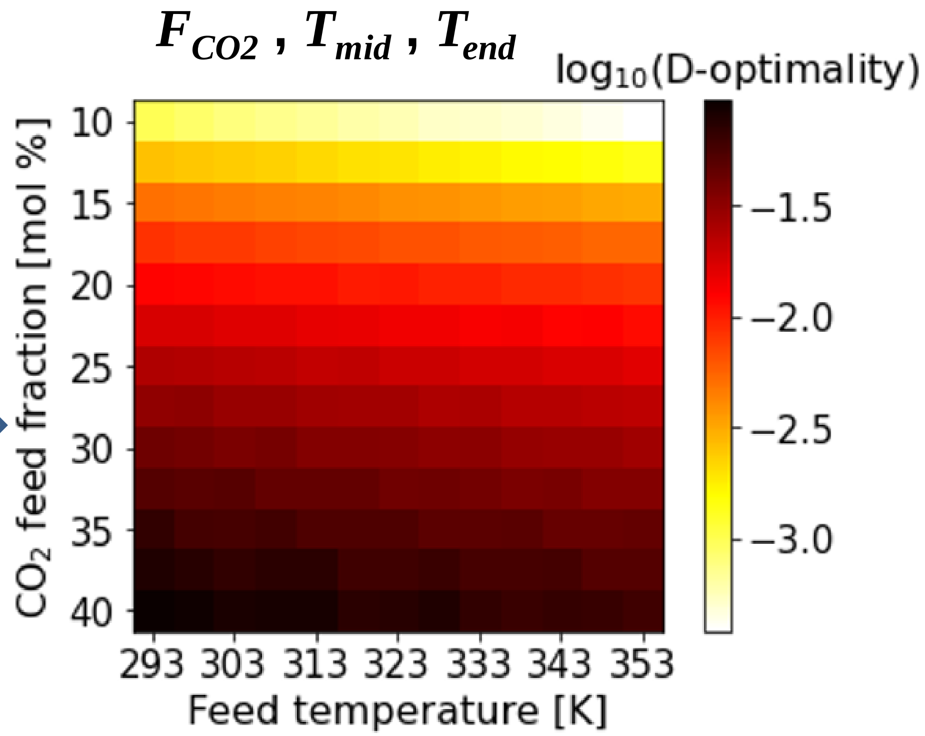
https://pyomo.readthedocs.io/en/stable/contributed_packages/doe/doe.html

- Utilize science based models
- Better design experimental devices and measurements to ensure identifiability of the process
- Extendable to dynamic experimental designs





Add two ***T*** measurements



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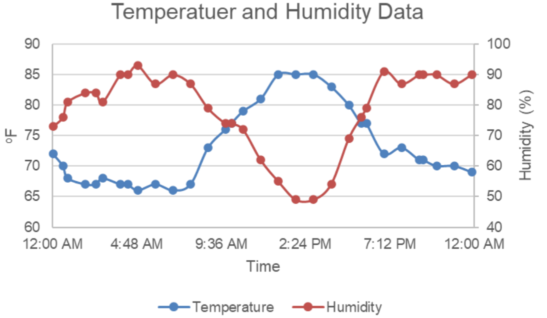
Wang, Jialu, and Alexander W. Dowling. "Pyomo. DOE: An open-source package for model-based design of experiments in Python." *AIChE Journal* 68.12 (2022): e17813.

