2023 PSE+ Stakeholder Workshop: Carbon Capture Simulation for Industry Impact ($CCSI^2$)

Michael Matuszewski
$CCSI^2$ Associate Technical Director

Westin Hotel and Conference Center
Tysons Corner, VA
10/11/2023

CCSI^2 – Modeling, Optimization, and Technical Risk Reduction

CCSI^2

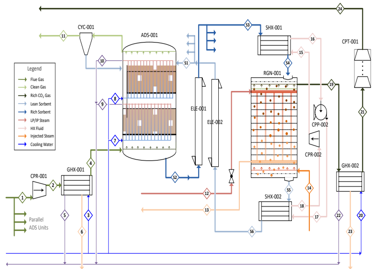
Carbon Capture Simulation for Industry Impact

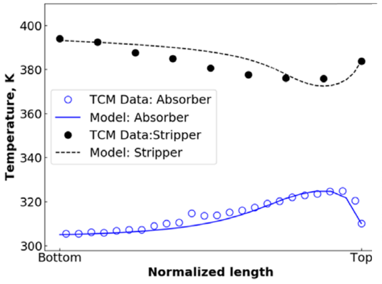
Multi-lab modeling initiative to support carbon capture technology development

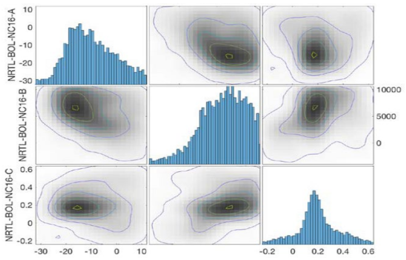
NATIONAL ENERGY TECHNOLOGY LABORATORY | BERKELEY LAB | Lawrence Livermore National Laboratory | Los Alamos NATIONAL LABORATORY EST. 1943 | Pacific Northwest NATIONAL LABORATORY | OAK RIDGE National Laboratory

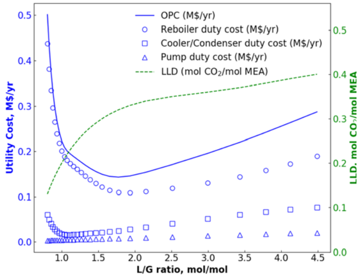
Carnegie Mellon | West Virginia University | UNIVERSITY OF NOTRE DAME | THE UNIVERSITY OF TEXAS AT AUSTIN | UT | UNIVERSITY OF PITTSBURGH

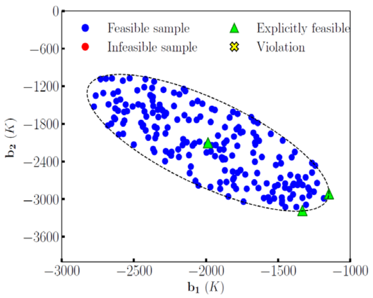
Modeling			Optimization	Risk Reduction	
High Fidelity Process Modeling	Model Validation	Uncertainty Quantification	Process Optimization	Robust Design	Maximizing Learning

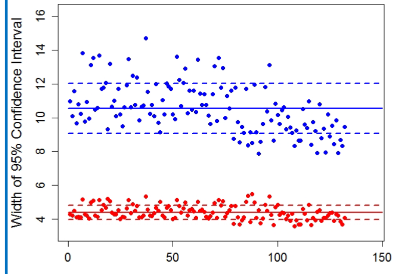












Open Source: github.com/CCSI-Toolset

Past and Present CCSI/CCSI² Industrial Collaborations

ADA: Solids heat exchanger modeling and bottlenecks
GE: Key characterizers of amino-silicone solvent performance
CAER: Dynamic CCS modeling and advanced process control (power/steel)
TDA Research: Sorbent pilot test support via DoE
RTI International: **NAS solvent process modeling and pilot support via SDoE**
SINTEF: **Solvent VLE and emissions modeling**
EPRI Electric Power Research Institute: EEMPA solvent and process modeling and optimization
MTR Membrane Technology & Research: Membrane module and process modeling for pilot support
CHART: Cryogenic capture process modeling
USS: Membrane module and process modeling (steel)
Honeywell UOP: Piperazine process modeling
SRI International: Requested to support mixed salt solvent pilot via SDoE
Chevron: Requested to support sorbent pilot via SDoE
National Carbon Capture Center: MEA Baseline Campaign process modeling and SDoE
CO_2 Technology Centre Mongstad: MEA Baseline Campaign process modeling and SDoE

*Highlighted by Marty Lail at 1:30 on Oct 11th
*Poster by Josh Morgan

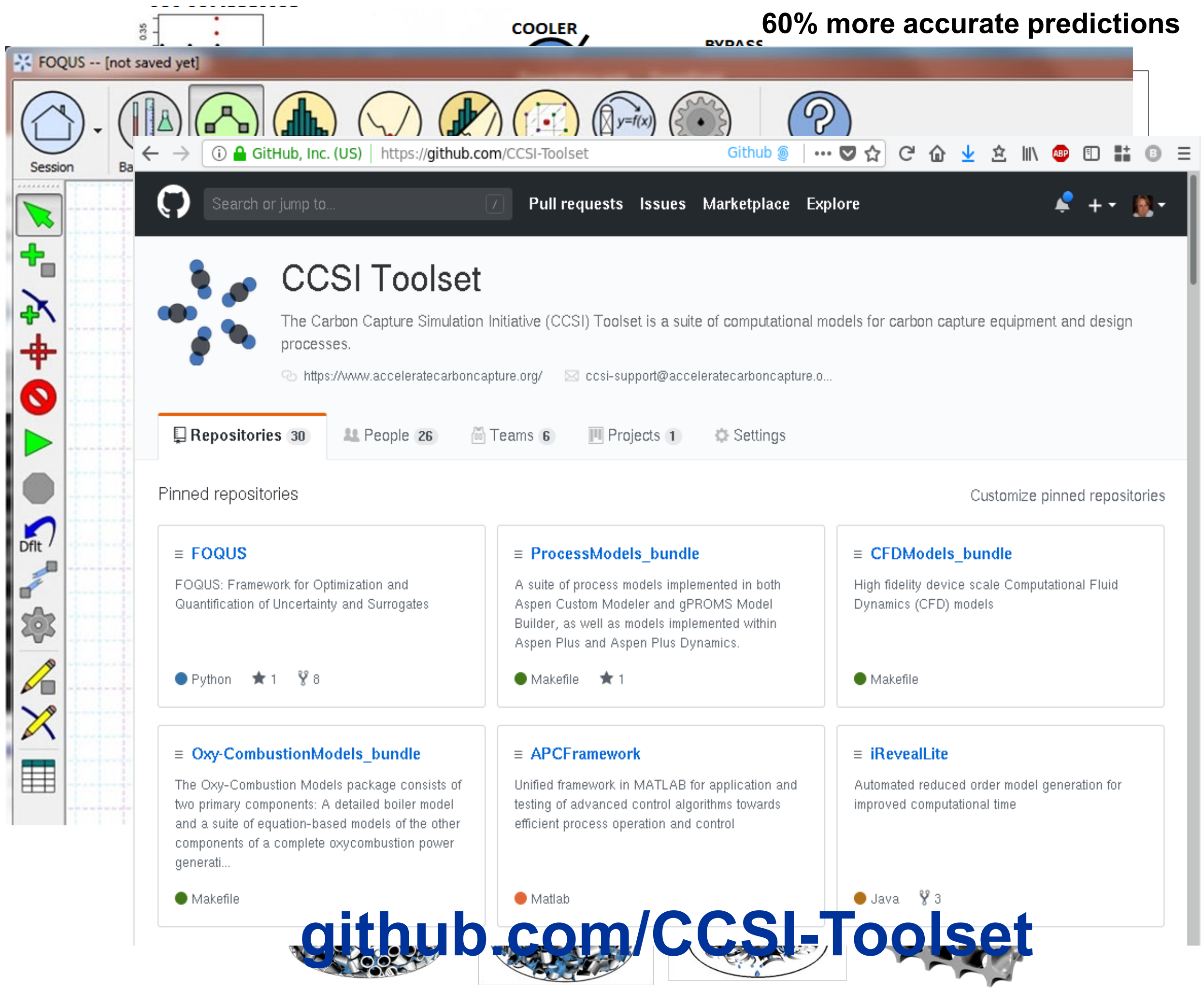
Since 2010 CCSI/CCSI² Supported 16 Carbon Capture projects $100MM+ in total project value (TRL 3-7)

