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Predictive models of carbon capture systems and their validation using bench scale and pilot scale data

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Predictive Models of Carbon Capture Systems and their Validation Using Bench Scale and Pilot Scale Data

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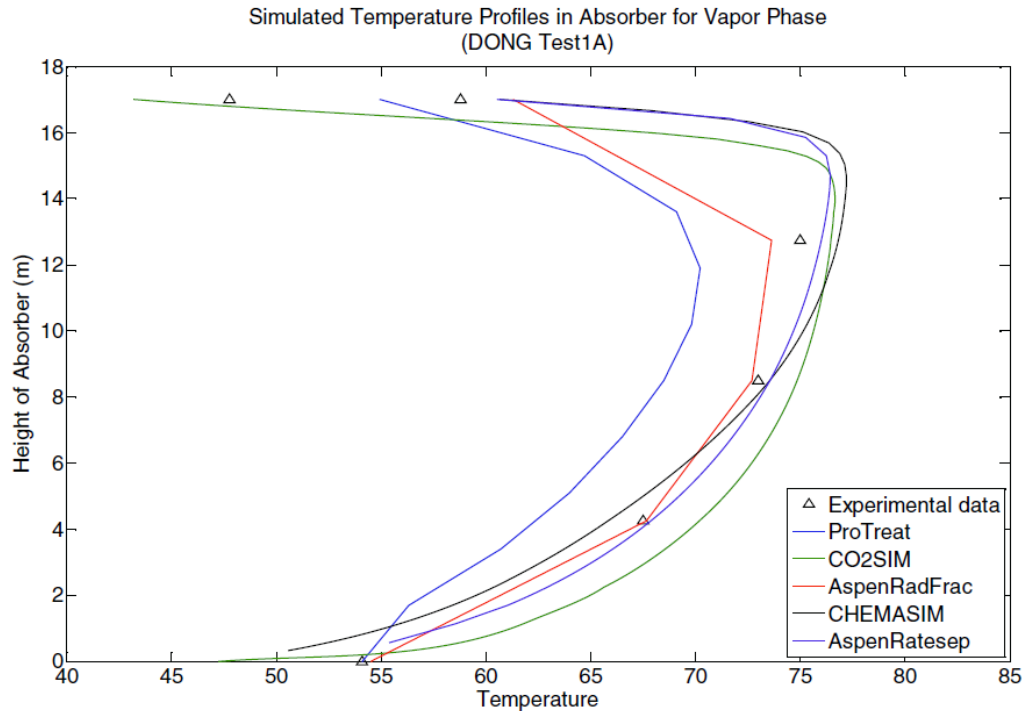
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CO₂ Summit II: Technologies and Opportunities
Santa Ana Pueblo, New Mexico
April 10-14, 2016

Motivations Behind CCSI Solvent System Process Models

- Development of a **Gold Standard** model for comparing different proposals for advanced solvent-based capture technologies
 - Open source
 - Validated framework
 - Well documented
 - Uncertainties quantified
 - Can be leveraged for scaleup studies
- Aqueous monoethanolamine (MEA) used as baseline
 - Industry standard
 - Extensive amount of data available
- Steady-state validation
- Dynamic validation