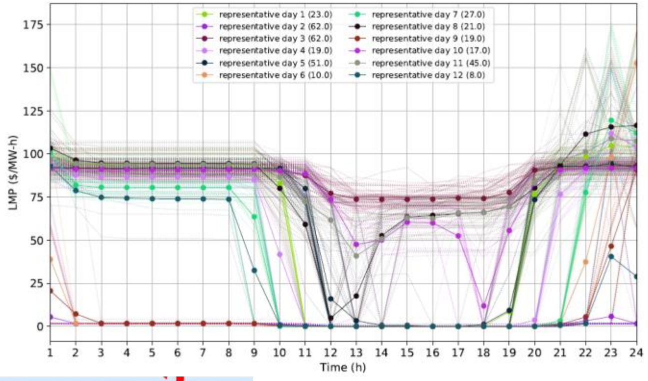
DAC Systems – Integrated Approach

Historical Time Series Data

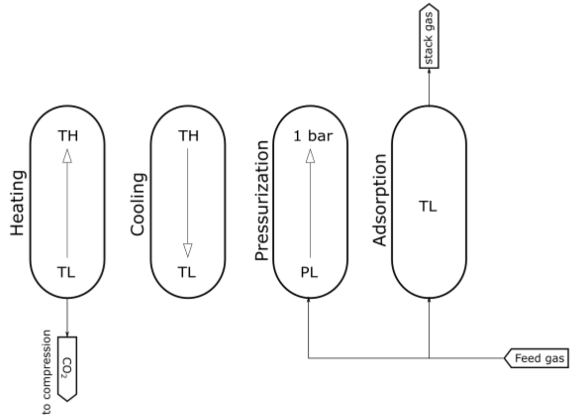
Historical Ambient Conditions data



Historical (or Future) Local Marginalized Prices of Electricity



Process Model



Multi-period Optimization Problem

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- Optimal Design
- Net Present Value Analysis (versus TEA)
- Dispatch schedule

- Performance of DAC process will likely vary via seasons and changing temperatures and humidities throughout the day
- Utilization of excess electricity from increased variable renewable generation may require optimal dispatch schedules
- Weather, seasonal patterns may be correlated with electricity price

TEA may be insufficient

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Multi-period Optimizations and NPV Analysis: FLExible Carbon Capture and Storage (FLECCS)

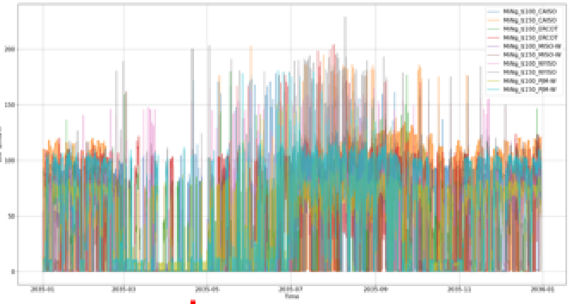
Sponsor: ARPA-E

Ext. Partners: Susteon, Svante, SoCalGas, LA DWP Los Angeles Department of Water & Power, West Virginia University

