CCSI²
Carbon Capture Simulation for Industry Impact

Computational Guidance for RTI Test Campaign

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National Energy Technology Laboratory (NETL)

2023 FECM/NETL Carbon Management Research Project Review Meeting Agenda

August 28, 2023

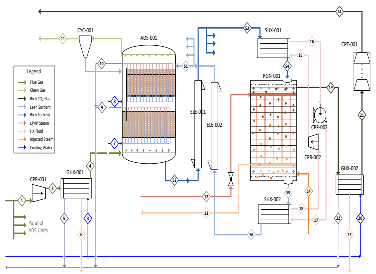
CCSI^2 – Modeling, Optimization and Technical Risk Reduction

CCSI^2
Carbon Capture Simulation for Industry Impact

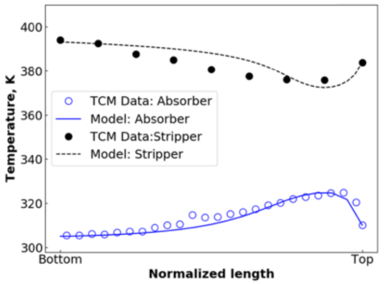
Multi-lab modeling initiative to support carbon capture technology development

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

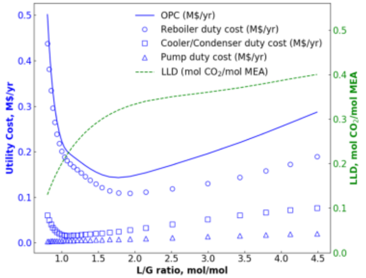
High Fidelity Process Modeling



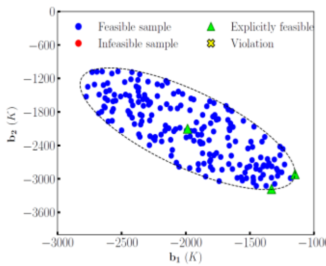
Model Validation



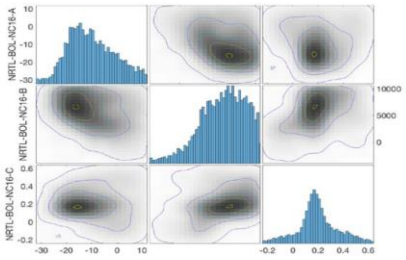
Process Optimization



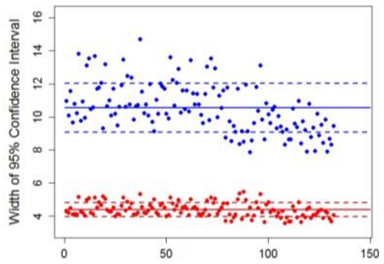
Robust Design

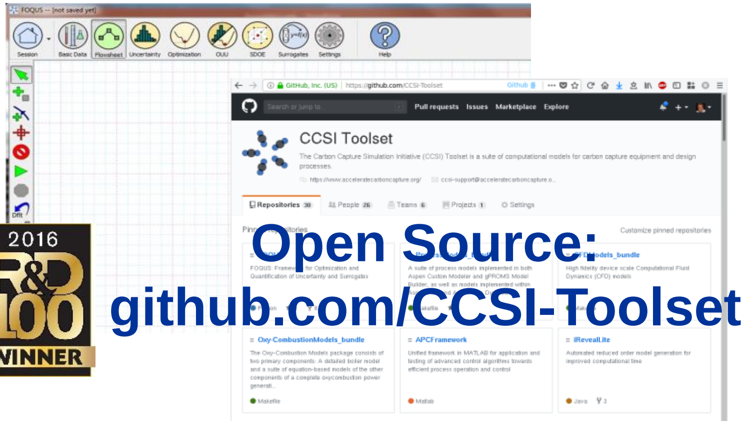


Uncertainty Quantification



Maximizing Learning





2016 R&D 100 WINNER

Open Source: github.com/CCSI-Toolset

IDAES
Institute for the Design of Advanced Energy Systems

2020 R&D 100 WINNER

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

U.S. DEPARTMENT OF ENERGY · National Energy Technology Laboratory · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory EST.1943 · 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