Deficiencies in Existing Steady State Models



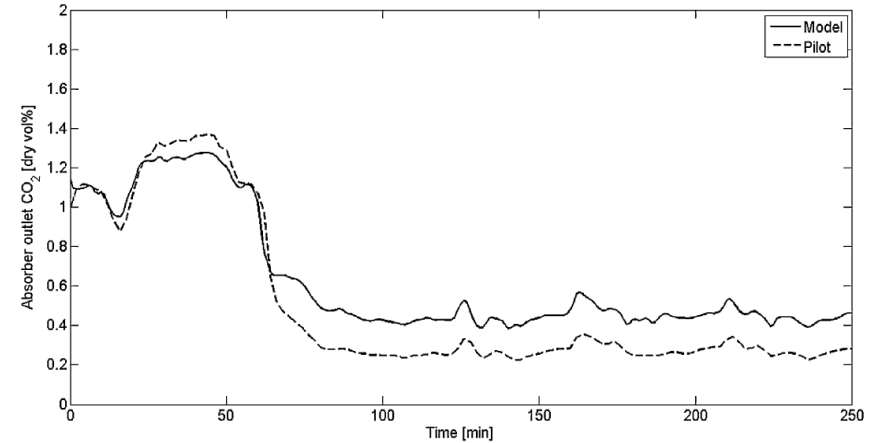
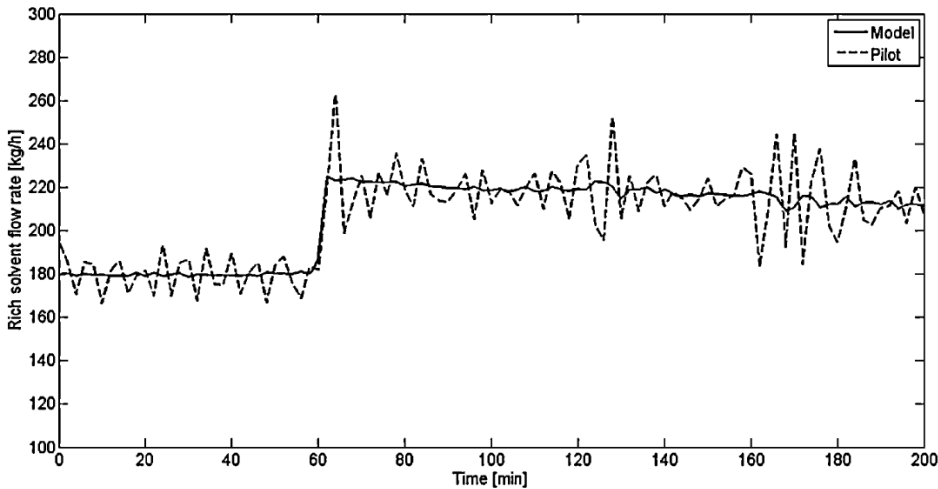
- Limited data from large scale pilot plants
- Limited variability in operating conditions and hardware (such as no of beds, intercoolers) while collecting experimental data
- Discrepancy in temperature profile and solvent loading estimation

ProTreat-Optimized Gas Treating, Inc.; CO2SIM-NTNU/SINTEF
CHEMASIM-BASF SE; AspenRatesep-modified by IFP

Luo et al., "Comparison and validation of simulation codes against sixteen sets of data from four different pilot plants", Energy Procedia, 1249-1256, 2009

