2024 PSE+ Stakeholder Workshop:
Carbon Capture Simulation for Industry Impact ($CCSI^2$)

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$CCSI^2$ Associate Technical Director

Pittsburgh Marriott City Center
Pittsburgh, PA
9/18/2024

CCSI² – CCS Modeling, Optimization, and Technical Risk Reduction

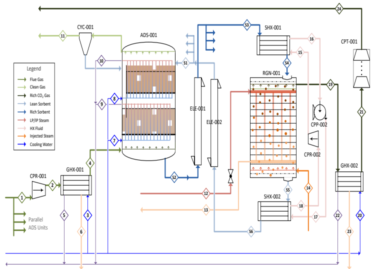
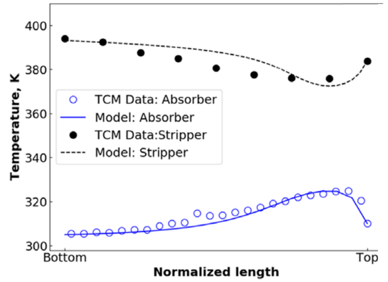
CCSI² Carbon Capture Simulation for Industry Impact

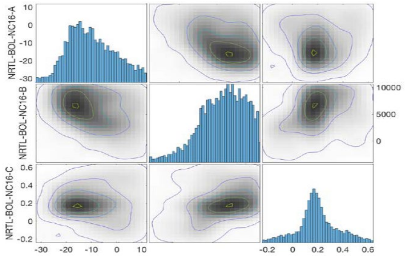
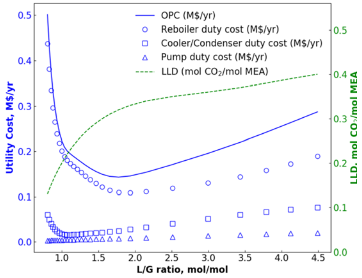
Multi-lab modeling initiative to support carbon capture technology development

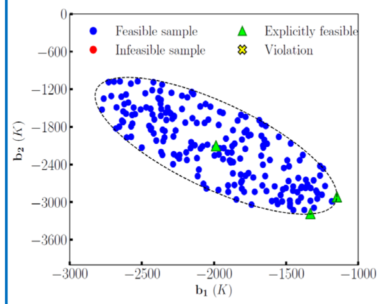
NATIONAL ENERGY TECHNOLOGY LABORATORY · BERKELEY LAB · Lawrence Livermore National Laboratory · Los Alamos NATIONAL LABORATORY EST.1943 · Pacific Northwest NATIONAL LABORATORY

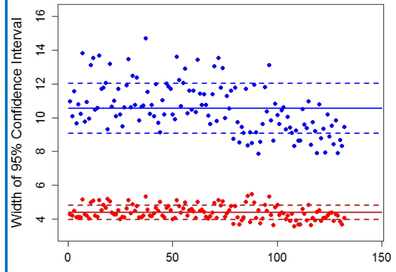
Carnegie Mellon · West Virginia University · UNIVERSITY OF NOTRE DAME · THE UNIVERSITY OF TEXAS AT AUSTIN · UT · UNIVERSITY OF PITTSBURGH

Modeling			Optimization	Risk Reduction	
High Fidelity Process Modeling	Model Validation	Uncertainty Quantification	Process Optimization	Robust Design	Maximizing Learning





IDAES Institute for the Design of Advanced Energy Systems

CCSI^2 Applies IDAES Toolset

IDAES
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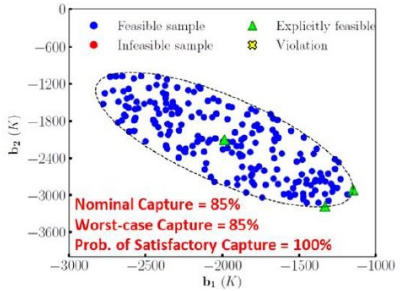
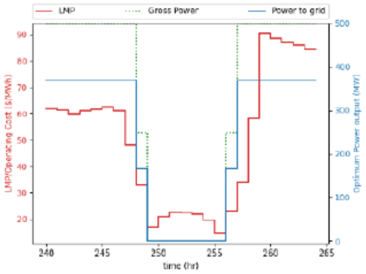
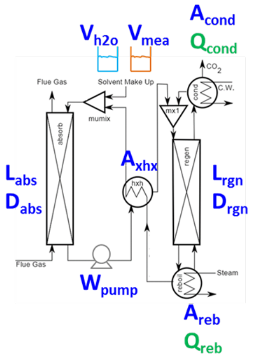
*Burgard Wed at 9:15

PyROS







Robust Optimization

*Chrysanthos Thu at 2:30

Multi-period Optimization

*Radhakrishna Thu at 9:30

MEA Process Model

*Poster by Doug Allan

CCSI^2
Carbon Capture Simulation for Industry Impact

Mission: Ensure Maximum Value to Tech Developer Pilots

- **First principles based process models** are a key component in demonstrating **risk reduction** for process scale-up
- **Model demonstration and validation** at pilot scale is understood to be an **important component** of relevant funding opportunity announcements (FOA)
- **All pilots** in FOA 2614 Round 3 expected to **develop and validate process models** of their technology
  - Models **do not** have to be provided to NETL/FECM, however details of models and submodels, data sets, and validations will be examined
- **CCSI² can provide support** for model development, optimal DoE, uncertainty quantification and validation

Present CCSI^2 Industrial Collaborations

*Matuszewski Wed at 3:30

Dynamic CCS modeling and advanced process control (power/steel)

NAS solvent process modeling and pilot support via SDoE

Solvent VLE and emissions modeling

EEMPA solvent and process modeling and optimization

Membrane module and process modeling for pilot support

Membrane module and process modeling (steel)

Piperazine process modeling

Requested to support mixed salt solvent pilot via SDoE

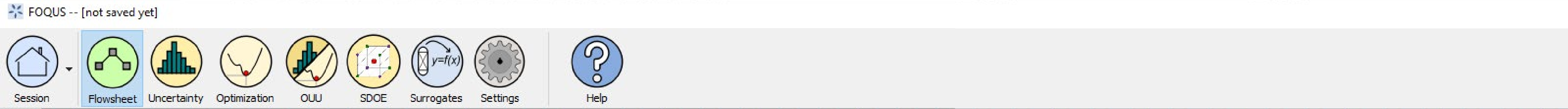
MEA Baseline Campaign process modeling and SDoE

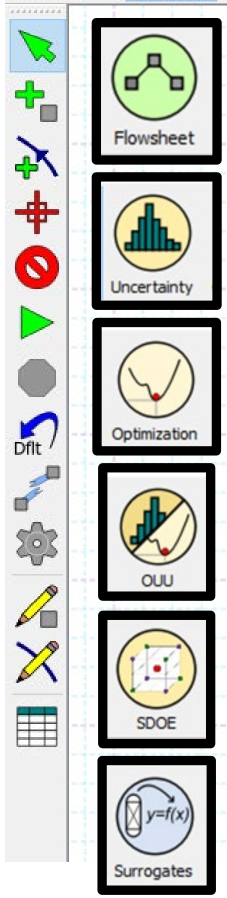
MEA Baseline Campaign process modeling and SDoE

Facilitated Transport Membrane modeling and SDoE

Requested to support solvent modeling and SDoE

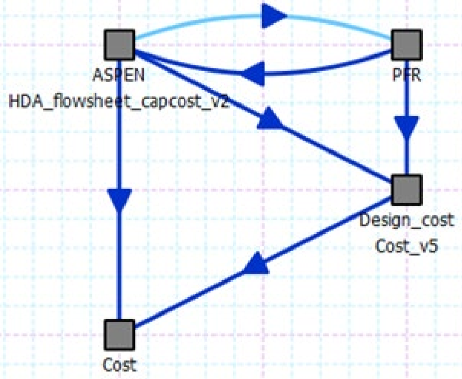
How CCSI² Adds Value: FOQUS Framework





- Interface connecting commercial and open source modeling platforms (Aspen, gPROMS, Python, Pyomo, Excel). Uses your models.

- Propagates uncertainty through modeling hierarchy. Data visualization, parameter screening.



- Simulation based optimization of modeling ensemble.

- Optimization of modeling ensemble incorporating parameter-based uncertainty.

- Sequential Design of Experiments (SDoE) maximize learning from experimentation. Uniform and non-uniform space filling. Ordering.

- Surrogate modeling capabilities to reduce computational burden of simulation-based engineering. Now coupled with optimization.