Presentation Overview

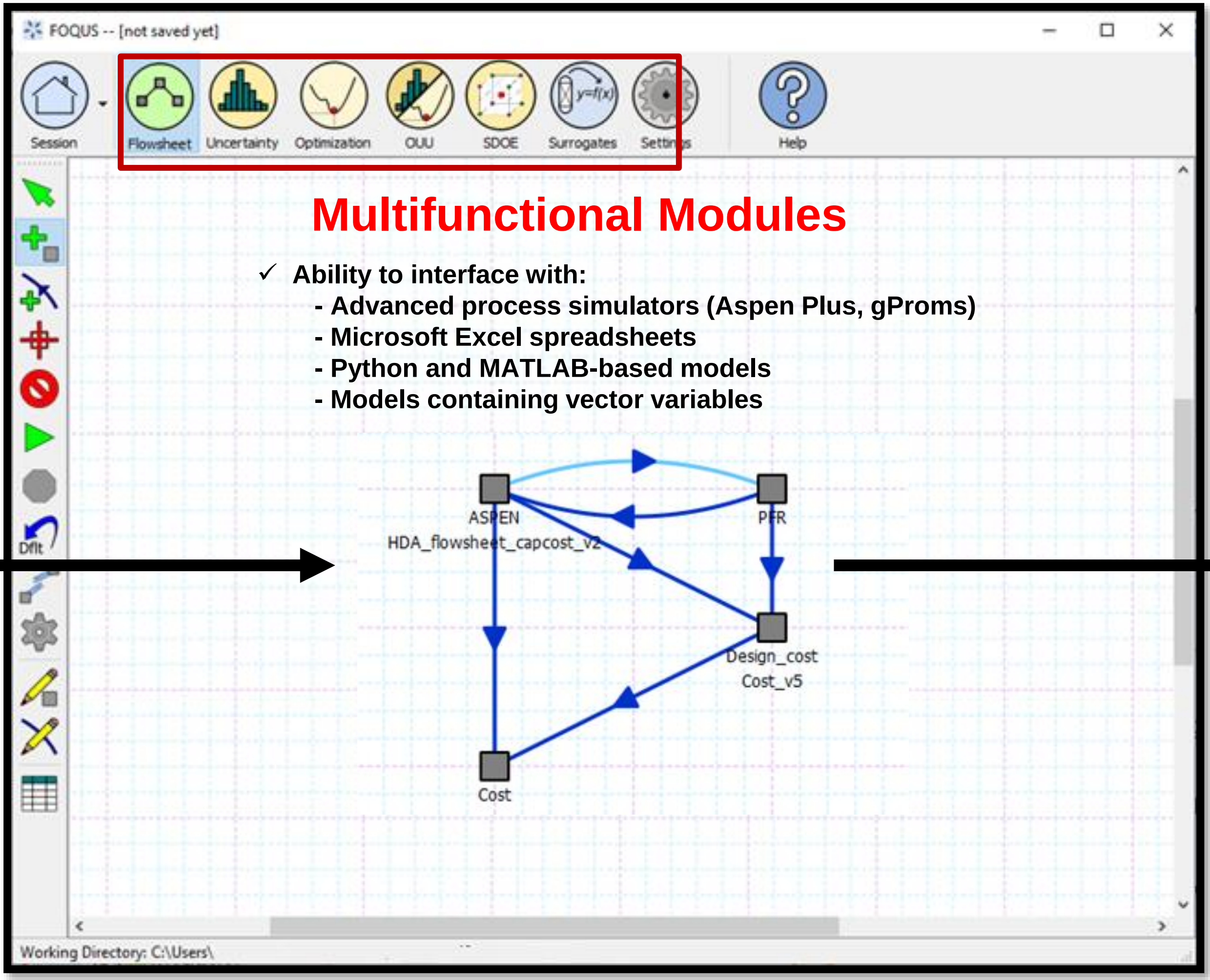
- Overview of CCSI^2 Modeling Capabilities
- CCSI^2-RTI Collaboration
  - SDoE work for TCM pilot campaign
  - Process modeling
  - Transition to new project for modeling of GEN2NAS
- Summary and Future Work

FOQUS – Framework for Optimization, Quantification of Uncertainty, and Surrogates

Advanced Process Simulators and Modeling Environments

PYOMO

IDAES
Institute for the Design of Advanced Energy Systems



Multifunctional Modules

✓ **Ability to interface with:**
- **Advanced process simulators (Aspen Plus, gProms)**
- **Microsoft Excel spreadsheets**
- **Python and MATLAB-based models**
- **Models containing vector variables**