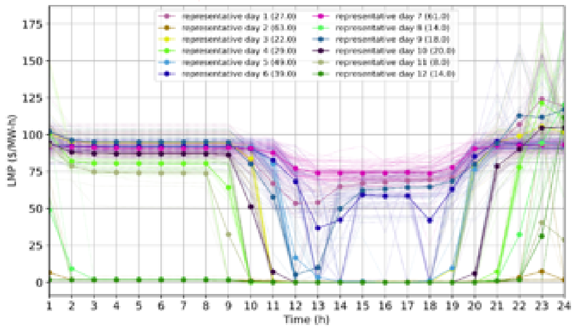
Gooty, et. al., Applied Energy, 2023

Process LMP Signals

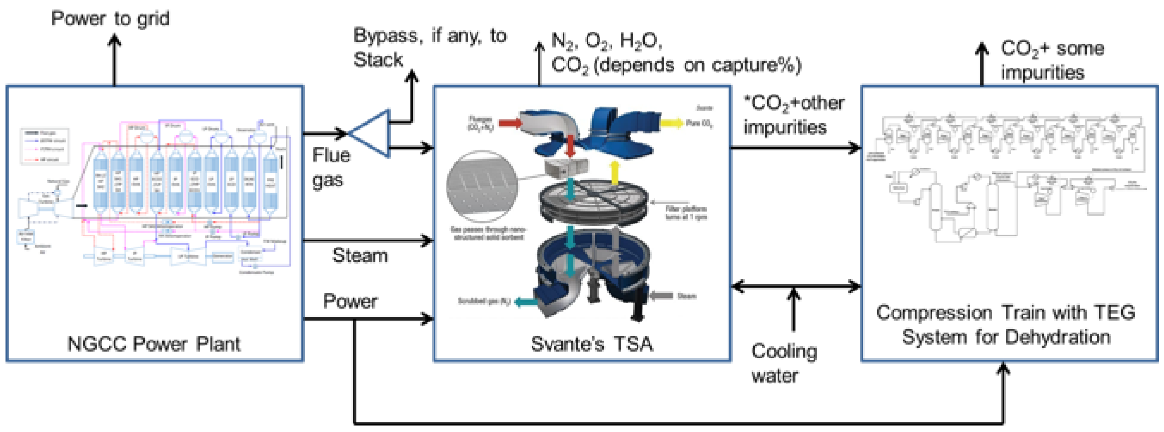
Input from ARPA – E
- Locational Marginal Price (LMP) signal (in \$/MWh)



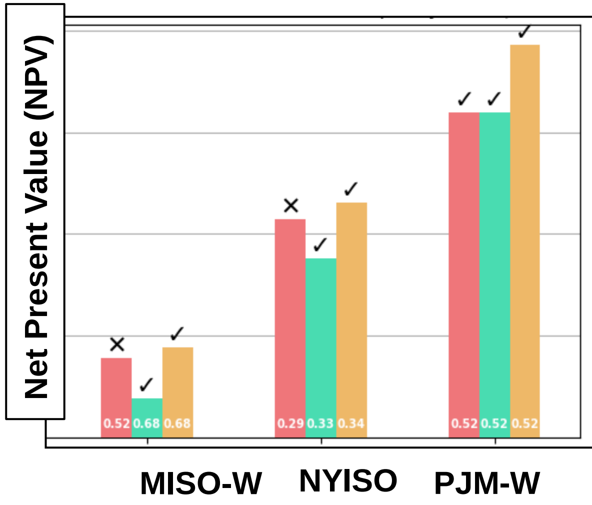
Identify representative days



Develop Rigorous and Reduced-order (surrogate) Process Models



Example Scenario: \$150/ton CO_2 tax
Build Capture System?
Capture System Must Be Built
Build Capture System if Capex/Opex Reduced by 20%?



Formulate and Solve Multi-period Optimization Problem

Result: Optimal solution maximizing the Net Present Value (NPV)
- Optimal design of the capture system
- Optimal power schedule
- Detailed cash flows

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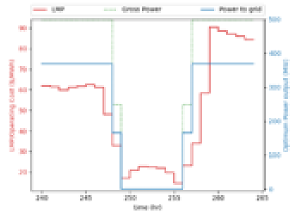

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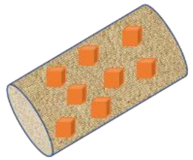
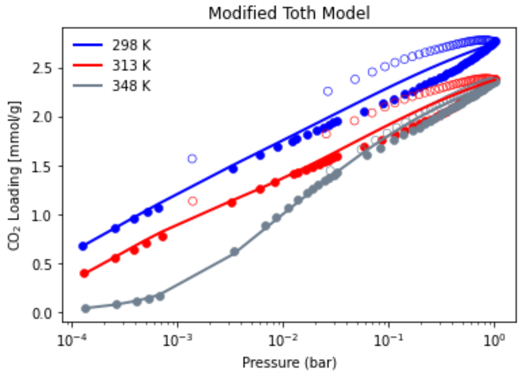
CCSI² Support For NETL DAC Technology