CCSI² Summary, Capabilities, Highlights

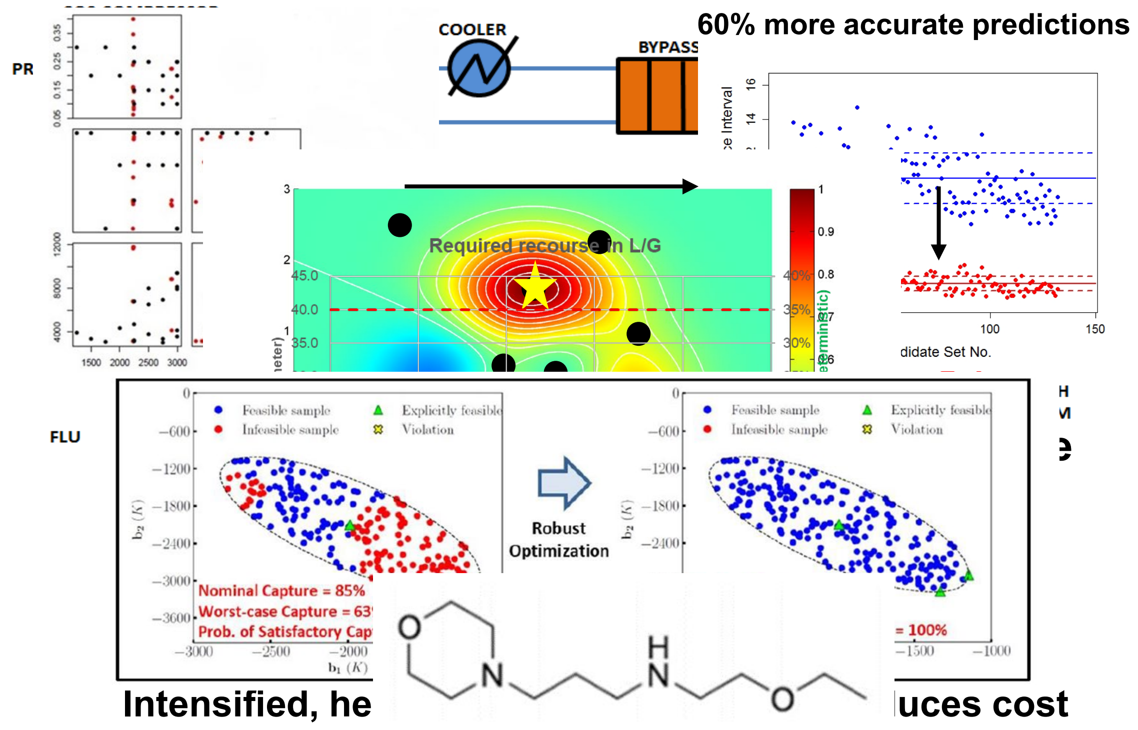
- **Sequential Design of Experiments for lab-, bench-, or pilot-testing**
  - Improves model **while** optimizing lab- or pilot-scale experimental data generation – **can save years off of pilot test schedule**
    - NCCC and TCM MEA pilot models accurate on CO_2 Capture percentage within **3-6% with 95% confidence**

- **Uncertainty Quantification**
  - Perspective on whether **fixed process design/operation** is sufficient
  - **Which design variables** are most effective at improving performance

- **Robust Optimization**
  - Optimization **amidst uncertainty** to **ensure** safe, feasible operation
  - **Cost-optimal over-design**

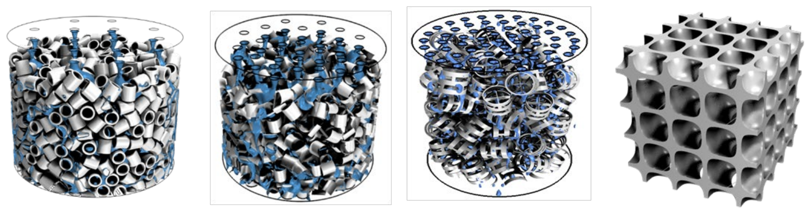
- **Novel Solvent and Process Optimization**
  - CFD to **optimize contactor geometry**, elucidate novel solvent/packing interaction, contact angle, interfacial areas, etc.
  - Rigorously balances cost and performance, gaining **>10% reduction in captured cost** over designs not using optimization (e.g. EEMPA).

- **Machine Learning**
  - **Increased speed** of CFD based hydrodynamic simulations **by 4000x** for 13-22% accuracy (or 14x with better accuracy)



CO2BOL - EEMPA

(a) Raschig Ring (b) Pro-Pak (c) Pall Ring (d) TPMS: Schwarz-D



CCSI² Part of a Family of PSE Projects

Multi-scale Process Modeling and Optimization

Uncertainty Quantification and Technical Risk Reduction

Design and Operation of Dynamic, Interacting Systems

Optimization-based Decision Support/Operations Research

PSE Application Areas (non-exhaustive):

- Point Source and Direct Air Capture
- Blue Hydrogen
- Low emission Power Generation
- Solid Oxide Fuel/Electrolyzer Cells
- Supercritical CO_2 Power Cycles
- Integrated Energy Systems
- Rare Earth Element/Critical Mineral Processing
- Water Treatment
- Produced Water Management & Optimization
- Methane Mitigation

Part of Several Collaborative Efforts Aimed at National and DOE Priorities:

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Carbon Capture Simulation for Industry Impact

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PARETO
The Produced Water Optimization Initiative

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

PRIMO

Water TAP

Acknowledgements

The CCSI[2] team gratefully acknowledges support from the U.S. DOE's Point Source Carbon Capture Program

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University of Pittsburgh: Katherine Hornbostel

University of Toledo: Glenn Lipscomb

University of Texas at Austin: Gary Rochelle, Miguel Abreu, Ben Drewry, Athreya Suresh, Miguel Torres

CCSI[2] Carbon Capture Simulation for Industry Impact

CCSI²

Carbon Capture Simulation for Industry Impact

For more information

https://www.acceleratecarboncapture.org/

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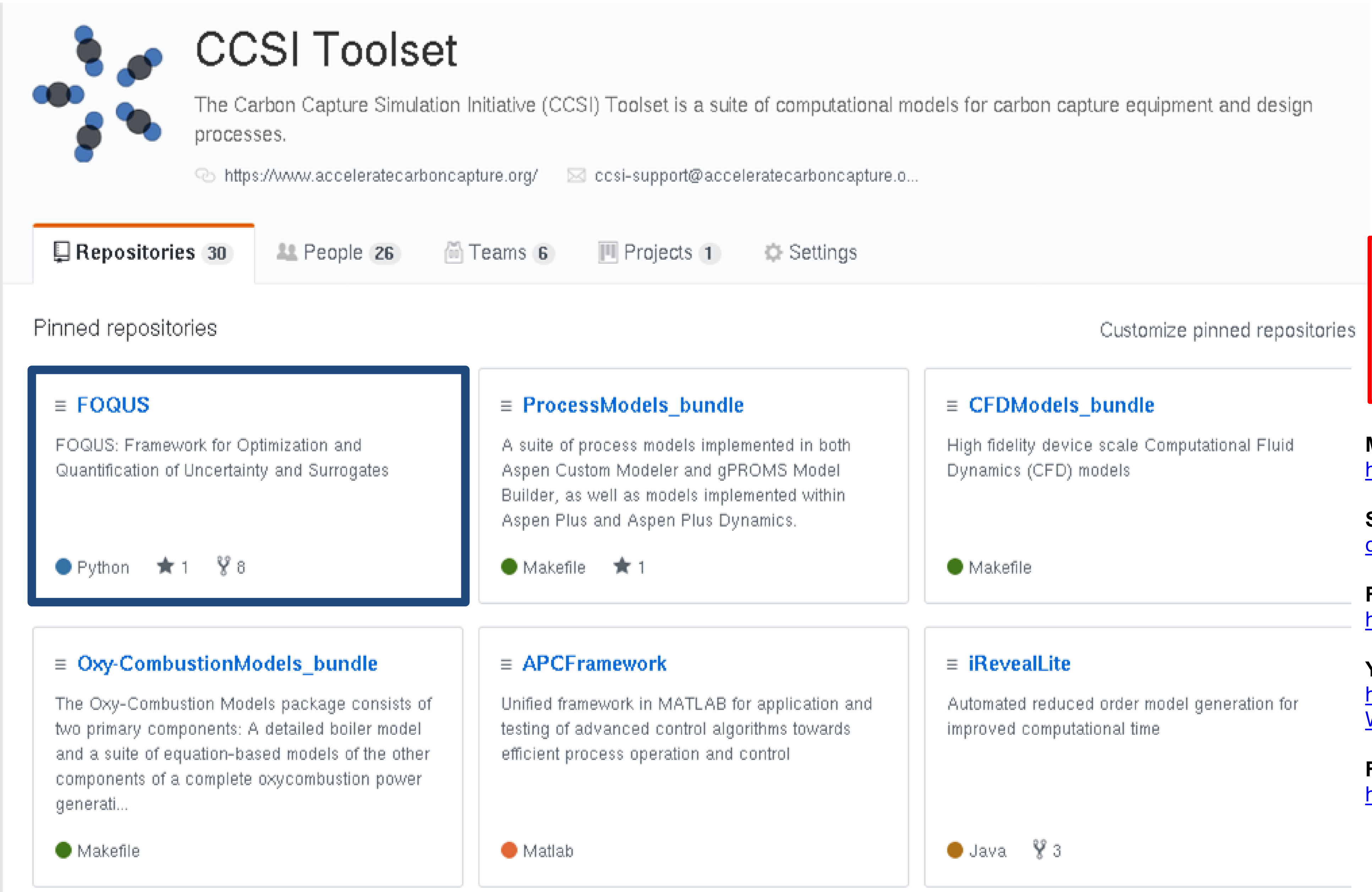
2023 Joint CCSI²/IDAES Technical Team Meeting, Lawrence Berkeley National Lab