Comprehensive Analysis of Process Systems

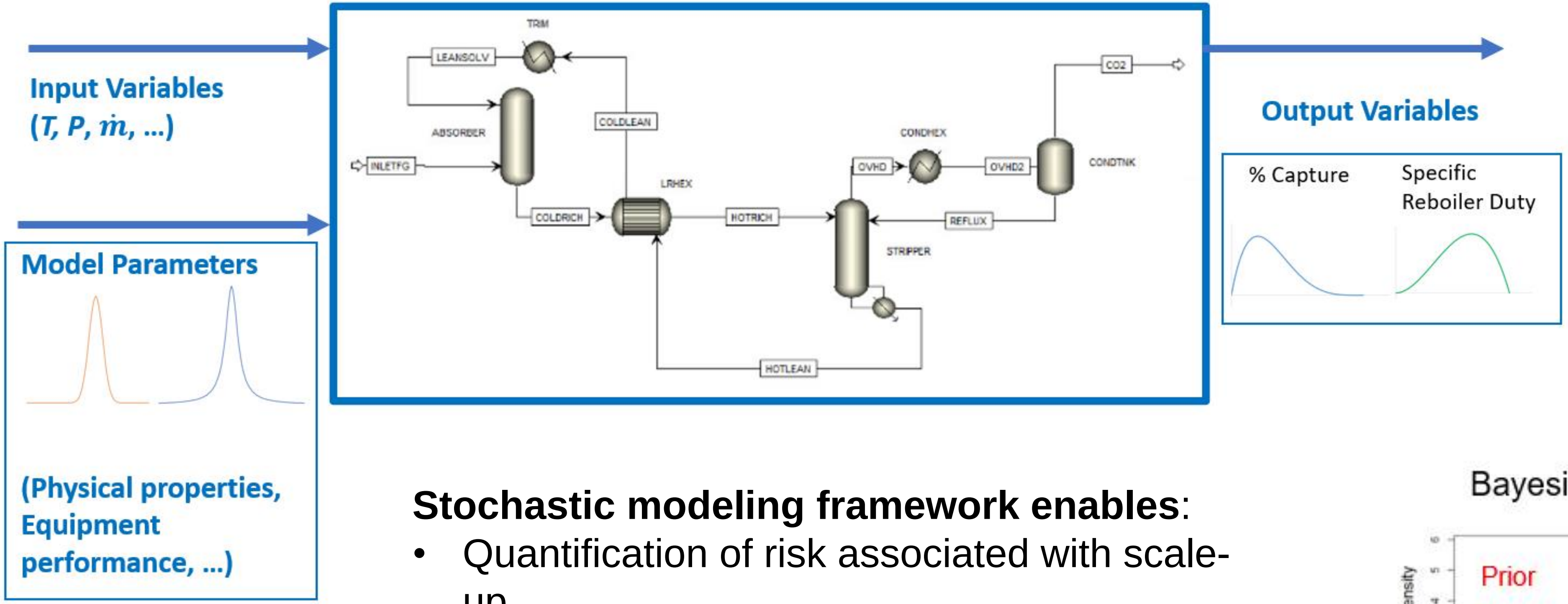
- Uncertainty Quantification
- Simulation-Based and Mathematical Optimization
- Surrogate Modeling

- Sequential Design of Experiments
- Optimization Under Uncertainty

Nodes: Contain Individual Models

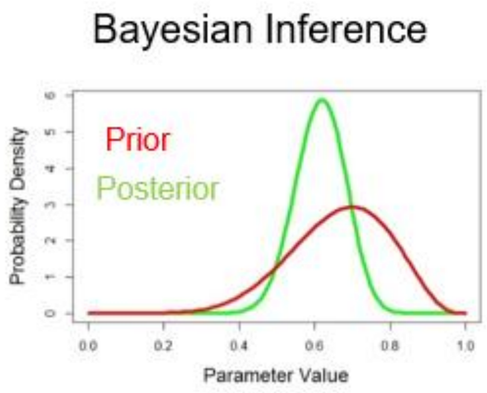
Edges: Transfer variables between nodes

CCSI^2 Capabilities – Uncertainty Quantification (UQ) and Stochastic Modeling



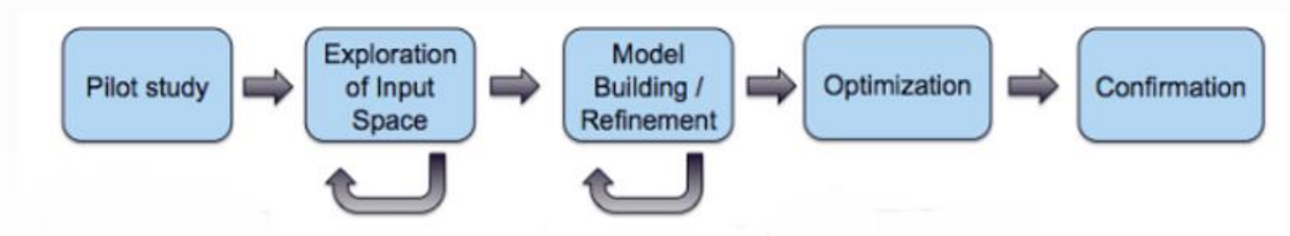
Stochastic modeling framework enables:

- Quantification of risk associated with scale-up
- Robust design and optimization
- Reduction of epistemic uncertainty through data collection (Bayesian inference)



Sequential Design of Experiments (SDoE)

- **Design of experiments (DOE)** is a powerful tool for accelerating learning by targeting maximally useful input combinations to match experiment goals
- **Sequential design of experiments (SDoE)** allows for incorporation of information from an experiment as it is being run, by updating selection criteria based on new information
- Specific algorithms can be tailored to match experimental goals. Options available in the CCSI Toolset include:
  - Uniform Space Filling (USF)
  - Non-Uniform Space Filling (NUSF)
  - Input-Response Space Filling (IRSF)
  - Robust Optimality-Based Design of Experiments (ODoE)
- Recommended to run experiments in phases to take advantage of SDoE capabilities and customize test designs to meet expected project outcomes



Detailed discussion on SDoE:

Technical Risk Reduction: Sequential Design of Experiments and Uncertainty Quantification (Abby Nachtsheim – LANL)
Thursday (8/31/2023) @ 9:30 AM during Point Source Carbon Capture Breakout Session

Highlights of CCSI^2 – RTI Collaboration

- Collaboration initiated in 2019 with early CCSI^2 work focused on computational support for modeling RTI's non-aqueous solvent (NAS) system and evaluating model performance against small pilot data

- Development of tools for amine emissions and aerosol formation

- Contributed sequential design of experiments (SDoE) capabilities to design a portion of the test campaign for NAS at TCM in 2022

- SLB forms partnership with RTI to support and accelerate industrialization of RTI solvent systems
  - CCSI^2 met with SLB and RTI (March 2023) to develop strategy for future work and demonstrate capabilities of CCSI^2 Computational Toolset

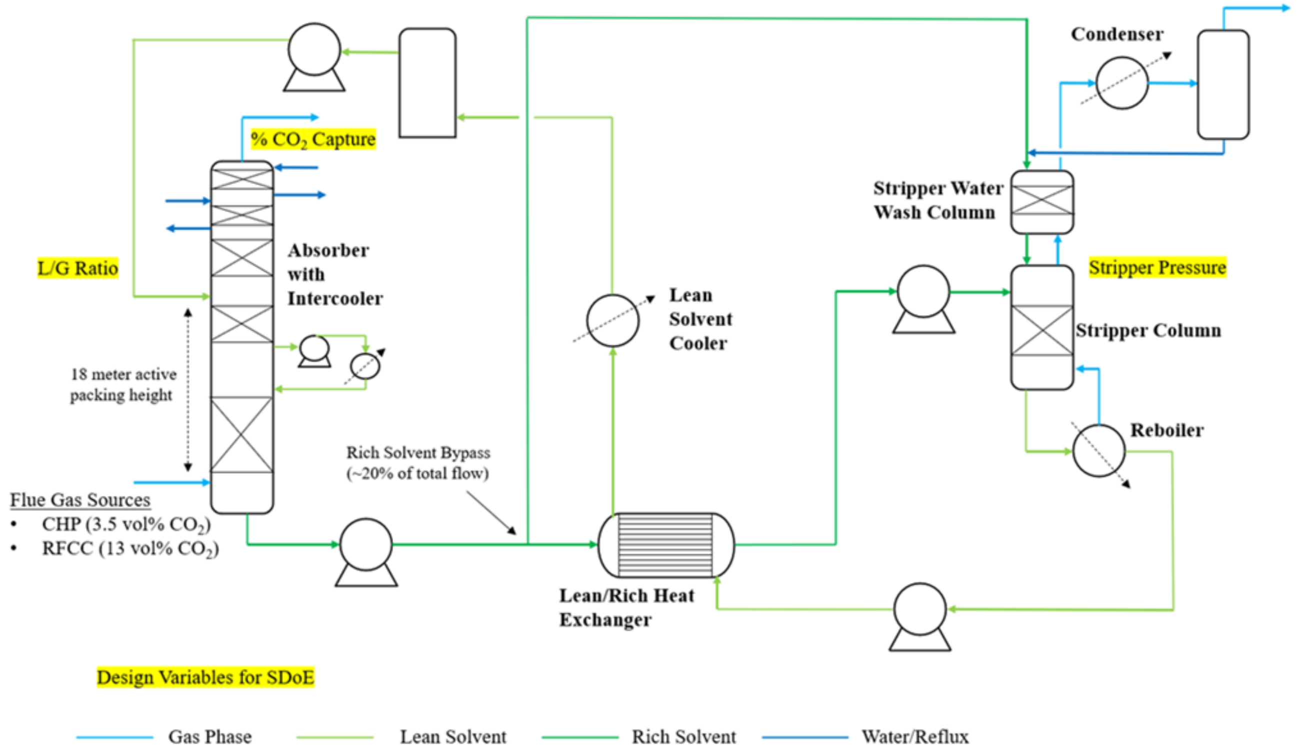
- Current work focused on refining process models of NAS and transition into new project in support of new project for next-generation solvent system

TCM Test Campaign for RTI NAS Solvent

- Leveraged SDoE to guide NAS test campaign at TCM → focused on demonstrating high levels of CO_2 capture with low solvent emissions and regeneration energy requirement

- CCSI[2] team contributed separate designed experiments for gas-fired combined heat and power (CHP) [3.7 vol% CO_2] and residual fluidized catalytic cracker (RFCC) [13.5 vol% CO_2] flue gas sources

- Each designed experiment includes a series of test matrices with 12-22 proposed operating conditions for flexibility in design size



Design factors:
CO_2 Capture: 85 – 95%
Absorber L/G Ratio: 2.5 – 6.5 kg/kg
Stripper Pressure: 0.9 – 3.2 barg