CCSI² Carbon Capture Simulation for Industry Impact

Past
Present
Non-FECM Funded

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**
- **Novel Solvent and Process Optimization**
  - CFD to elucidate novel solvent/packing interaction, contact angle, interfacial area.
  - Rigorously ensures proper balance of cost and performance. Minimize captured cost of 1. PNNL CO_2BOL Process **(>10% improvement over baseline)**, 2. Advanced Solvent Flash Stripper Process (optimization performed for multiple solvents)
- **Process Intensification/Equipment Design**
  - Intensified solvent absorber design can **improve capture rates by >10%**
- **Machine Learning**
  - **Increased speed** of CFD based hydrodynamic simulations **by 4000x** for 13-22% accuracy (or 14x with better accuracy)
- **Computational Toolset Maintenance**
  - Regular software updates and revision management – **open source**



Toolset Publicly Available

*More Detail by Ryan Hughes at 1:15 on Oct 12th

github.com/CCSI-Toolset

CCSI Toolset

The Carbon Capture Simulation Initiative (CCSI) Toolset is a suite of computational models for carbon capture processes.

https://www.acceleratecarboncapture.org/ ccsi-support@acceleratecarboncapture.o...

Repositories 30 People 26 Teams 6 Projects 1 Settings

R&D 100

2016 R&D 100 Awards

Pinned repositories

FOQUS
FOQUS: Framework for Optimization and Quantification of Uncertainty and Surrogates
Python ★ 1 8

ProcessModels_bundle
A suite of process models implemented in both Aspen Custom Modeler and gPROMS Model Builder, as well as models implemented within Aspen Plus and Aspen Plus Dynamics.
Makefile ★ 1

CFDModels_bundle
High fidelity device scale Computational Fluid Dynamics (CFD) models
Makefile

Oxy-CombustionModels_bundle
The Oxy-Combustion Models package consists of two primary components: A detailed boiler model and a suite of equation-based models of the other components of a complete oxycombustion power generati...
Makefile

APCFramework
Unified framework in MATLAB for application and testing of advanced control algorithms towards efficient process operation and control
Matlab

iRevealLite
Automated reduced order model generation for improved computational time
Java 3

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

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

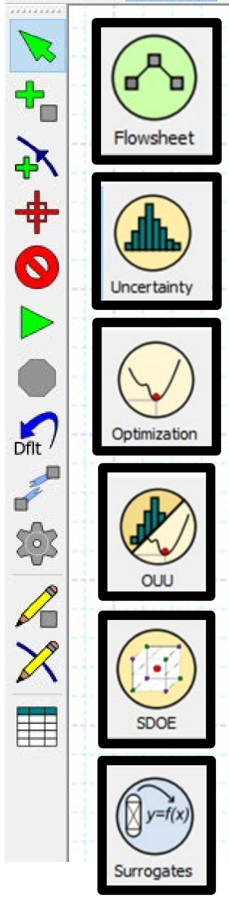
FOQUS User Documentation:
https://foqus.readthedocs.io

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

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

CCSI² FOQUS Framework

*Demonstration by Ryan Hughes at 1:15 on Oct 12th

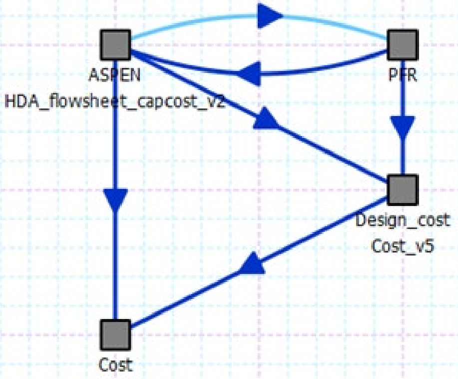


- Interface connecting commercial and open source modeling platforms (Aspen, gPROMS, Python, Pyomo, Excel). Uses your models.

- 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.

*More Detail by Abby Nachtsheim and Alex Dowling at 1:15 on Oct 12th and Poster by Jialu Wang

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

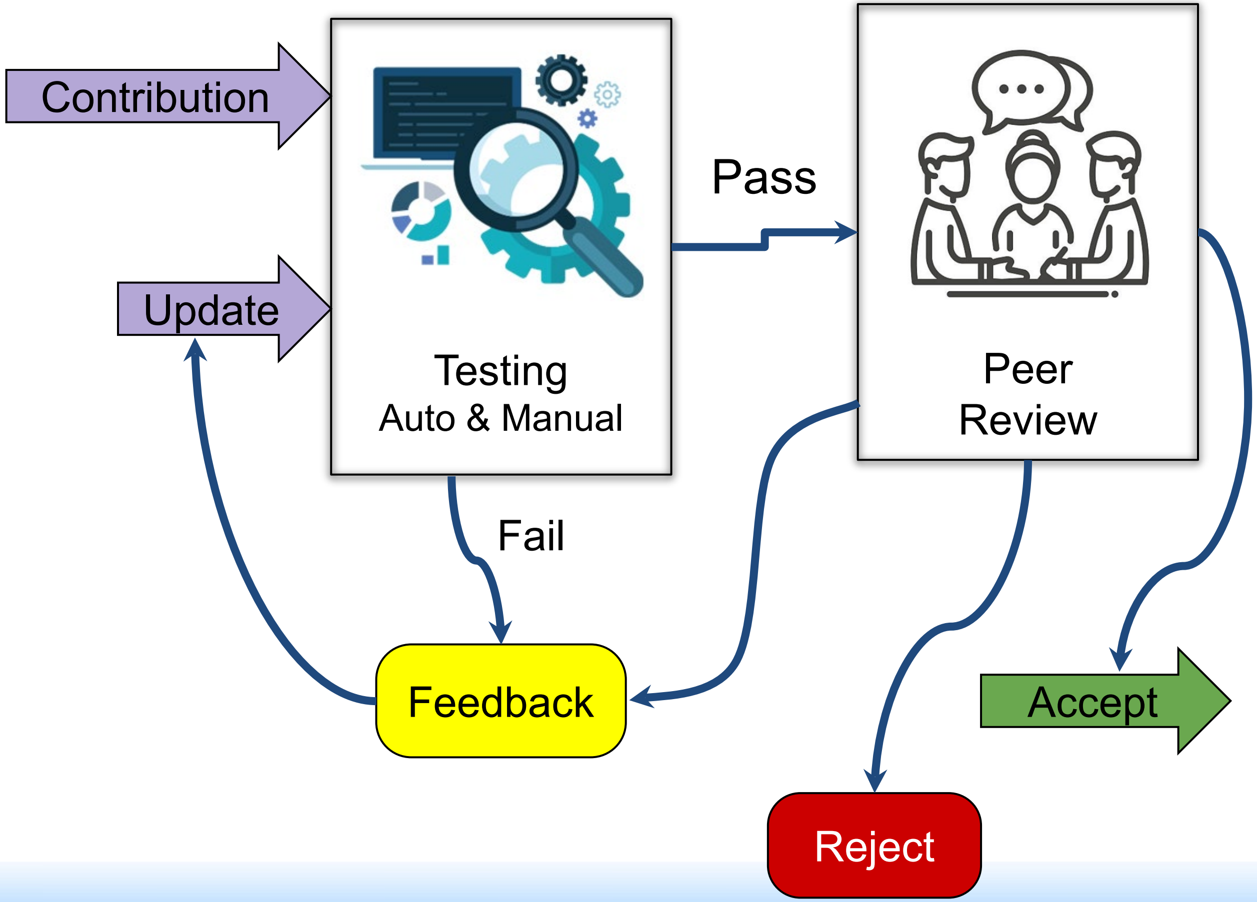
Open Source Toolset Development and Maintenance