U.S. DEPARTMENT OF ENERGY · NATIONAL ENERGY TECHNOLOGY LABORATORY · BERKELEY LAB · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · West Virginia University · University of Notre Dame · The University of Texas at Austin · UT · University of Pittsburgh · Carnegie Mellon

Toolset Publicly Available



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

Main website:
https://www.acceleratecarboncapture.org/

Support/Contact Us email:
ccsi-support@acceleratecarboncapture.org

FOQUS User Documentation:
https://foqus.readthedocs.io

YouTube Channel - tutorials:
https://www.youtube.com/channel/UCBVjFnxrsWpNlcnDvh0_GzQ/

FOQUS GitHub repo - development:
https://github.com/CCSI-Toolset/FOQUS

Capture Modeling and Analysis Capabilities

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

*Posters by: Morgan, Panagakos, Xu, Summits, Tsouris

*Posters by: Morgan, Hughes, Hedrick

*Demo by: Hughes, Hedrick

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Carbon Capture Simulation for Industry Impact

2016 R&D 100 WINNER

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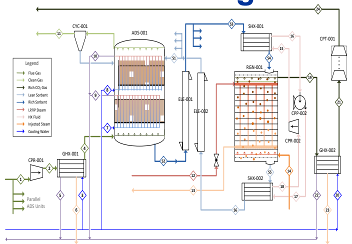
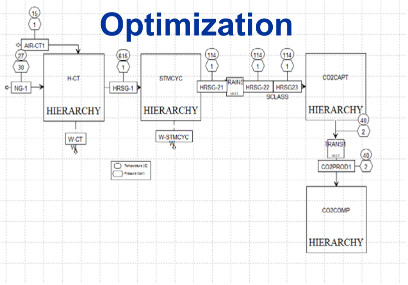
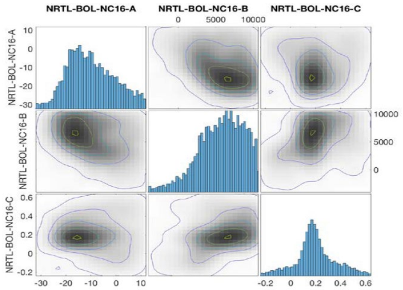
High-Fidelity, Multi-Scale Modeling



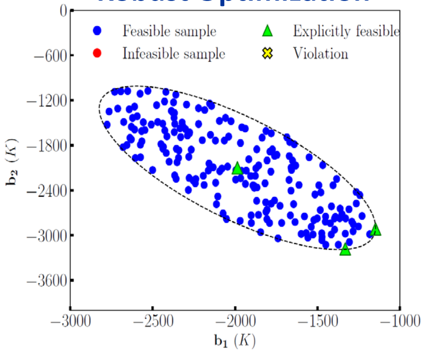
Process-level TEA Optimization



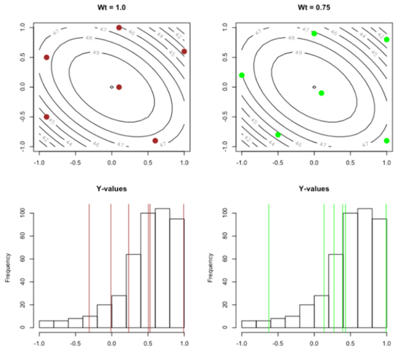
UQ and Parameter Optimization



Robust Optimization



Optimal DoE



Foundational Capabilities

- High-Fidelity CCS Modeling (sorbents, solvents, membranes)
- 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

*Poster by: Sherman

*Posters by: Nachtsheim, Wang

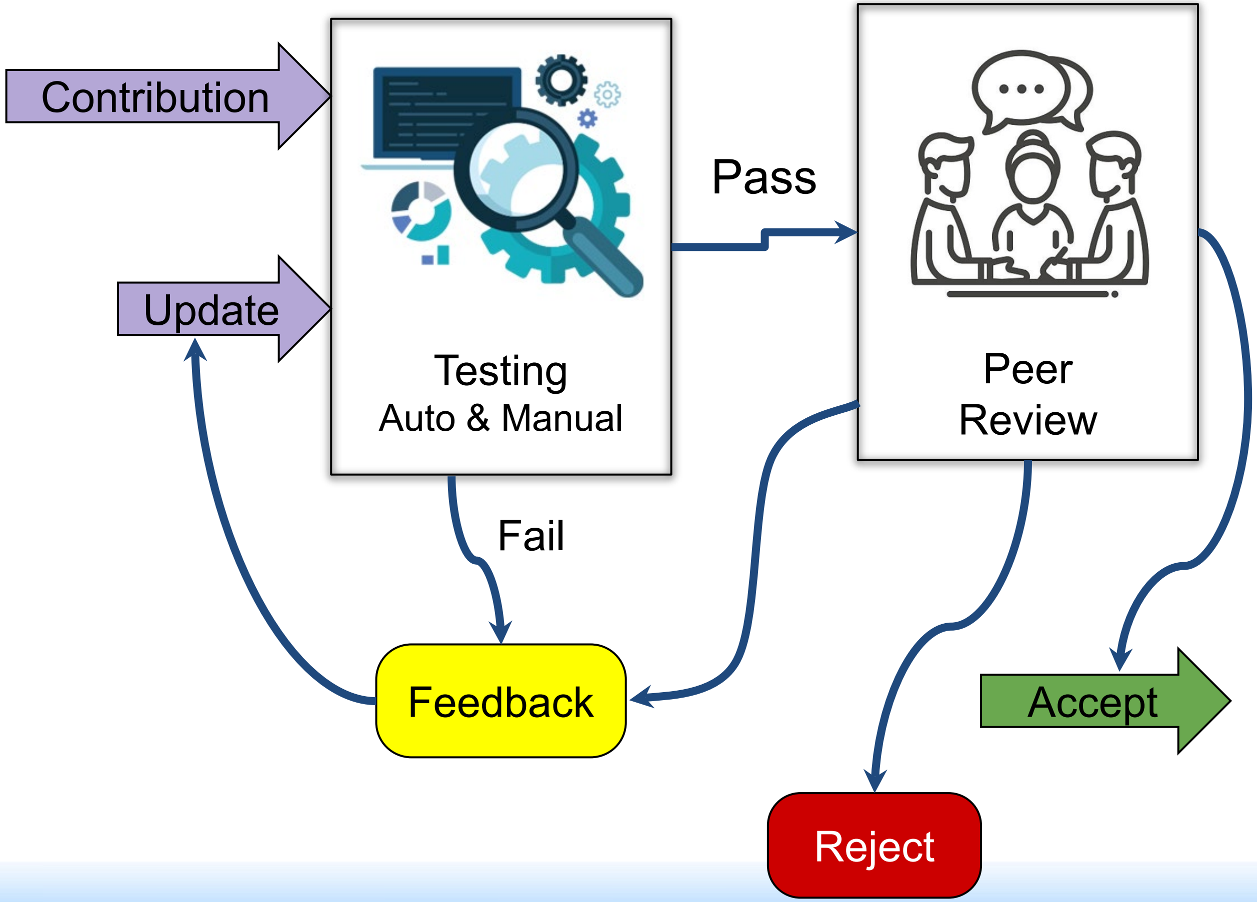
Open Source Toolset Development and Maintenance

- Code publicly available since 2017
- Permissive 3-clause BSD license
- All may use, modify or distribute (with attrib.)
- Examination and contributions welcomed

All Changes Tested and Reviewed

- Currently being used by dev team
- Contributions are tested (manual & auto)
- Peer reviewed by core team members
- Feedback, conversation, changes…
- Change is accepted or rejected
- NDA-Protected IP uses identical process

Two-Stage Code Review Process



Solvent Model Validation Hierarchy

Rationale

- **Fundamental interactions between CO_2 solvent and absorber packing** are poorly propagated between material and process length scales.
- Absorber packing sizing and performance predictions are largely empirically based, and **often use low fidelity engineering safety factors** to account for unknown commercial scale uncertainties.