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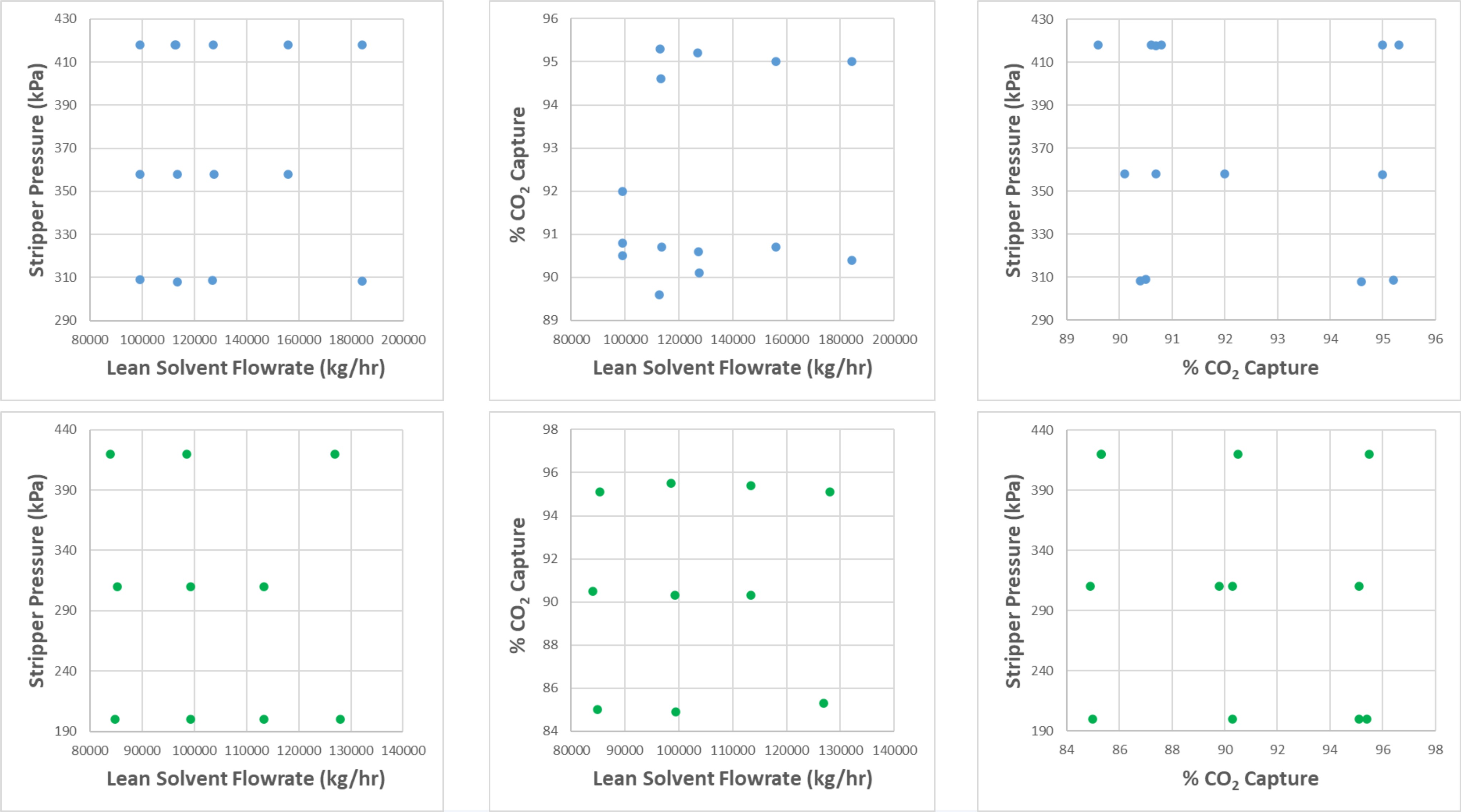
SDoE Results – Data Collection at TCM

Data sets generated for SDoE demonstrate good coverage of operation space:



- Coal-based flue gas
- NGCC flue gas

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CCSI² Process Modeling Support – Current Work Goals

- Evaluate quality of fit to pilot data of current version of process model
  - Coal-based flue gas (analysis in progress)
  - Natural gas-based flue gas (analysis forthcoming)
- Identify needs for refinement of individual sub-models through re-calibration and/or parametric UQ
- Leverage CCSI² Toolset to determine best practices for solving robustness issues associated with these models
  - Ensure modeling framework is sufficiently robust in order to extend to new solvent formulations