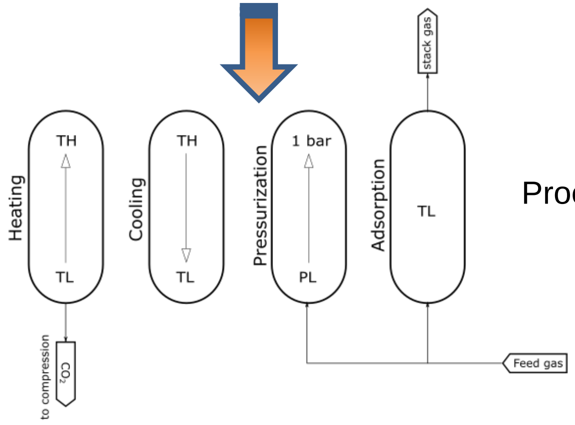
- Support analysis of NETL developed PIM-1-AO-TAEA sorbent
- Help guide data collection to properly inform process scale
- Work with high fidelity (CFD) modeling teams to inform mass transfer, hydrodynamics submodels
- Estimate performance with varying regeneration methods (temperature swing, vacuum assisted vacuum swing, etc.)
- Perform cost analysis (12/31/23)
- Characterize performance under varying air conditions (3/31/23)
- Long term goal – support testing at NETL DAC center