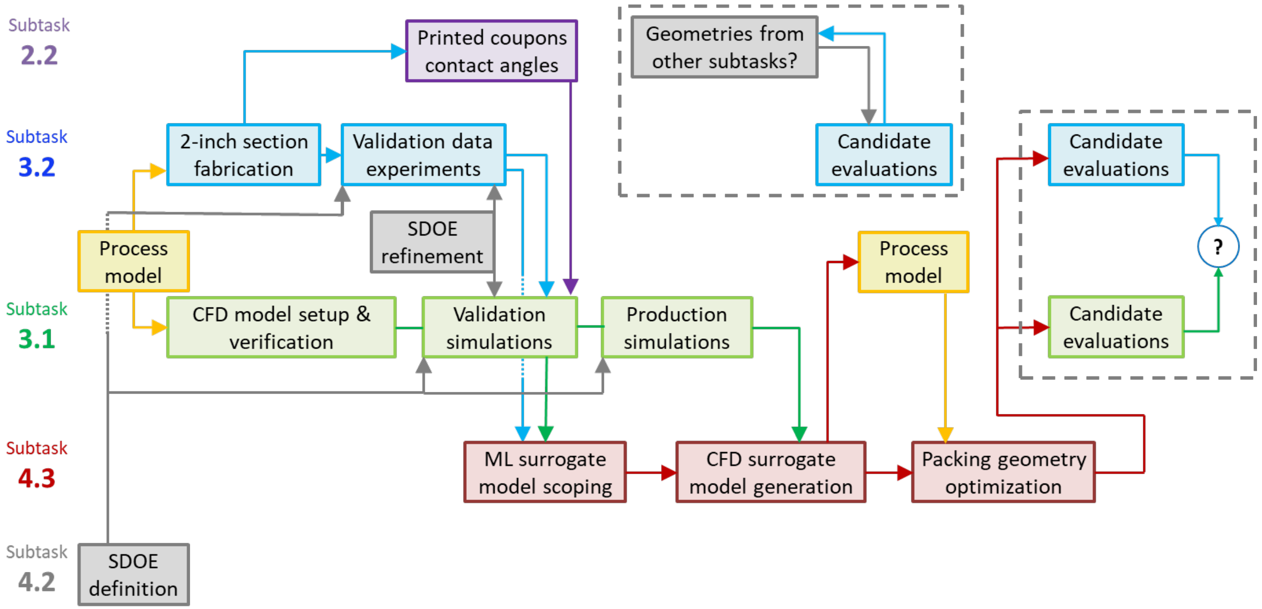
Approach

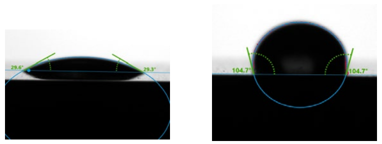
- Develop fundamental models of governing phenomena at **each length scale**
- **Couple multi-scale and multi-physics models**, reduce model complexity while retaining sufficient accuracy for meaningful performance predictions
- **Validate models** by generating prototype packing and testing carbon capture performance across a range of conditions, including arbitrary heat management throughout the column length.

Outcome

- A **cohesive modeling framework** that can propagate behavior induced by solvent, packing geometry, and packing material choices from the droplet scale through the process scale.
- Fundamental understanding of how to **optimize absorber design/operation for arbitrary solvents and capture targets**.

Solvent Model Validation Hierarchy Workflow

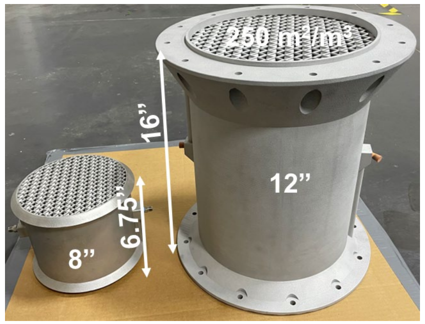




Solvent Contact Angle

8” column

12” column

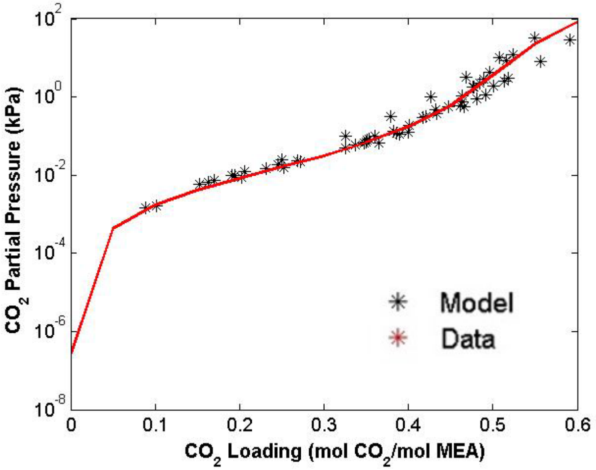


3D printed intercooled packing

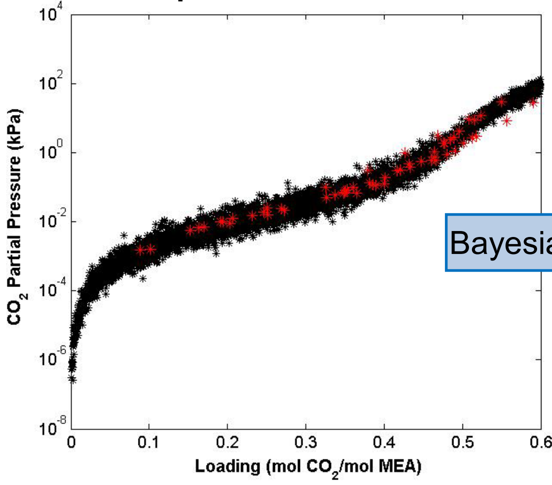
Uncertainty Quantification Bayesian Inference Example: VLE Models