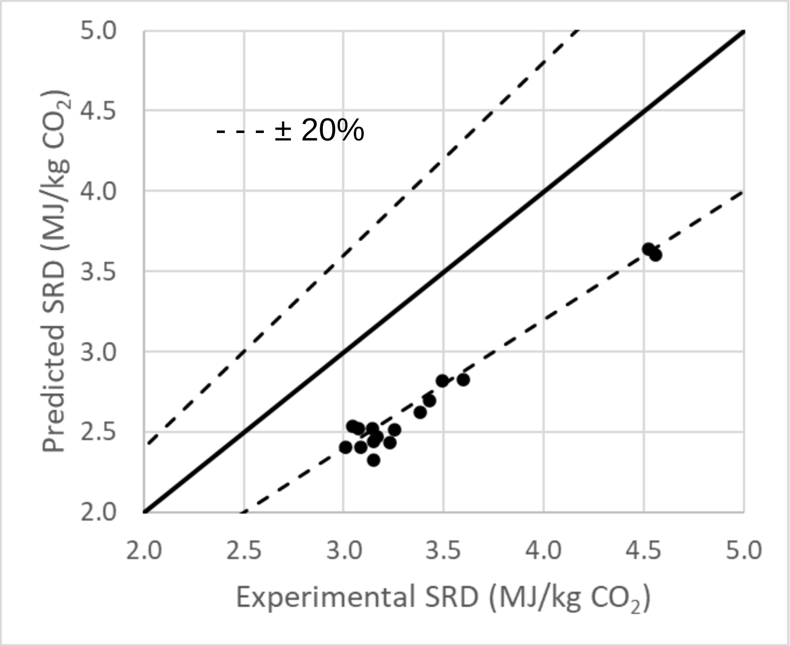
Preliminary Process Modeling Results - Absorber

- Initial efforts to model absorber have revealed computational challenges that must be addressed in order to successfully execute future scope
  - Incorporation of solvent intercooling and kinetic models have strong effect on model robustness
  - Plan to explore options for leveraging FOQUS tool to improve model performance
- CO_2 capture percentage generally overpredicted (~6% on average)
  - Performance of absorber highly sensitive to thermodynamic models in comparison to aqueous systems (MEA, CESAR1)
  - Uncertainty in model inputs (e.g., CO_2 loading, intercooler duty, solvent temperature) could potentially have an impact

Preliminary Process Modeling Results - Stripper

- Modeled stripper section as stand-alone process with CO_2 capture level constrained based on experimental data
- Stripper inlet temperature fixed to experimental value by adjusting lean/rich heat exchanger
- Compared experimental and model predictions of specific reboiler duty (SRD):

$$SRD = \frac{Q_{reb}}{\dot{m}_{CO_2-captured}}$$



Identify bias in which the model consistently underpredicts heat of absorption by 20% - can attribute in part to heat of absorption calculation

Preliminary Process Modeling Results - Stripper

$$Q_{reb} = Q_{sensible} + Q_{CO_2\ Desorption} + Q_{H_2O\ Evaporation}$$

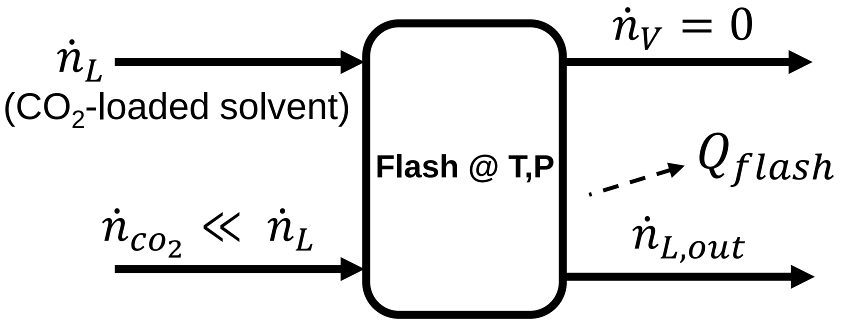
Potential sources of discrepancy:

- Thermodynamic model (VLE, heat of absorption, heat capacity)
- Uncertainty in boundary conditions (lean/rich CO_2 loading, temperature, pressure)

Heat of absorption calculation:

- For water-lean solvent, term associated with H_2O evaporation should be negligible
- For thermodynamic consistency in e-NRTL model, calculations of differential heat of absorption expected to be consistent with Gibbs-Helmholtz equation

Differential Heat of Absorption:



$$\dot{n}_L \text{ (}CO_2\text{-loaded solvent)}, \quad \dot{n}_{co_2} \ll \dot{n}_L, \quad \dot{n}_V = 0, \quad Q_{flash}, \quad \dot{n}_{L,out}$$