Sorbent data collection

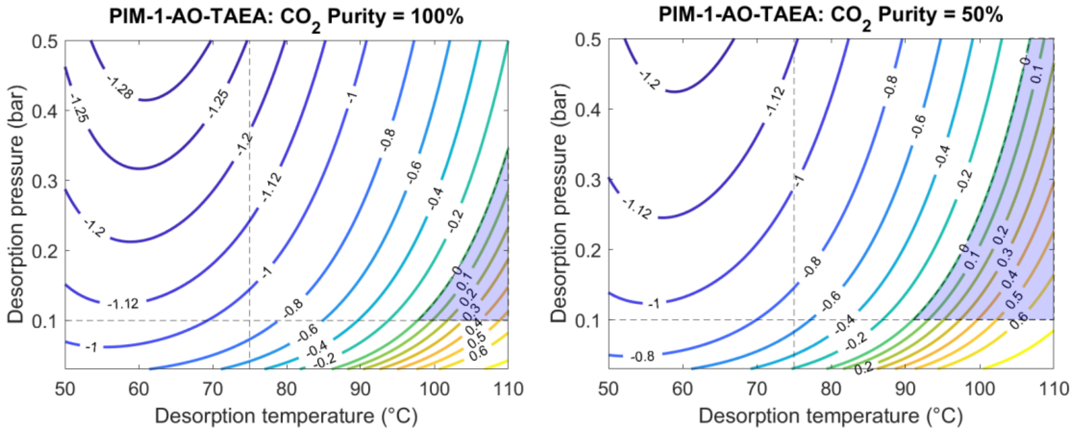


Property Model



Process Model

CO_2 Cyclic Working Capacity Analysis



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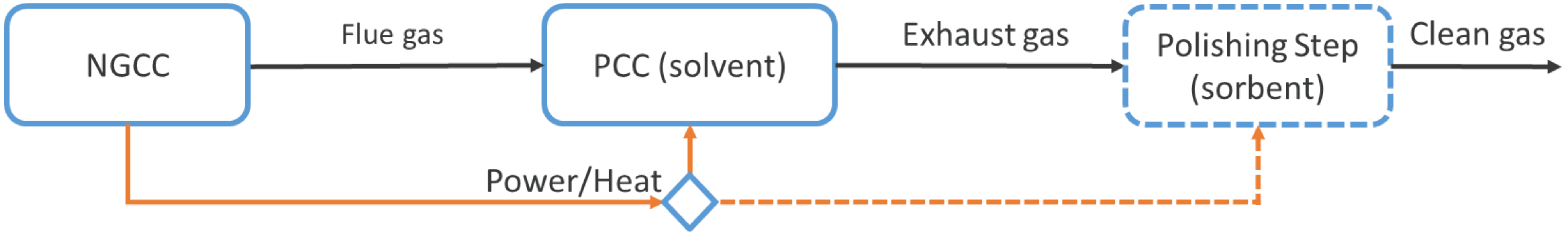
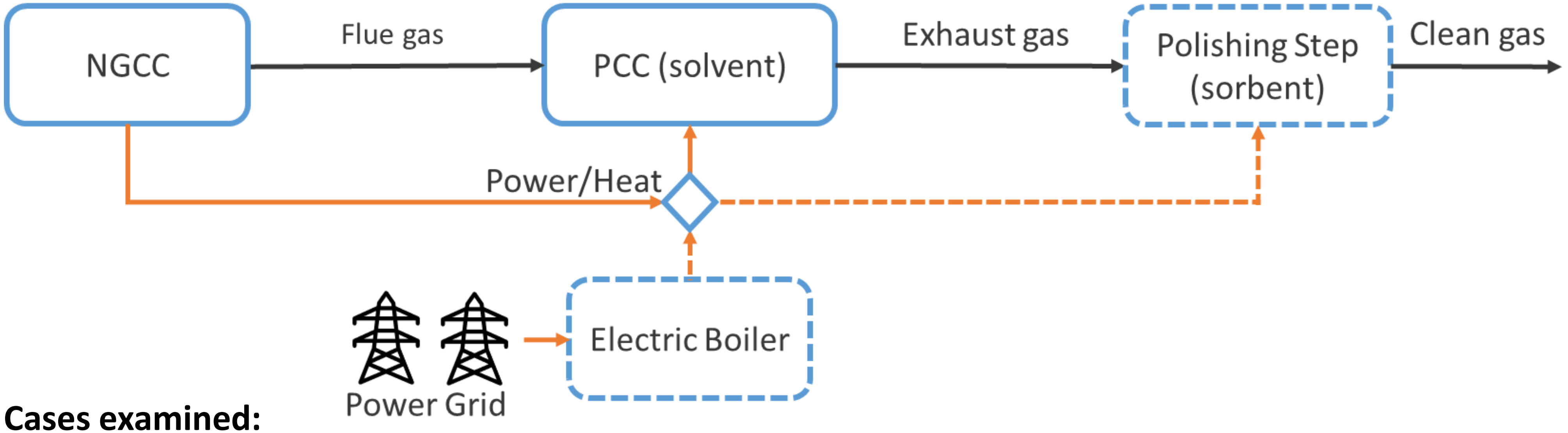
Optimization of Integrated Capture Process: Achieve Net-zero Emissions for NGCC Power Plant



Cases examined:

1. **Integrated NGCC and TSA: Net-zero achieved via polishing step**
2. NGCC + Electric Boiler (steam + power for TSA) + TSA: Net-zero achieved via polishing step. Electric boiler added to provide steam and power for DAC system.
3. Integrated NGCC and DAC: DAC meets net-zero requirement
4. NGCC + Electric Boiler (steam + power for DAC) + DAC: DAC meets net-zero requirement. Electric boiler added to provide steam and power for DAC system

Optimization of Integrated Capture Process: Achieve Net-zero Emissions for NGCC Power Plant



Cases examined:

1. Integrated NGCC and TSA: Net-zero achieved via polishing step
2. **NGCC + Electric Boiler (steam + power for TSA) + TSA: Net-zero achieved via polishing step. Electric boiler added to provide steam and power for DAC system.**
3. Integrated NGCC and DAC: DAC meets net-zero requirement
4. NGCC + Electric Boiler (steam + power for DAC) + DAC: DAC meets net-zero requirement. Electric boiler added to provide steam and power for DAC system