VLE Data/Model Comparison at 40°C

Deterministic sub-model

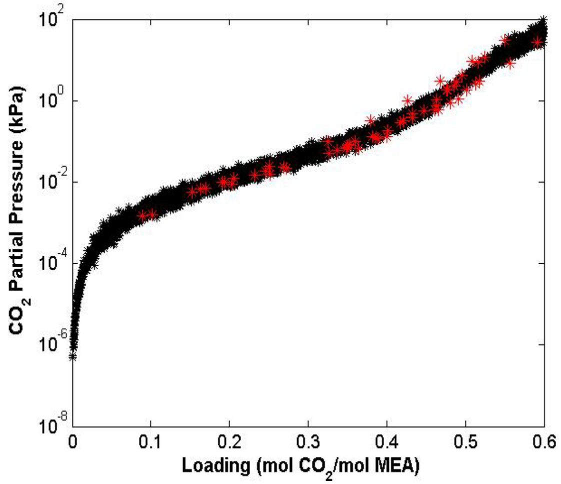


Using best initial guess of parameter set

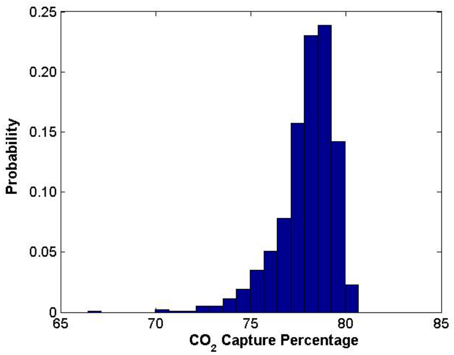


Bayesian inference

Refined parameter set

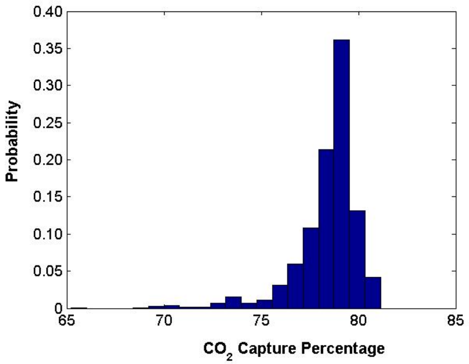


Process Model



high uncertainty

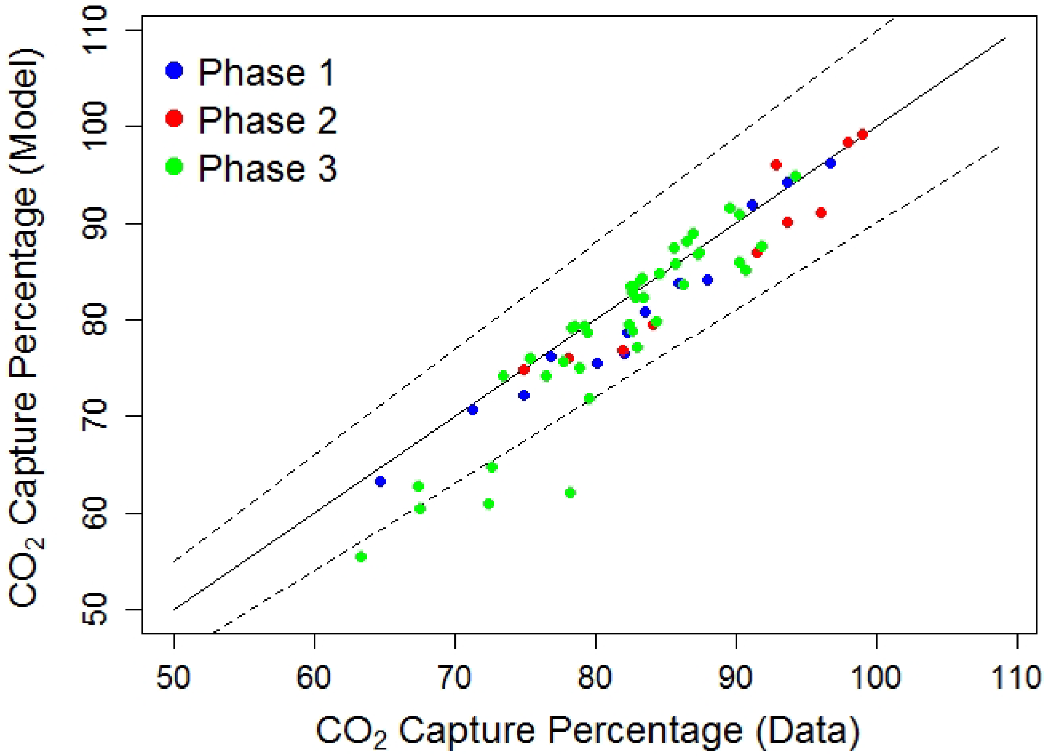
Process Model



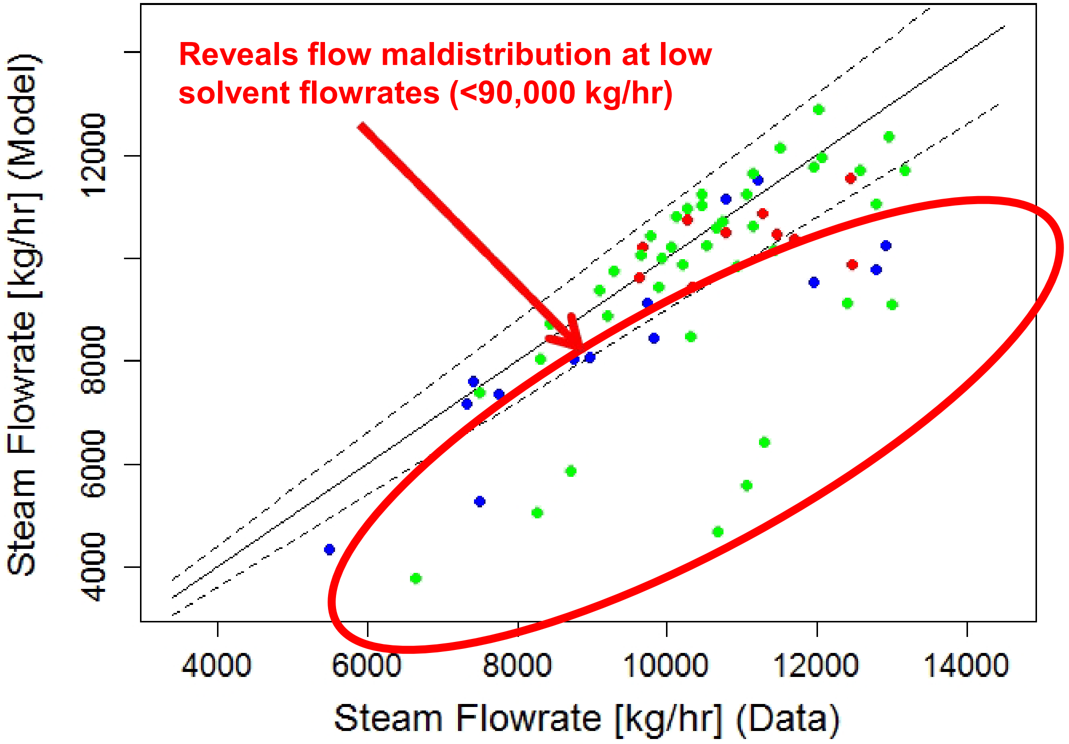
reduced uncertainty

Model Based Insight into Operational Non-Idealities

TCM Absorber Performance*



TCM Stripper Performance*



Fundamental Model Insight into Data Aberrations

*MEA solvent. Data include variation in flowrates of solvent, flue gas, steam, and CO_2 composition

SDoE Executive Summary

- **First-principles modeling** serves as the foundation for pilot campaign designs
- UQ can be used to **identify data gaps and their effect on key metrics**
- SDoE leverages UQ to more **efficiently inform data collection**
  - Improves MEA CO_2 capture rate prediction by ~60%
- Improved models support **better optimizations**
- Optimization under more refined uncertainty leads to more **robust designs**
- Modeling insights can be used to **guide future R&D decisions** more efficiently

Deterministic Solvent Modeling Framework

Vapor-Liquid Equilibrium

$$\hat{f}_i^V = \hat{f}_i^L \longrightarrow \hat{\varphi}_i y_i P = \gamma_i^* x_i H_i \quad \text{(for solutes)}$$

Activity Coefficient

$$ln(\gamma_i) = \frac{1}{RT}\frac{\partial(nG^{ex})}{\partial n_i}\bigg|_{T,P,n_{j\neq i}} \qquad \gamma_i^* = \frac{\gamma_i}{\lim\limits_{x_i\to 0}\gamma_i}$$

Reaction Equilibrium Constant

$$\Delta G_{rxn} = -RT ln(K)$$

Enthalpy Equations

Excess Enthalpy

$$H^{ex} = -RT^2 \sum_i x_i \left(\frac{\partial \ln \gamma_i}{\partial T}\right)\bigg|_{P,x}$$

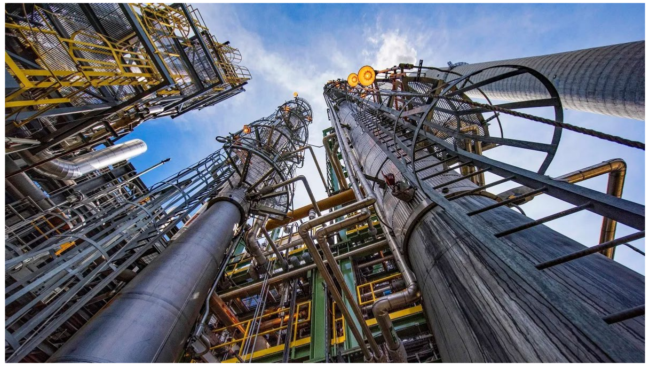
Heat Capacity

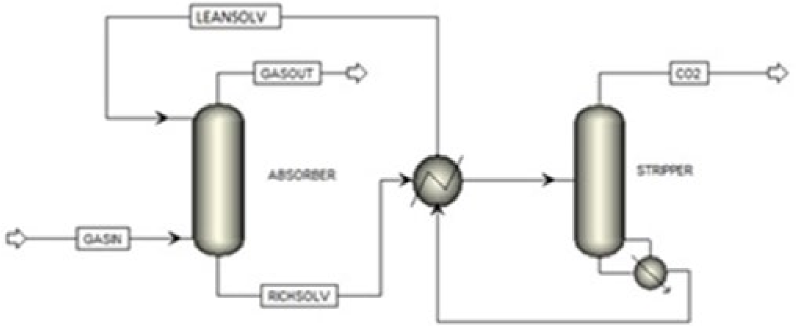
$$H_m{}^l(T+\Delta T) - H_m{}^l(T) = \int_T^{T+\Delta T} C_{p,m}{}^l dT$$

Heat of Absorption

$$\Delta H_{abs} = \frac{n_{final}H_{final} - n_{initial}H_{initial} - n_{CO_2}H_{CO_2}}{n_{CO_2}}$$

Deterministic Solvent Modeling Framework





- Validated for National Carbon Capture Center (NCCC) (MEA solvent)
- Validated for Technology Centre Mongstad (TCM) (MEA solvent)

Novel Solvent-Specific Uncertainty Quantification

Activity Coefficients

$$\ln \gamma_i = \frac{\sum_j X_j G_{j,i} \tau_{j,i}}{\sum_k X_k G_{k,i}} + \sum_j \frac{G_{i,j} X_j}{\sum_k G_{k,j} X_k} \cdot \left(\tau_{i,j} - \frac{\sum_m X_m G_{m,j} \tau_{m,j}}{\sum_k X_k G_{k,j}} \right)$$

$$\ln H_{ia} = \boxed{A_{ia}} + \frac{B_{ia}}{T}$$

$$\tau_{i,j} = A_{i,j} + \frac{B_{i,j}}{T}$$

$$\ln P_i^{vap} = A_i + \frac{B_i}{T + C_i}$$

$$G_{i,j} = e^{(-\alpha_{i,j} \tau_{i,j})}$$

Mass Transfer

$$k_G = D_G C_G \left(\frac{a}{d_H} \right)^{0.5} Sc_G{}^{0.333} Re_G^{0.75} \sqrt{\frac{1}{\varepsilon - h_L}}$$