- 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



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

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

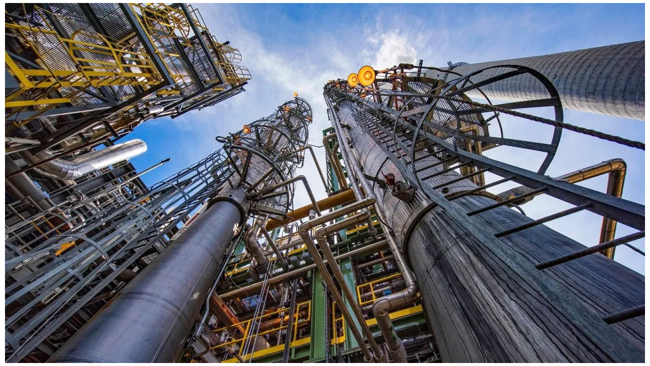
Heat Capacity

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

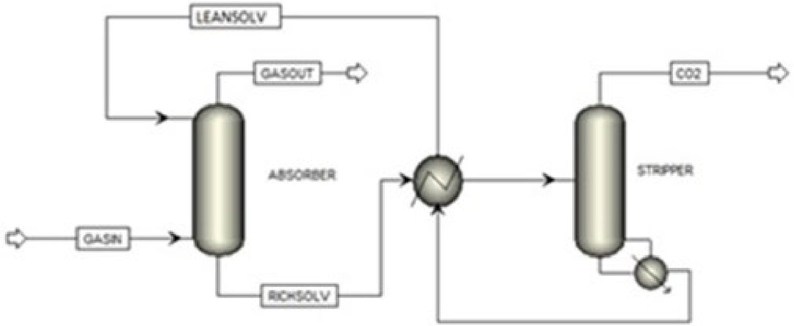
Heat of Absorption

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

Deterministic Solvent Modeling Framework



NATIONAL CARBON CAPTURE CENTER



TECHNOLOGY CENTRE MONGSTAD

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

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.

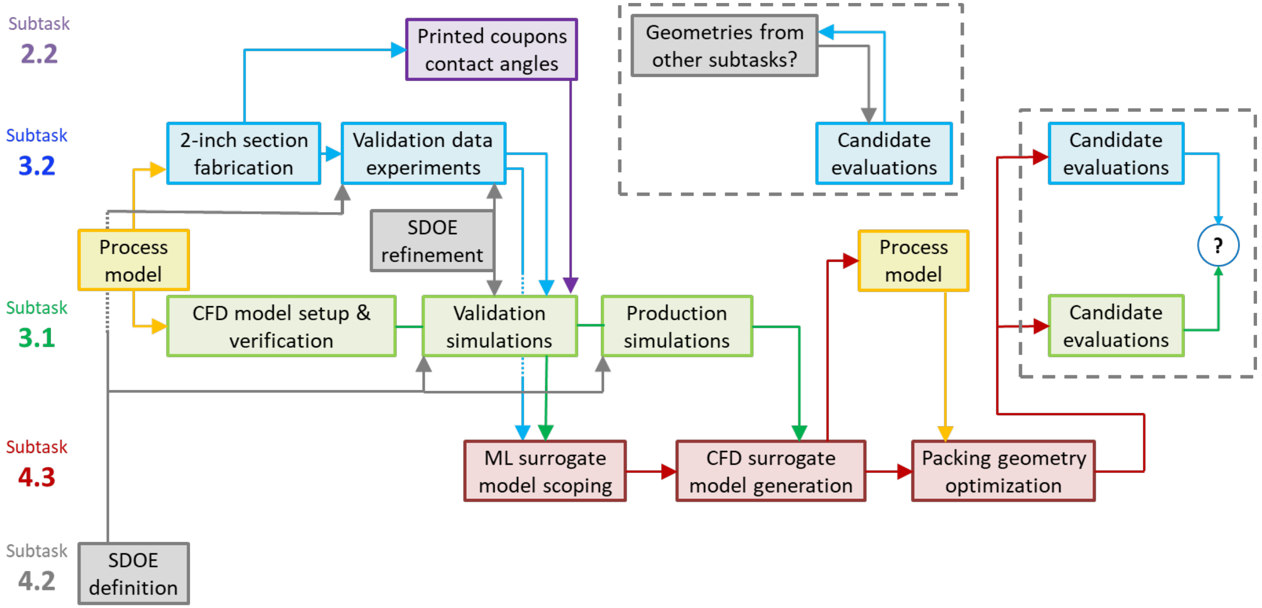
Approach

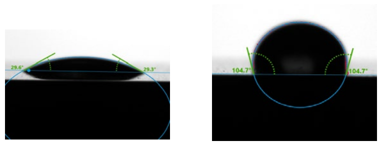
- Develop fundamental models of governing phenomena at **each length scale**
- **Couple multi-scale and multi-physics models**, reduce model complexity while retaining sufficient accuracy for meaningful performance predictions
- **Validate models** by generating prototype packing and testing carbon capture 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