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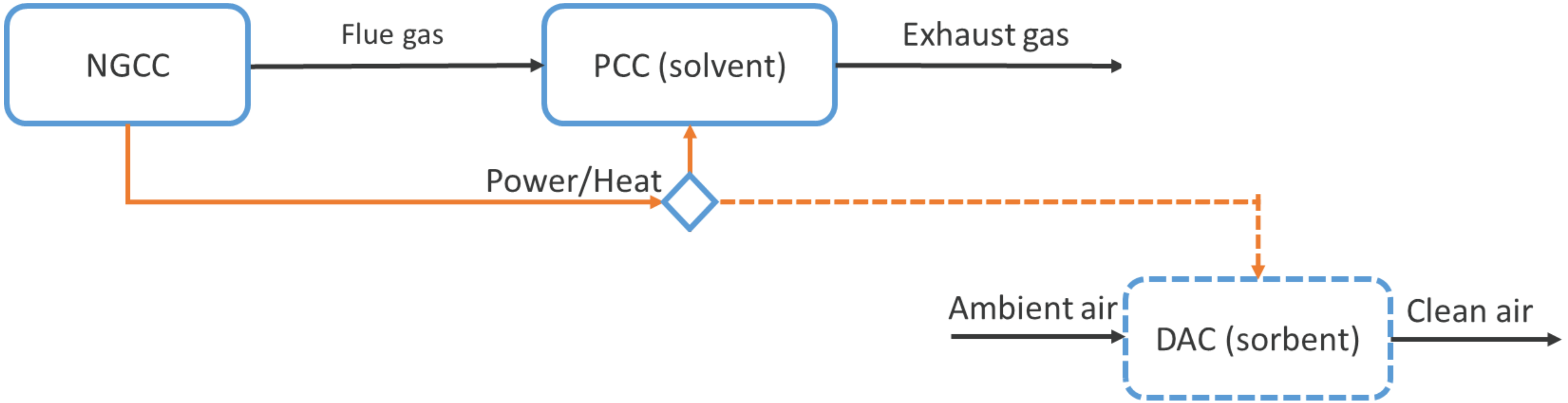
Optimization of Integrated Capture Process: Achieve Net-zero Emissions for NGCC Power Plant



Cases examined:

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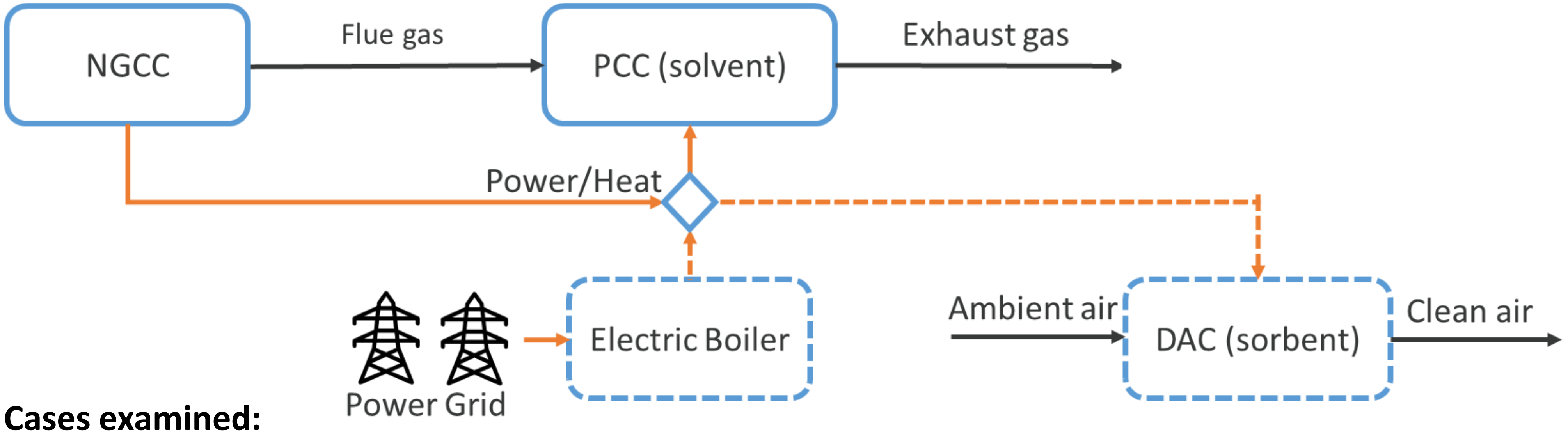