Viscosity

$$\ln \mu_{BOLs} = A_{BOLs} + \frac{B_{BOLs}}{T} + C_{BOLs} \cdot \ln T$$

$$w_{H2O} = \frac{\alpha_{H2O} \cdot MW_{H2O}}{\alpha_{H2O} \cdot MW_{H2O} + MW_{BOL}}$$

$$\mu_{BOLs-H2O} = \mu_{BOLs} \cdot (1 - w_{H2O}) + \mu_{H2O} \cdot w_{H2O} + D_{Binary} \cdot w_{H2O} \cdot (1 - w_{H2O})$$

$$\mu_{BOLs-CO2-H2O} = \mu_{BOLs-H2O} \cdot e^{\alpha_{CO2} \cdot E_{CO2}}$$

Kinetics

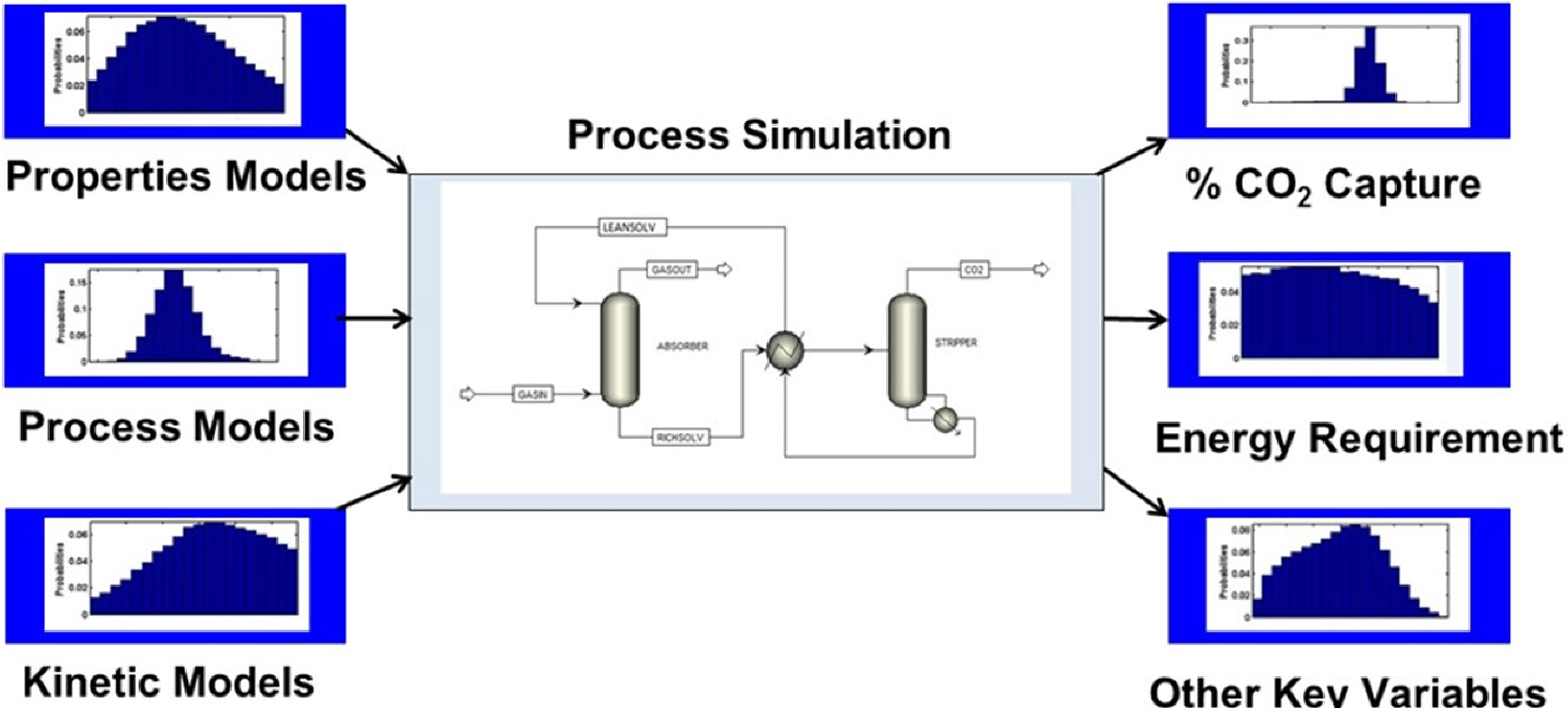
$$2CO_2 + 2BOL \leftrightarrow \{BOL - CD^+\} + \{BOL - CD^-\}$$

$$r_1 = k_1 \exp\left(-\frac{E_1}{R} \left(\frac{1}{T} - \frac{1}{T^{ref}} \right) \right) a_{CO_2} a_{BOL} \left(1 - \frac{a_{BOL-CD^+} a_{BOL-CD^-}}{(a_{CO_2} a_{BOL})^2 K_1} \right)$$

$$CO_2 + BOL + H_2O \leftrightarrow \{BOLH^+\} + \{HCO_3^-\}$$

$$r_2 = k_2 \exp\left(-\frac{E_2}{R} \left(\frac{1}{T} - \frac{1}{T^{ref}} \right) \right) a_{CO_2} a_{BOL} a_{H_2O} \left(1 - \frac{a_{BOLH^+} a_{HCO_3^-}}{K_2} \right)$$

Novel Solvent-Specific Uncertainty Quantification



Bayesian Inference

- **Bayesian Inference** provides a framework for updating beliefs of model parameters characterized by epistemic uncertainty in light of collection of new data

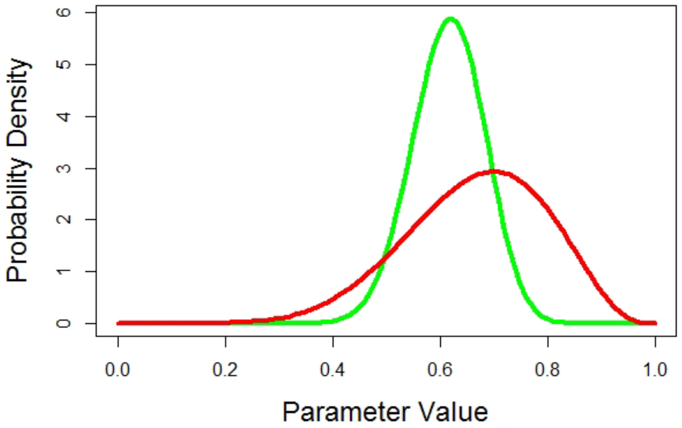
$$\pi(\theta|Z) \propto P(\theta) * L(Z|\theta)$$

Posterior **Prior** **Likelihood**

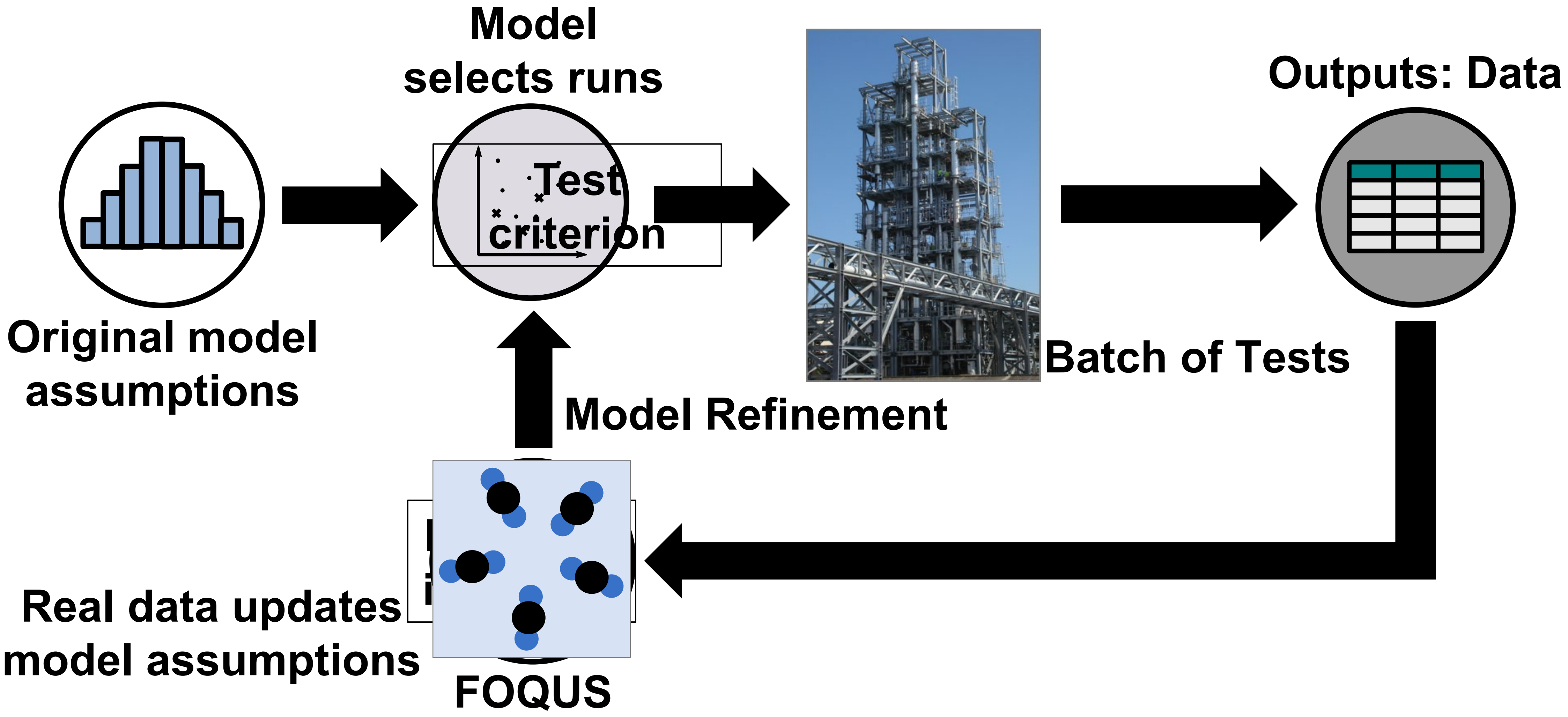
Typical likelihood function (represents discrepancy between model predictions and data values of the output:

$$L(Z|\theta) = exp\left(-0.5\sum_{i=1}^{M}\frac{\left[F^{*}(x_{i,}\theta) - Z(x_i)\right]^2}{M{\sigma_i}^2}\right)$$