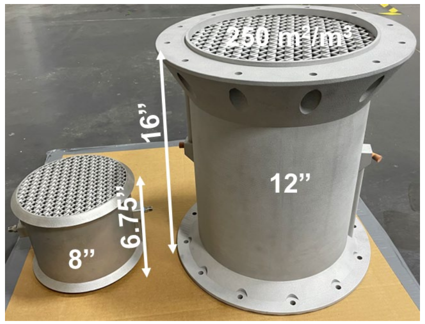




Solvent Contact Angle

8” column

12” column



3D printed intercooled packing

Novel Solvent-Specific Uncertainty Quantification

Activity Coefficients

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

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

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

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

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

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

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

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

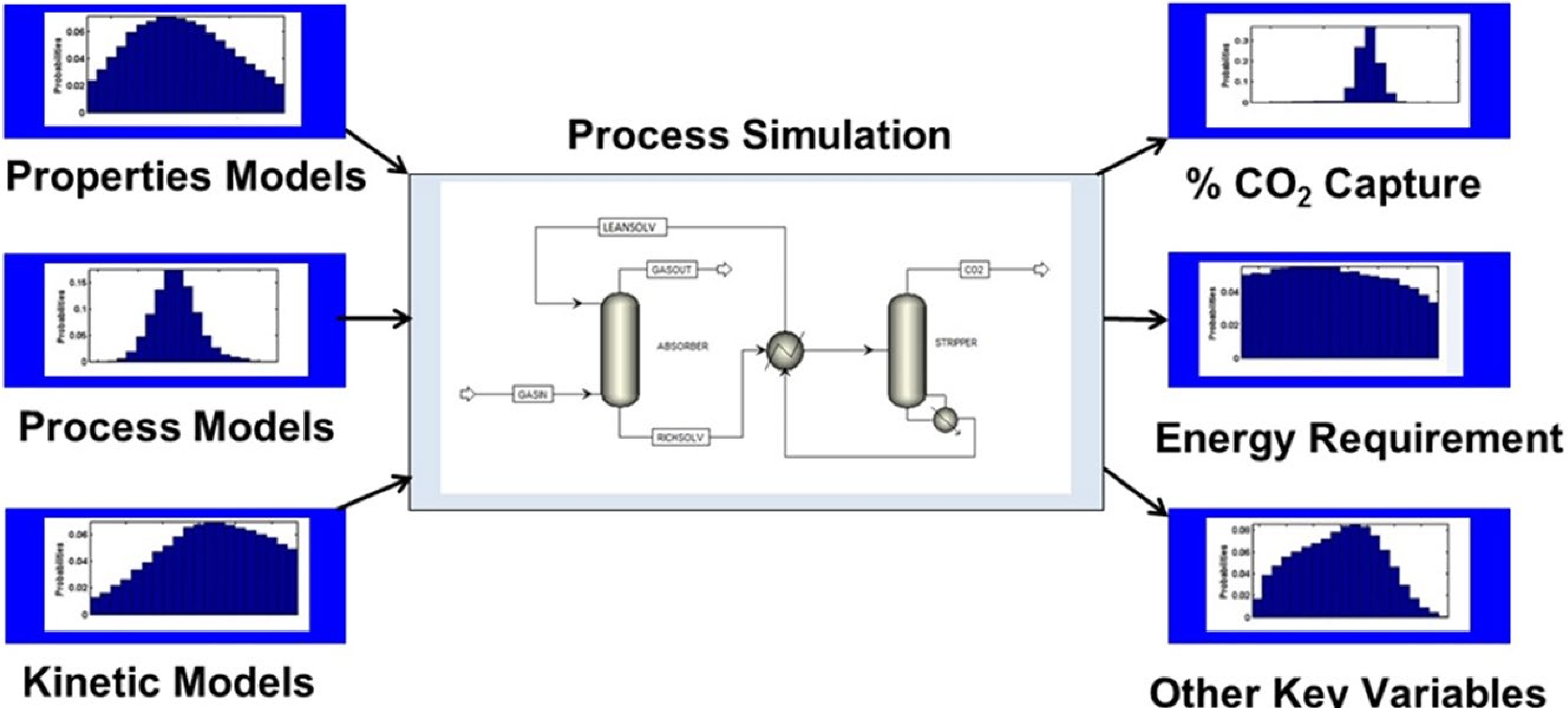
$$CO_2 + BOL + H_2O \leftrightarrow \{BOLH^+\} + \{HCO_3^-\}$$

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

Mass Transfer

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

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

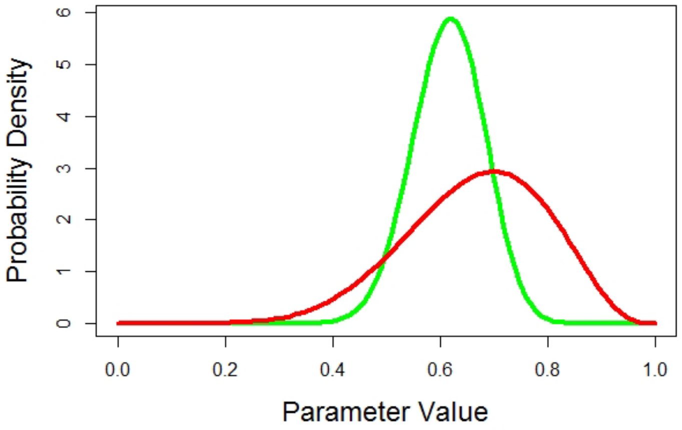
$$\pi(\theta|Z) \propto P(\theta) * L(Z|\theta)$$

Posterior **Prior** **Likelihood**

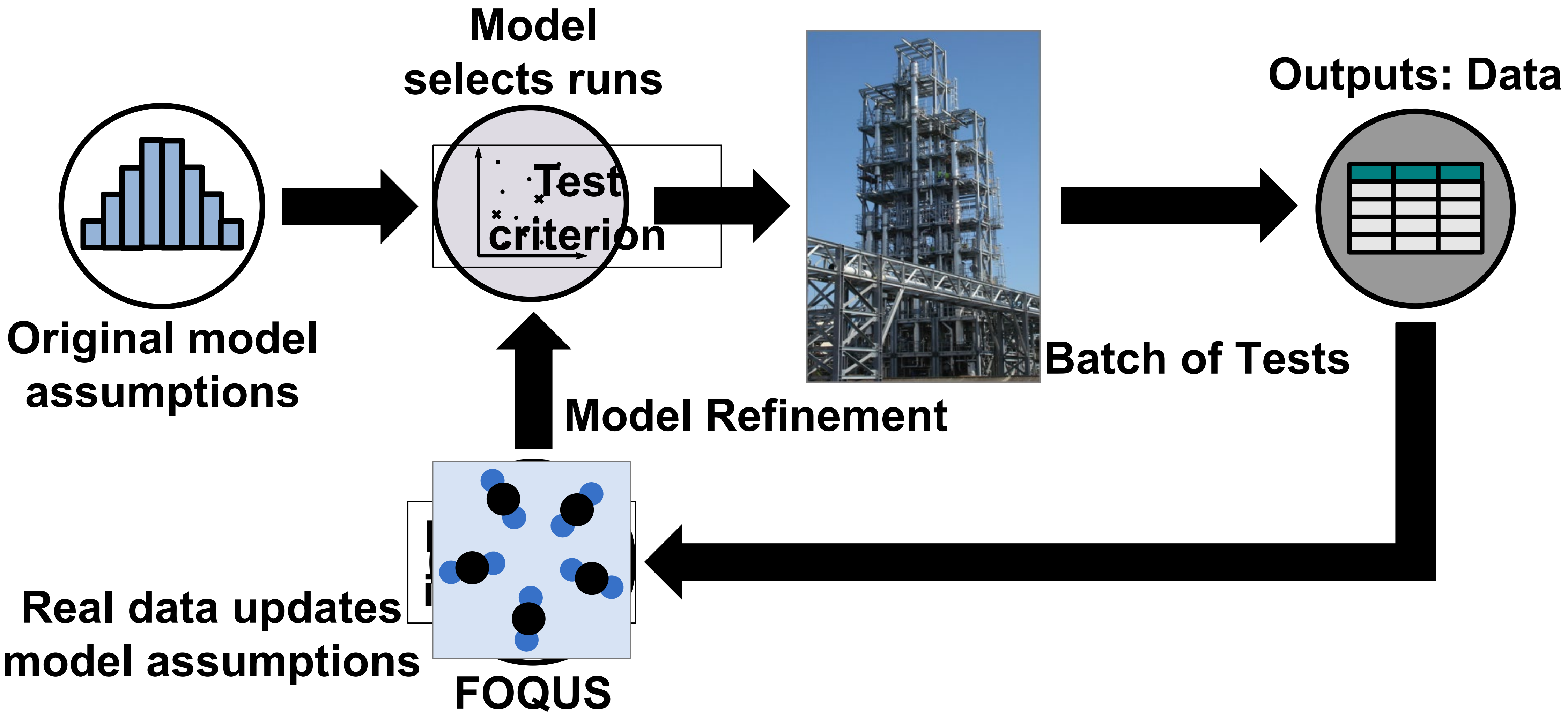
Typical likelihood function (represents discrepancy between model predictions and data values of the output:

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

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

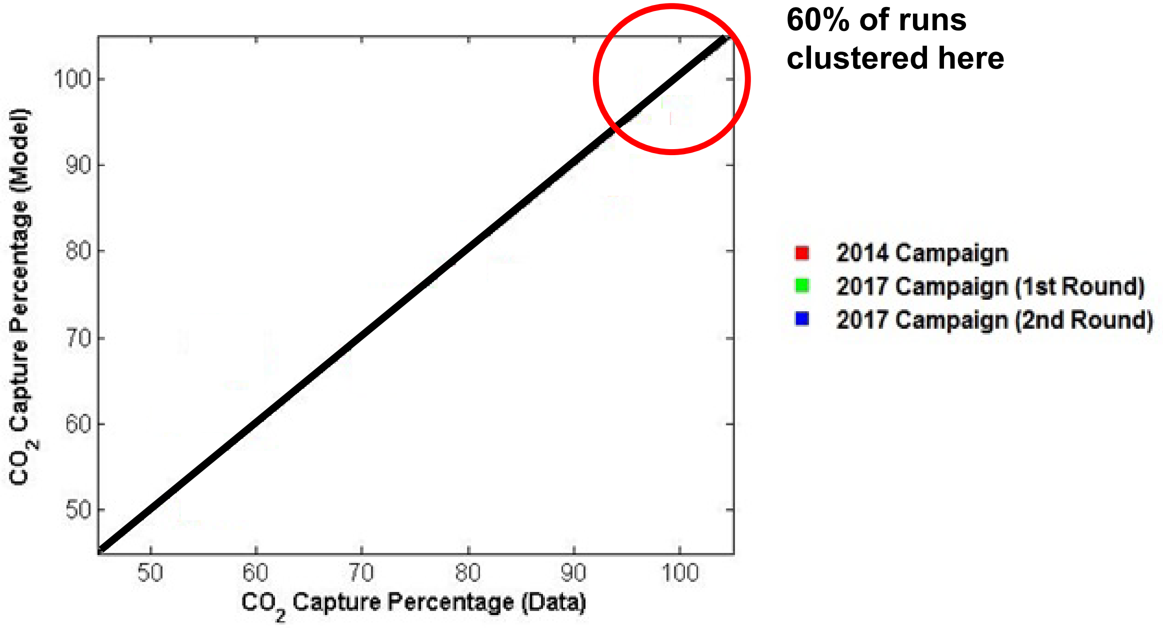


Sequential Design of Experiments Leverages Real Time Data Generation for Optimal Batch Generation



NCCC Model Improvement with SDoE Implementation

Three Beds with Intercooling Cases



2014 Campaign (Before SDoE)

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

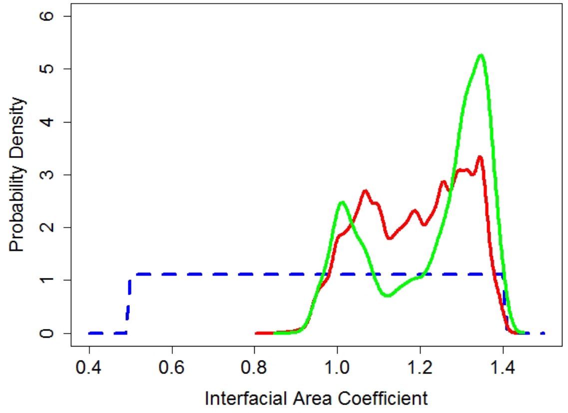
Wait 3 years….

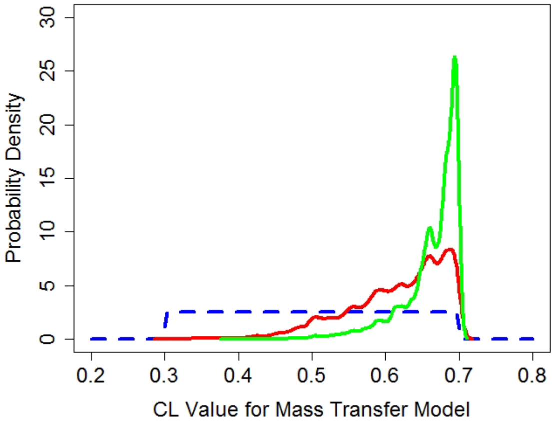
2017 Campaign (Using SDoE)

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

TCM Model Improvement with SDoE Implementation

Update in Parameter Distributions for Absorber Packing

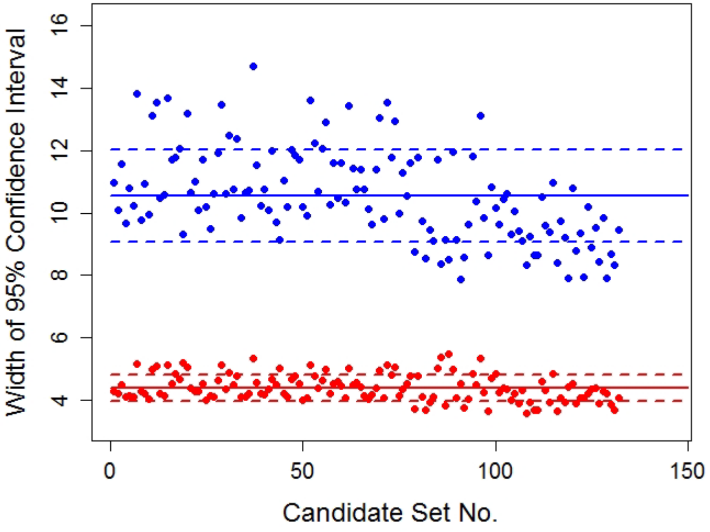




Mass transfer and interfacial area parameters are packing-dependent, and therefore are assigned uniform prior distributions over wide ranges, indicating assumption of relatively large uncertainty before collection of process data.

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

Reduction in CO_2 Capture Percentage Prediction Accuracy



Prior CI Width: (10.5 ± 1.5)%

Posterior CI Width: (4.4 ± 0.4)%

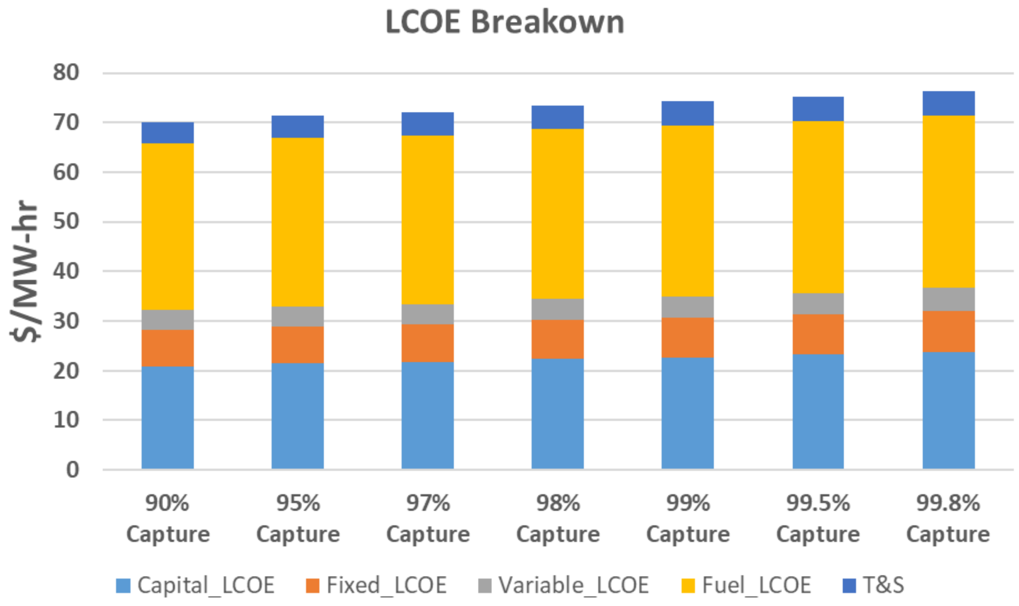
Average reduction in uncertainty: 58.0 ± 4.7%