Cases examined:

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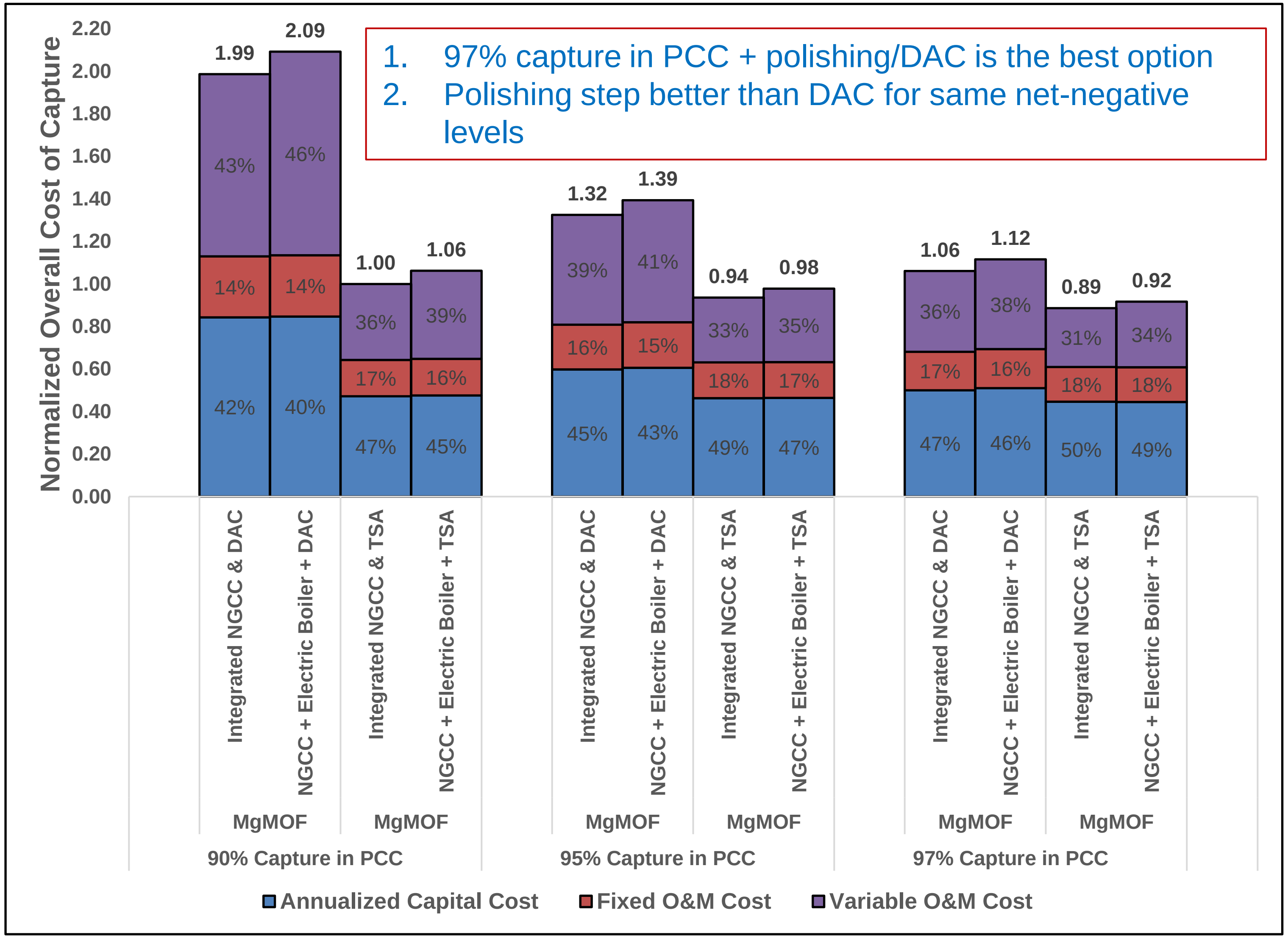
Summary of Results (Overall Cost of Capture PCC+TSA)