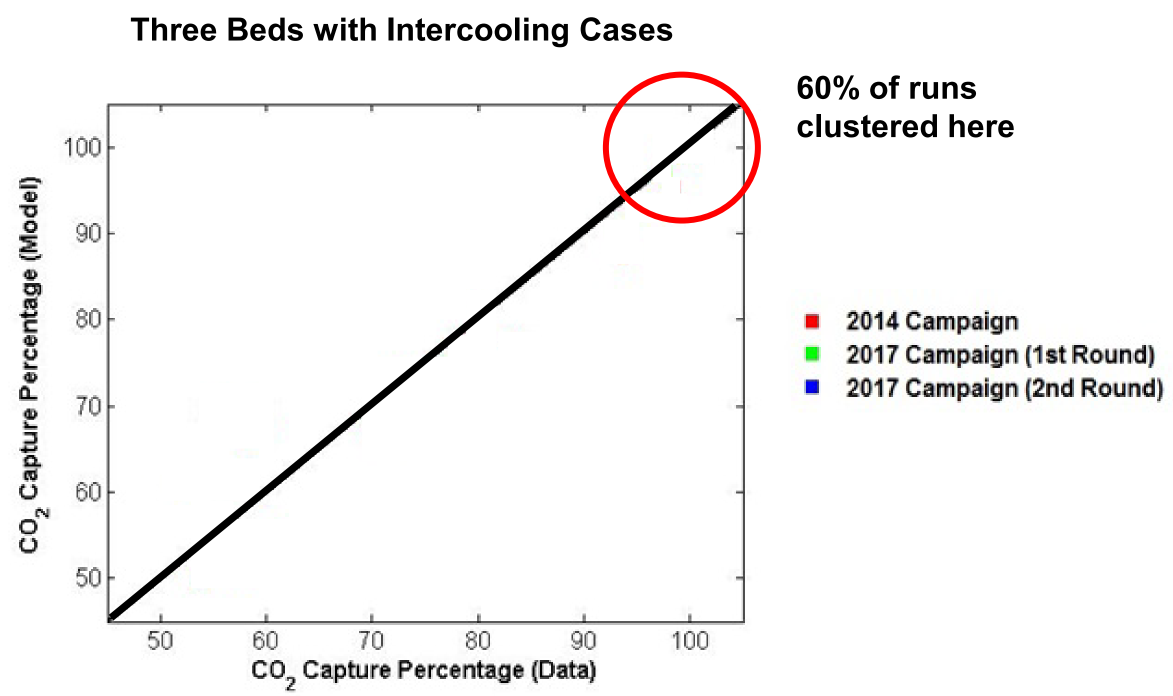
Representation of Prior and Posterior Distributions (reduction in uncertainty through data collection):



Sequential Design of Experiments Leverages Real Time Data Generation for Optimal Batch Generation



NCCC Model Improvement with SDoE Implementation



2014 Campaign (Before SDoE)

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

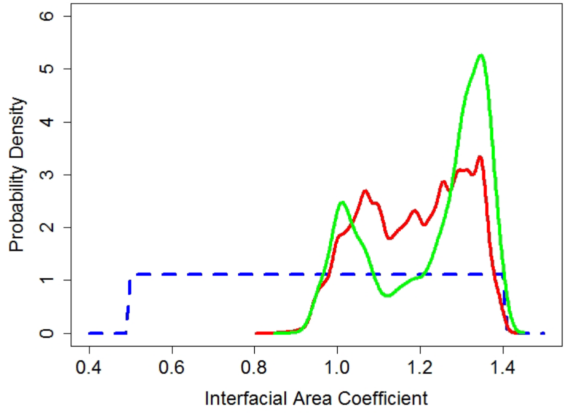
Wait 3 years….

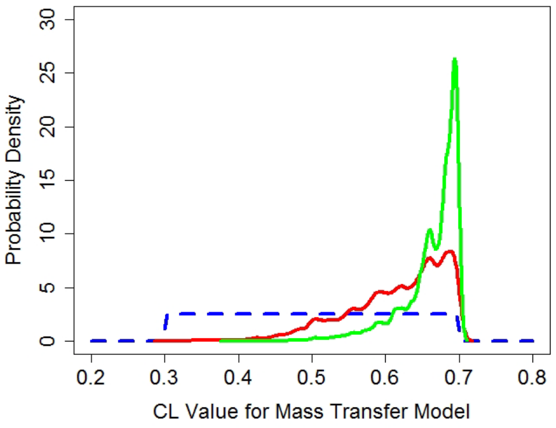
2017 Campaign (Using SDoE)

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

TCM Model Improvement with SDoE Implementation

Update in Parameter Distributions for Absorber Packing



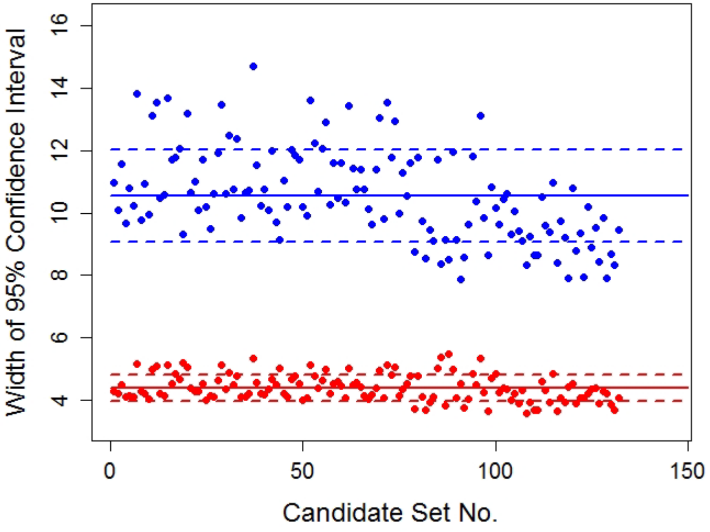


Mass transfer and interfacial area parameters are packing-dependent, and therefore are assigned uniform prior distributions over wide ranges, indicating assumption of relatively large uncertainty before collection of process data.

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

Prior
Posterior 1
Posterior 2

Reduction in CO_2 Capture Percentage Prediction Accuracy



Prior CI Width: (10.5 ± 1.5)%

Posterior CI Width: (4.4 ± 0.4)%

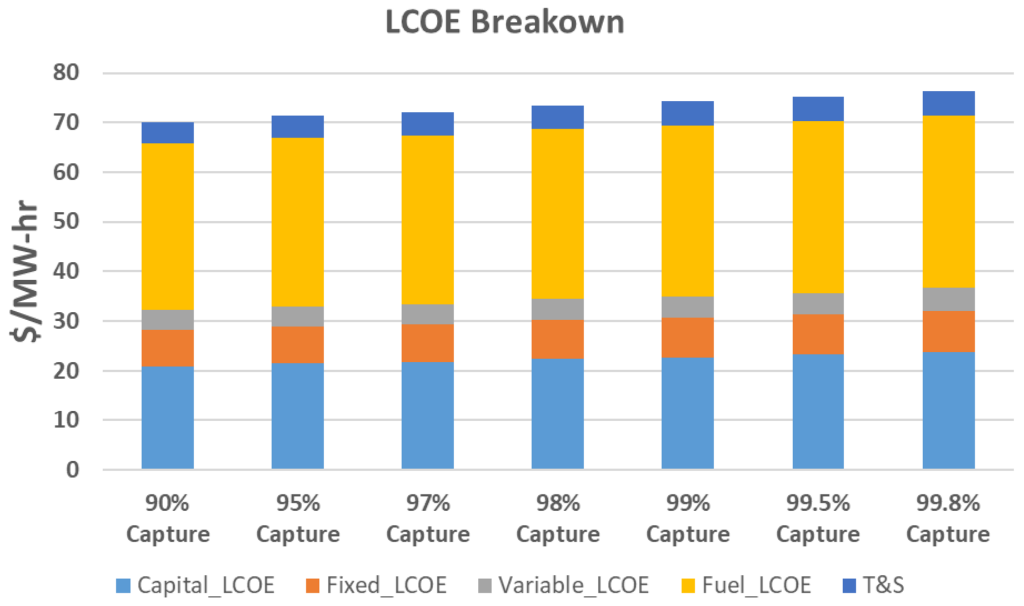
Average reduction in uncertainty: 58.0 ± 4.7%