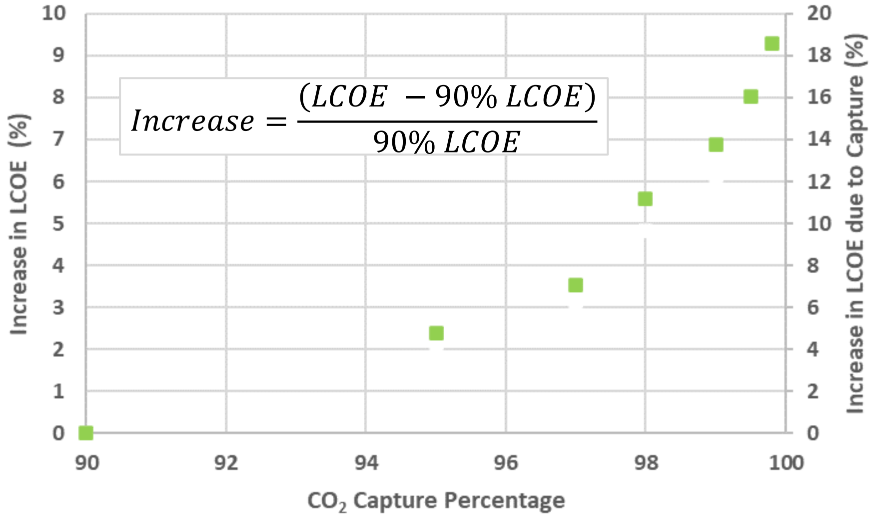
<u>Candidate set includes variation in</u>:

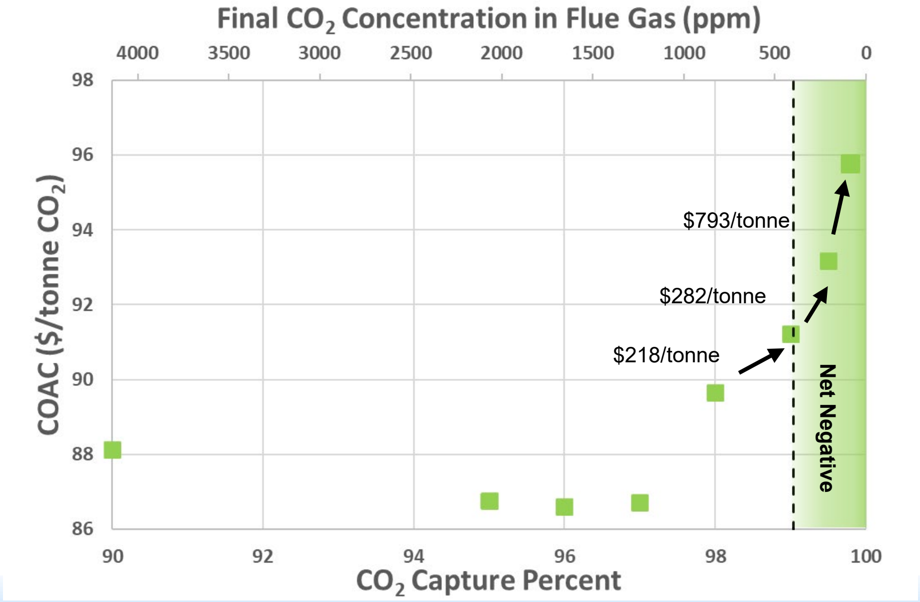
- **Solvent Circulation Rate**
- **Flue Gas flowrate and CO_2 concentration**
- **Reboiler steam flowrate**

High Capture Rates with MEA Solvent - NGCC

*More Detail in Poster by Ben Omell

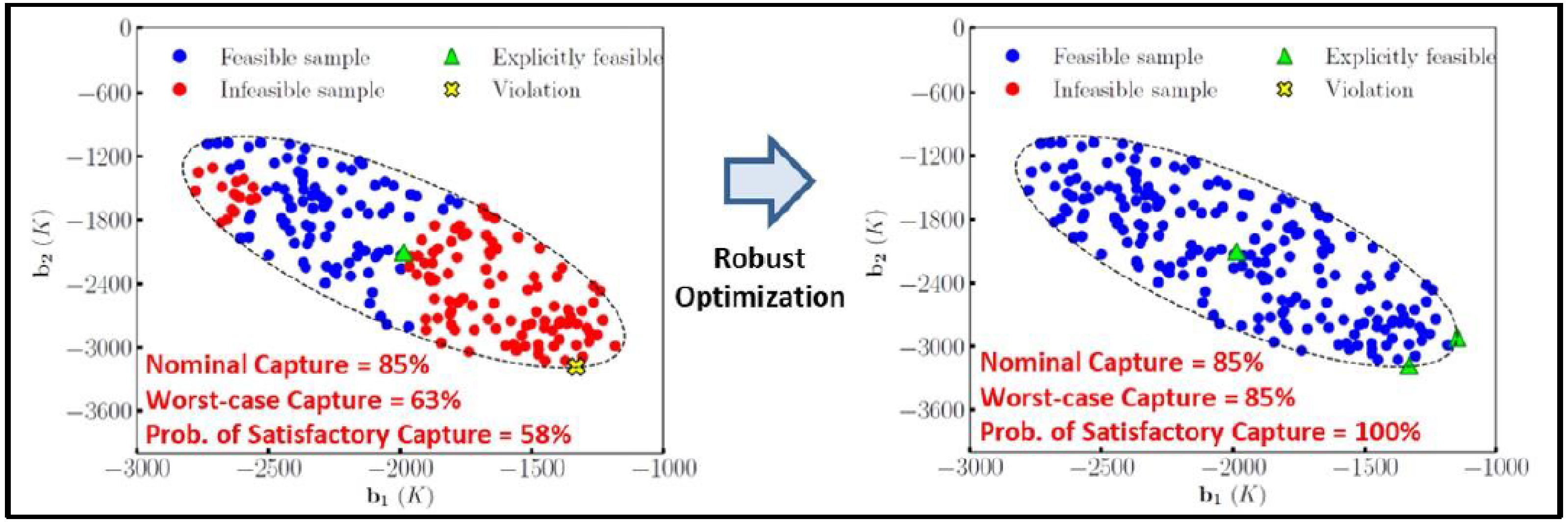




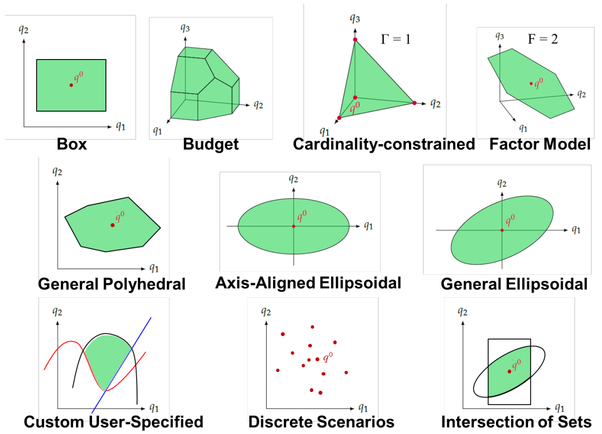


- **LCOE increases linearly from 90→98%,** relatively constant cost of avoided CO_2.
- Incremental **cost of avoided CO_2 significantly increases** in 98→99.8% capture range.
- Practical considerations (e.g., **need for aux boiler, flexible operation**) will increase LCOE further at high capture percentages