- 0D Equilibrium Model
  - FG polishing step – Integrated NGCC & e-boiler (90%, 95%, and 97%)
  - DAC – Integrated NGCC & e-boiler (90%, 95%, and 97%)

- Material used in TSA system MgMOF74, and assumed cost of $10/Kg
- Overall cost of capture = PCC capture cost + TSA capture cost
- All cases are "net-negative" at plant level
- FG Retrofit NGCC (polishing step) with 97% capture in PCC cheapest



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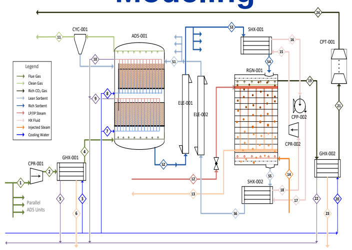
Modeling and Analysis Capabilities

Tools and process models to predict, optimize, and minimize risk in the scale-up of technologies

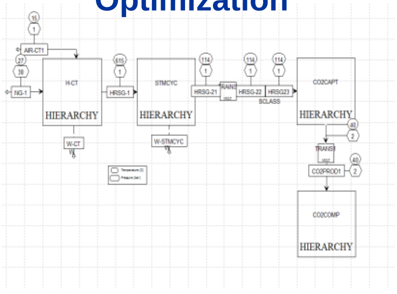
<u>Foundational Capabilities</u>

- High-Fidelity Modeling (sorbents, solvents, membranes)
- Optimal Design of Experiments
- Steady-State and Dynamic Process Optimization
- Electricity Grid Modeling / Expansion Planning
- Multi-Scale Modeling and Optimization (Materials/Process/Grid)
- Uncertainty Quantification
- Robust Optimization (i.e., Design Under Uncertainty)
- Machine Learning/AI

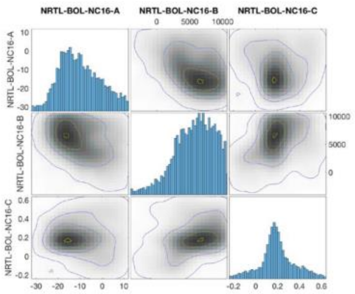
High-Fidelity, Multi-Scale Modeling



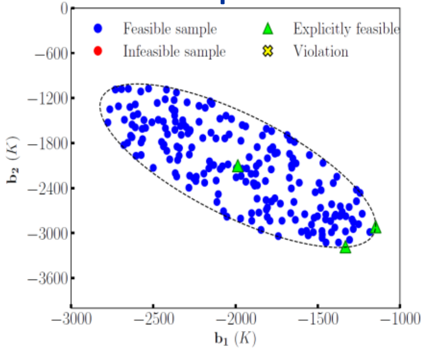
Process-level TEA Optimization



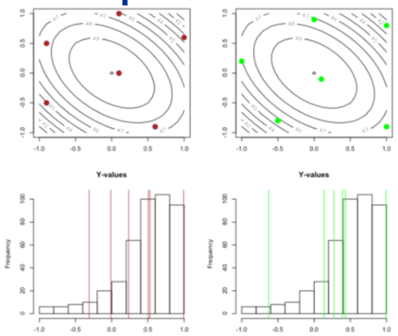
UQ and Parameter Optimization



Robust Optimization



Optimal DoE



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Disclaimer

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Carbon Capture Simulation for Industry Impact

For more information

https://www.acceleratecarboncapture.org/

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