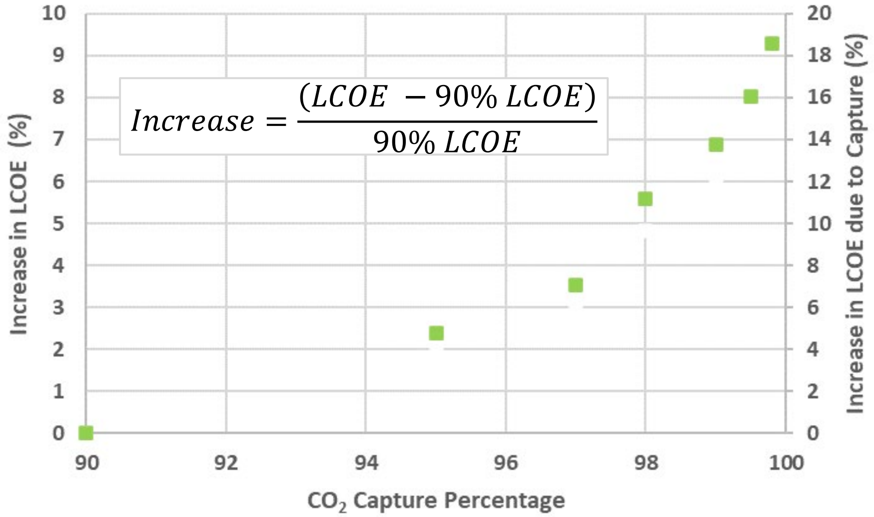
<u>Candidate set includes variation in</u>:

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

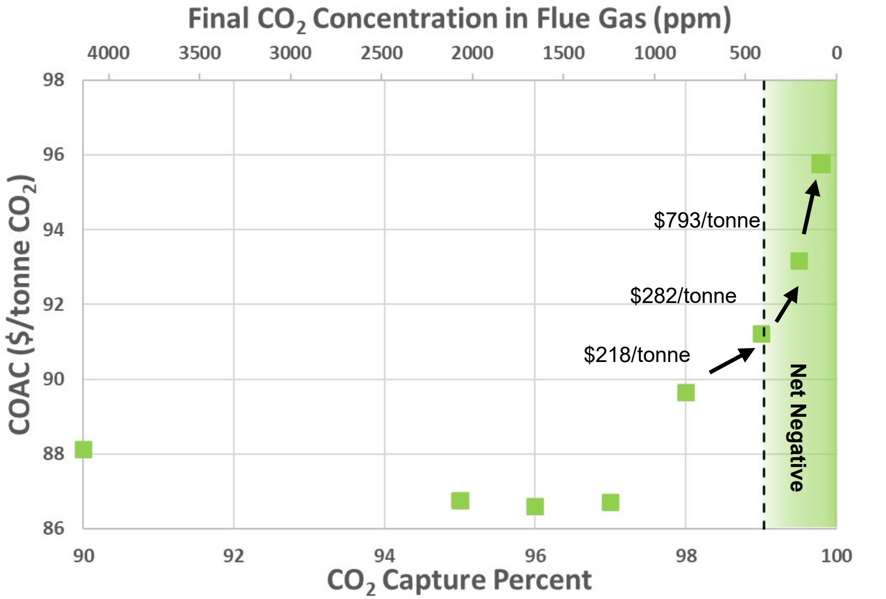
High Capture Rates with MEA Solvent - NGCC

*More Detail in Poster by Ben Omell



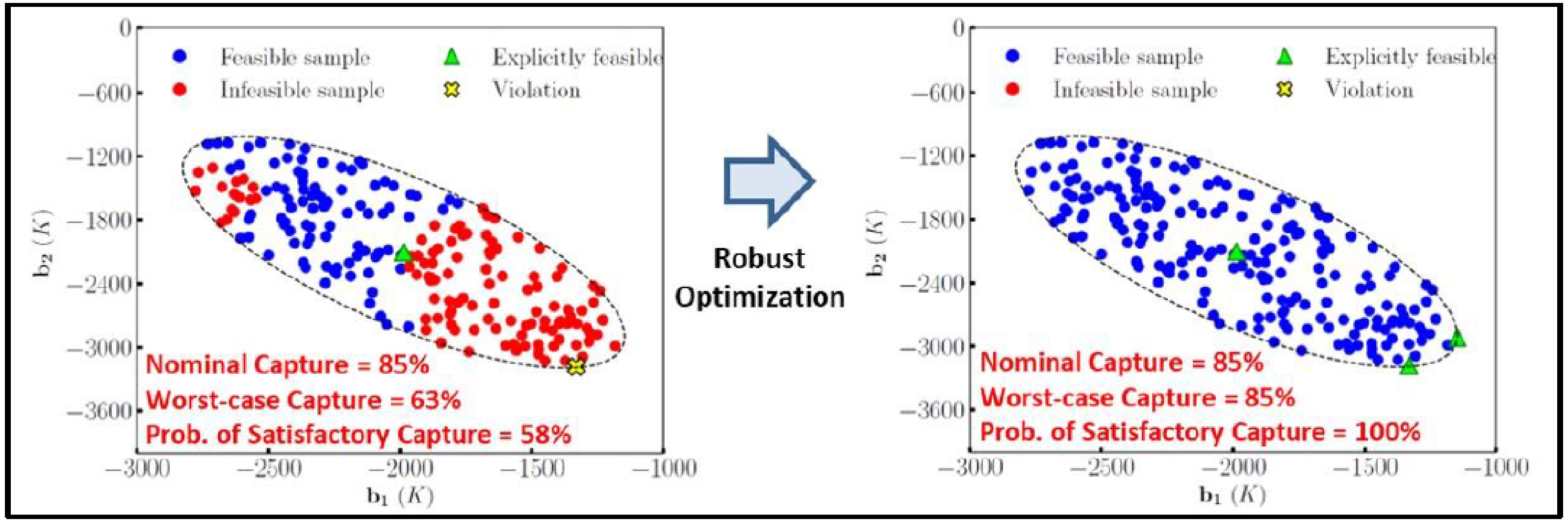


- **LCOE increases linearly from 90→98%,** relatively constant cost of avoided CO_2.
- Incremental **cost of avoided CO_2 significantly increases** in 98→99.8% capture range.
- Practical considerations (e.g., **need for aux boiler, flexible operation**) will increase LCOE further at high capture percentages

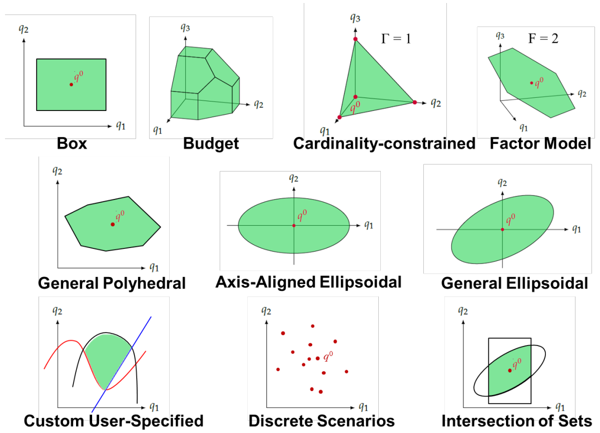


CCSI²
Carbon Capture Simulation for Industry Impact

PyROS: a Pyomo Robust Optimization Solver



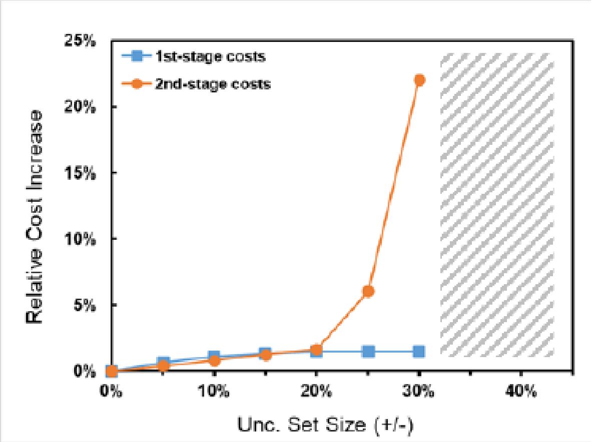
*More Detail in Poster by Jason Sherman



Designs optimized deterministically can easily become infeasible with moderate uncertainty

Robust optimized designs can ensure safety and performance constraints are met amidst anticipated uncertainty

Evolution of costs for increasingly robust designs



Price of robustness can be quantified, minimized