PyROS: a Pyomo Robust Optimization Solver



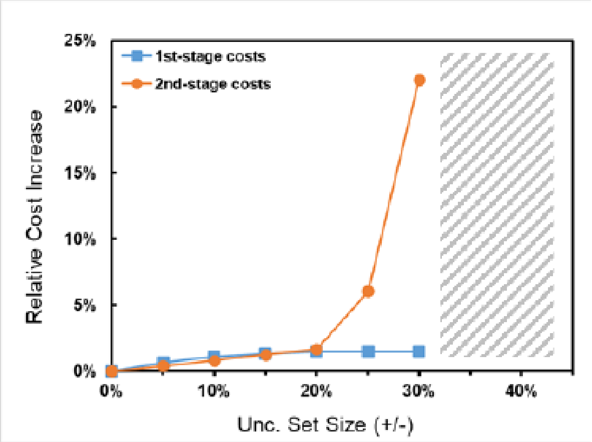
*More Detail in Poster by Jason Sherman



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

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

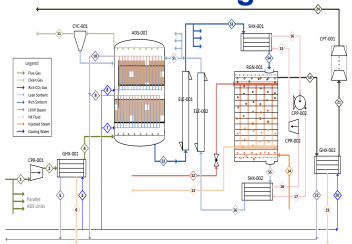
*Demo by: Hughes, Hedrick

CCSI[2]
Carbon Capture Simulation for Industry Impact

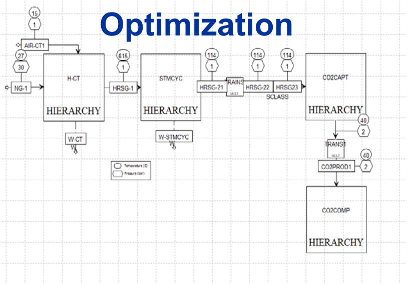
2016 R&D 100 WINNER

IDAES
Institute for the Design of Advanced Energy Systems

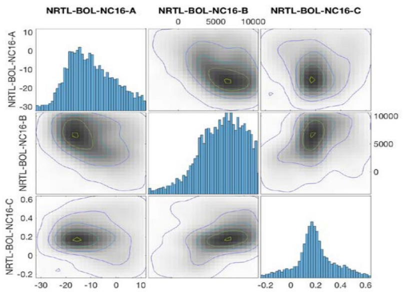
High-Fidelity, Multi-Scale Modeling



Process-level TEA Optimization



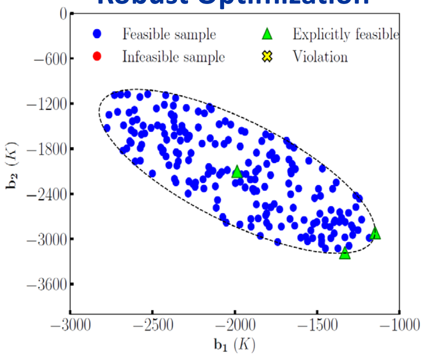
UQ and Parameter Optimization



Foundational Capabilities

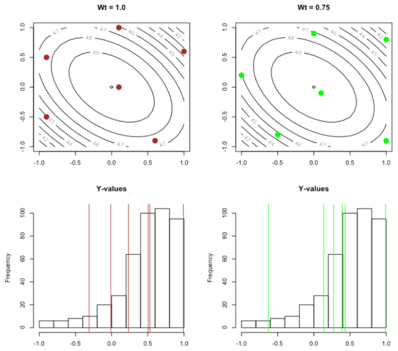
- High-Fidelity CCS Modeling (sorbents, solvents, membranes)
- Design of Experiments
- Steady-State and Dynamic Process Optimization
- Electricity Grid Modeling / Expansion Planning
- Multi-Scale Modeling and Optimization (Materials/Process/Grid)
- Uncertainty Quantification
- Robust Optimization (i.e.,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

Robust Optimization



*Poster by: Sherman

Optimal DoE



*Posters by: Nachtsheim, Wang

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Pacific Northwest National Laboratory: Jay Xu, Charles Freeman, David Heldebrant, Jie Bao, Yucheng Fu, Richard Zheng, Rajesh Singh

Los Alamos National Laboratory: Abby Nachstheim, Jim Gattiker, Sham Bhat, Miranda Martin

Lawrence Berkeley National Laboratory: Keith Beattie, John Shinn, Karen Whitenack, Josh Boverhof, Ludovico Bianchi, Sarah Poon

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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 | OAK RIDGE National Laboratory | West Virginia University | UNIVERSITY OF NOTRE DAME | THE UNIVERSITY OF TEXAS AT AUSTIN | UT | UNIVERSITY OF PITTSBURGH | Carnegie Mellon

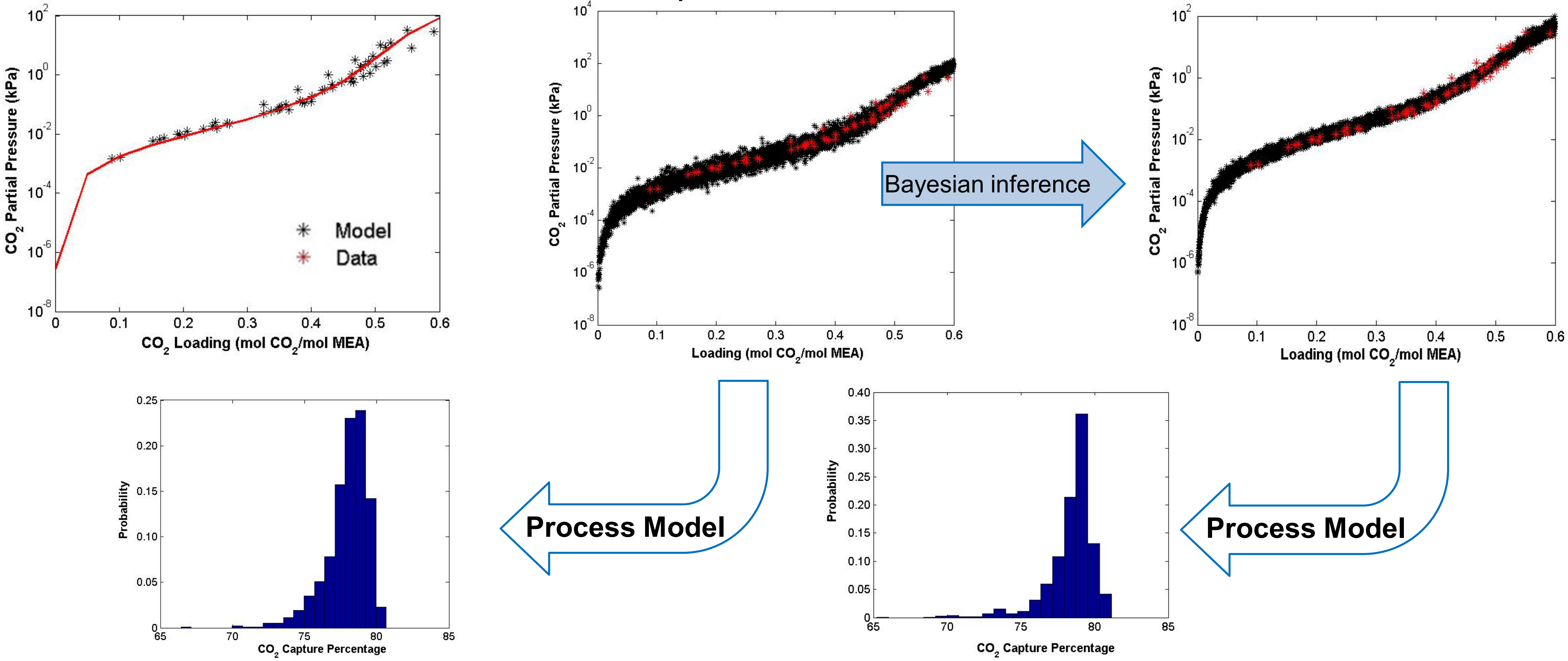
Uncertainty Quantification Bayesian Inference Example: VLE Models