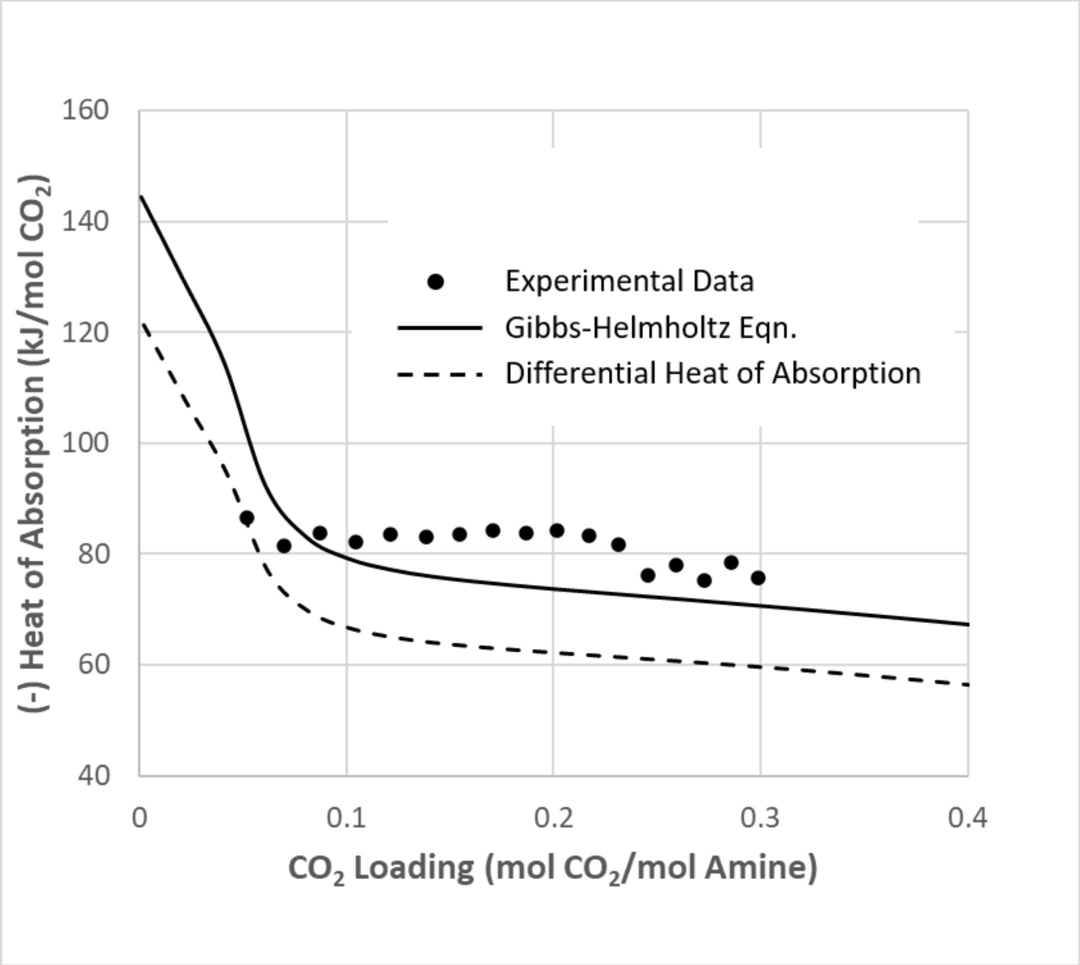
$$\Delta H_{co_2-abs} \approx \frac{Q_{flash}}{\dot{n}_{co_2}}$$

Gibbs-Helmholtz Equation:

$$\Delta H_{co_2-abs} \approx -R \left(\frac{\partial \ln(f_{CO_2})}{\partial \left(\frac{1}{T}\right)} \right) \Bigg|_{\sigma,\{x_0\}}$$

Preliminary Process Modeling Results - Stripper

Fit at 100°C:



- Heat of absorption not directly defined in Aspen Plus as physical property. Two options for including in thermodynamic model regression:
  - Differential heat of absorption – requires user subroutine
  - Gibbs-Helmholtz equation – use temperature perturbation on CO_2 partial pressure (*method used in this work*)
- With internally consistent thermodynamic framework, these methods should produce comparable results
- Magnitude of differential heat of absorption underpredicted – directionally consistent with bias in SRD prediction
- This discrepancy is not unique to this system – additional analysis is ongoing for multiple solvent systems

GEN2NAS Project

- RTI awarded new project (FE032218) to advance their non-aqueous capture technology with new solvent formulation
- Planned CCSI[2] contributions (EY23 – EY24):
  - Computational modeling to quantify effect of solvent properties (e.g., viscosity, thermodynamics) on equipment performance
  - Implement UQ work for assessment of risk associated with scale-up of process models
  - Explore use of SDoE strategies to aid in data collection for model and sub-model validation
- For more details on this project:
  - GEN2NAS Solvents for CO_2 Capture from NGCC Plants (FE0032218) (Jak Tanthana – RTI) – Wednesday (8/30/2023) @ 11:30 AM during Point Source Carbon Capture Breakout Session

Summary and Conclusions

- Collaboration with RTI has demonstrated successful application of $CCSI^2$ Toolset for development and refinement of process models of novel CO_2 capture processes
  - SDoE methods improve quality of data collection → essential for quantifying and reducing risk for process scale-up
- These tools and methodologies can be customized to support different technologies and test campaign goals
- Work is ongoing to finalize process models of first-generation NAS system, which will be leveraged to support development of models for new solvent formulation (GEN2NAS)