VLE Data/Model Comparison at 40°C

Deterministic sub-model

Using best initial guess of parameter set

Refined parameter set

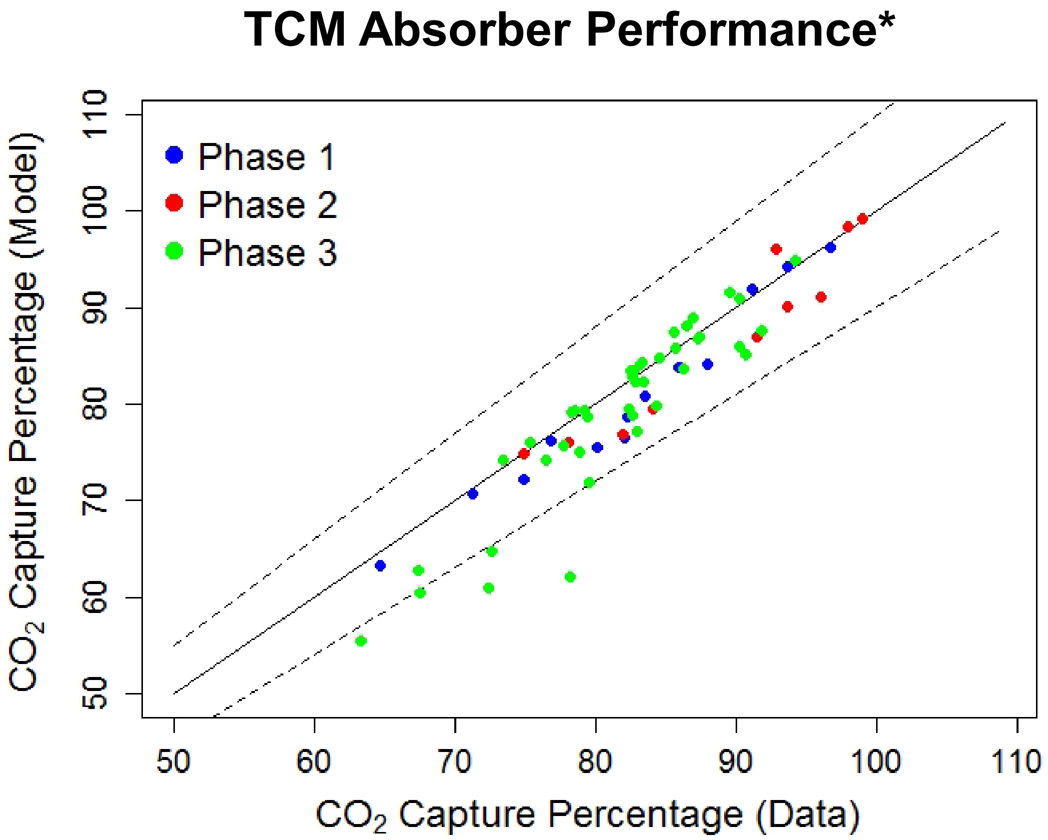


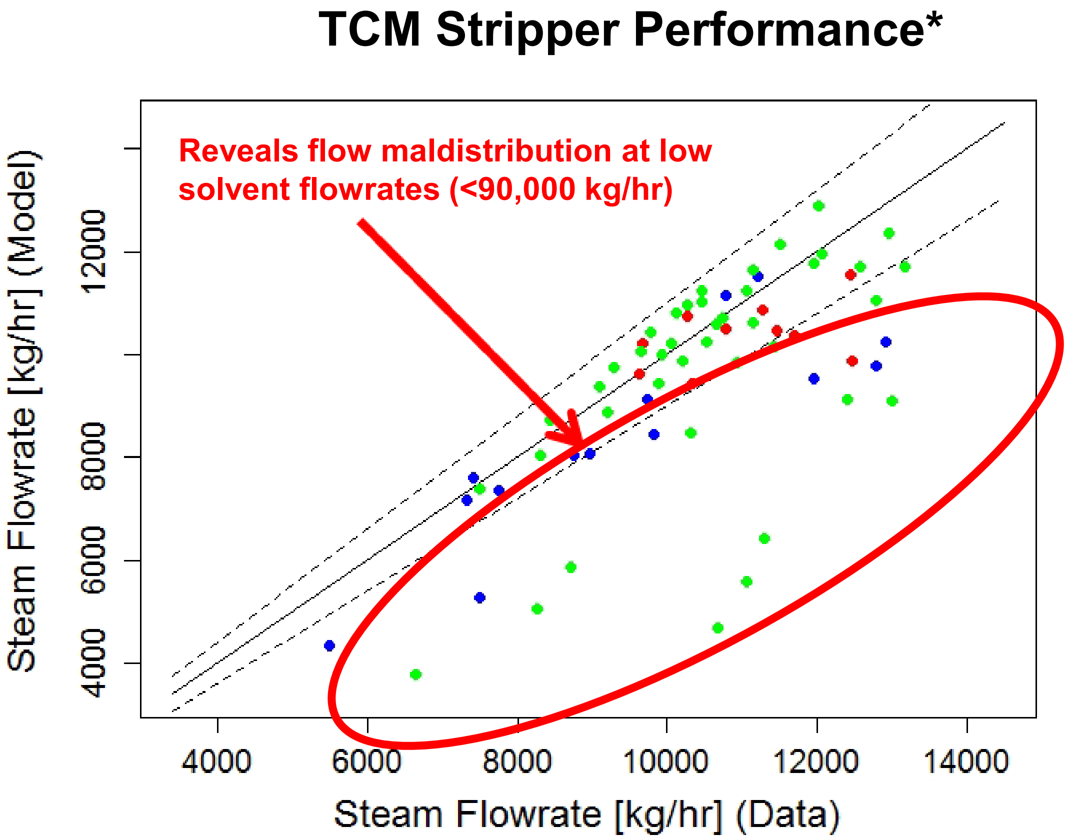
high uncertainty

reduced uncertainty

CCSI[2]
Carbon Capture Simulation for Industry Impact

Model Based Insight into Operational Non-Idealities





Fundamental Model Insight into Data Aberrations

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