Acknowledgements

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Disclaimer

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For more information

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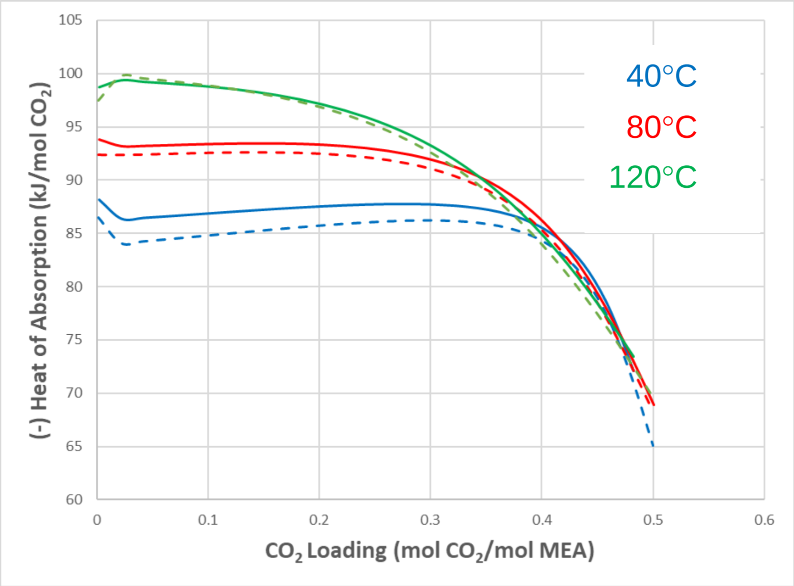
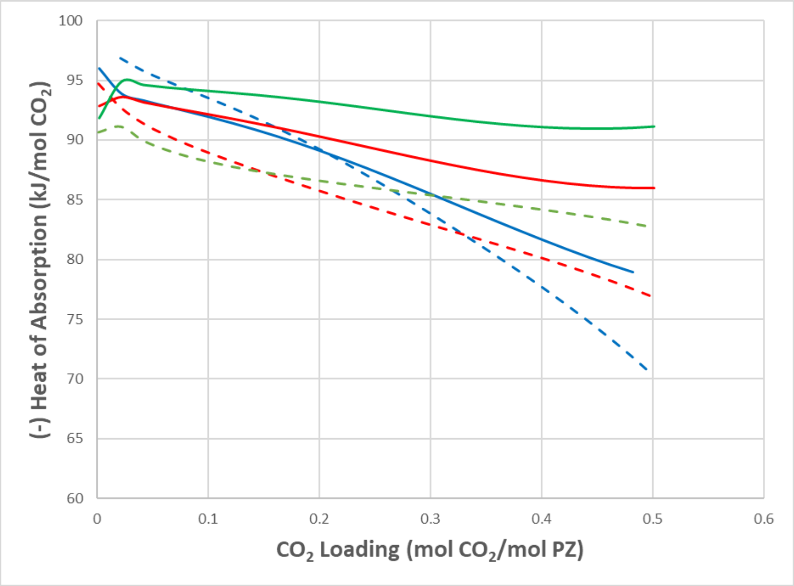
Backup Slides

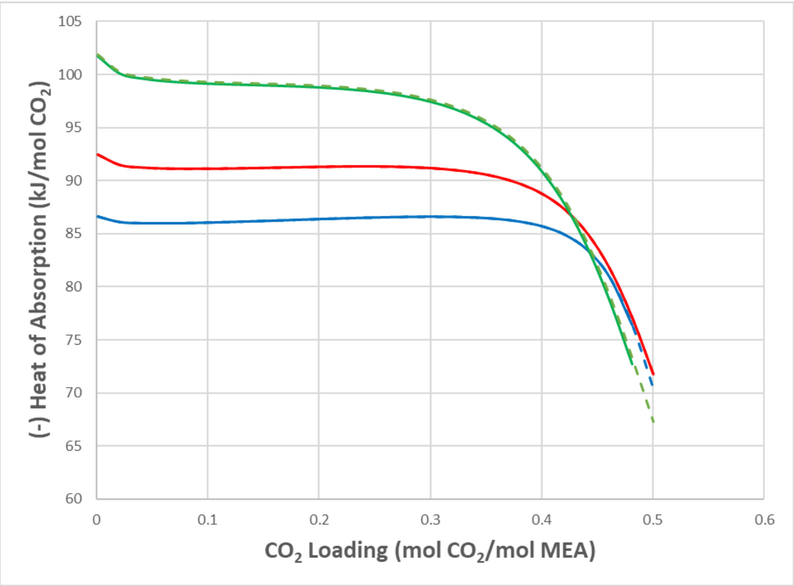
Heat of Absorption Calculation Inconsistency – Other Models



MEA model distributed with Aspen Tech software (ENRTL-RK thermodynamic method)



PZ model distributed with Aspen Tech software (ENRTL-RK thermodynamic method)



MEA model developed by CCSI team – Akaike information criterion (AIC) used to regress parameters to fit thermodynamic data - *does not include electrolyte pair parameters*
(ELECNRTL thermodynamic method)

——— Differential Heat of Absorption

– – – Gibbs-Helmholtz Equation

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