Deficiencies in Existing Dynamic Models

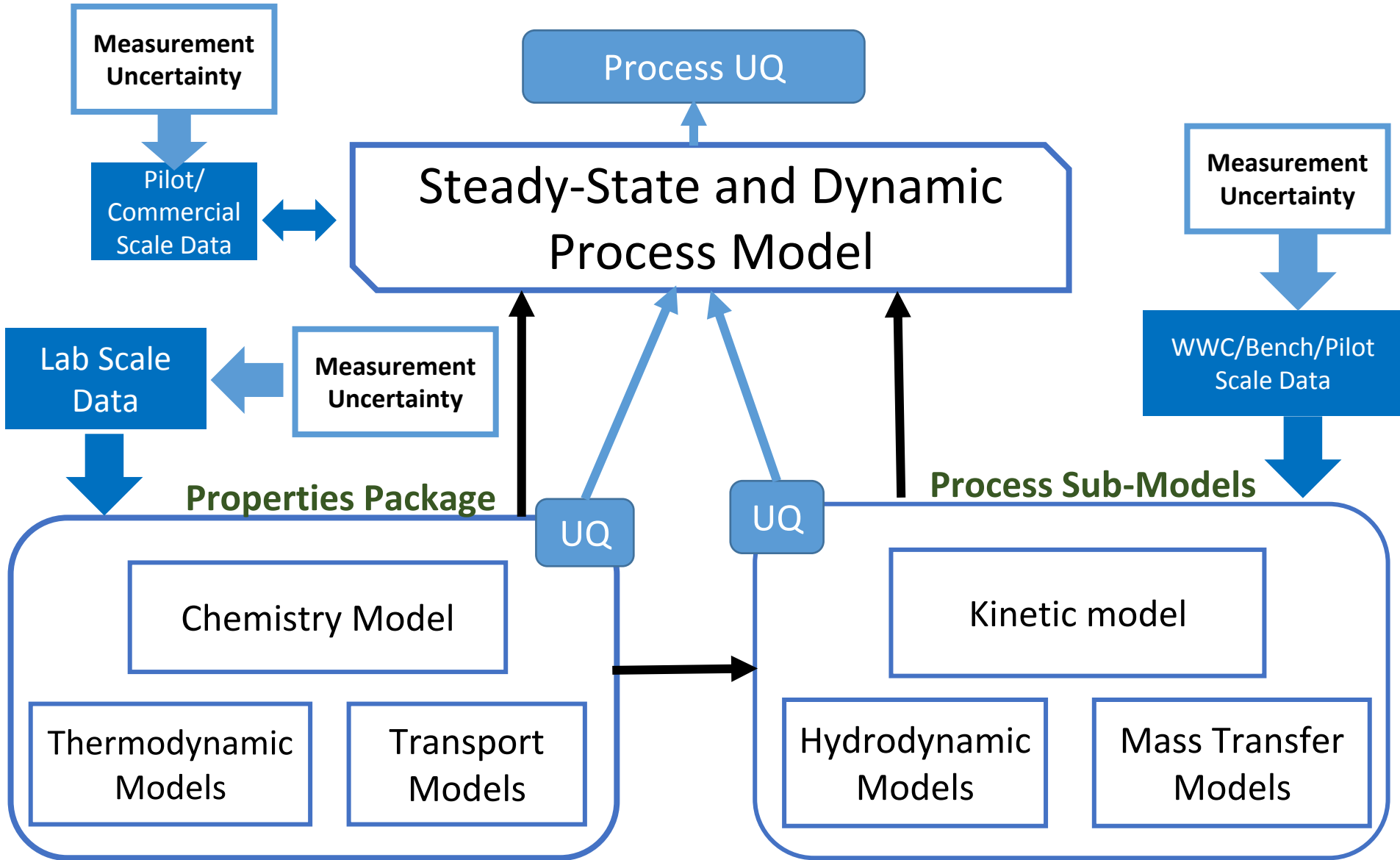
Dynamic Response due to Step Change in Lean Solvent Flowrate*



- Little work done so far
- Usually single step tests are done without maintaining persistence of excitation
- Mass and energy balance errors and noise in the data are either neglected or manually removed

Enaasen Flø et al., Dynamic Model Validation of Post-Combustion CO₂ absorption Process, International Journal of Greenhouse Gas Control, 41, 127-141, 2015

How did we develop the gold standard model?



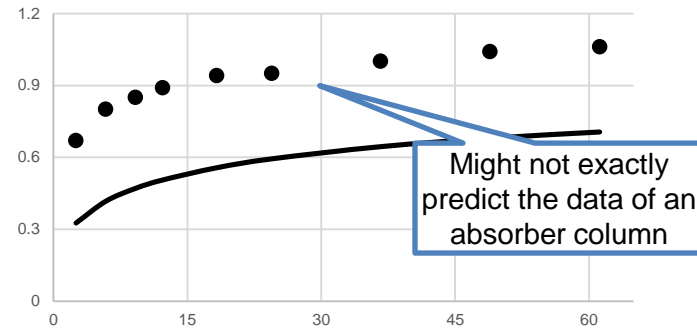
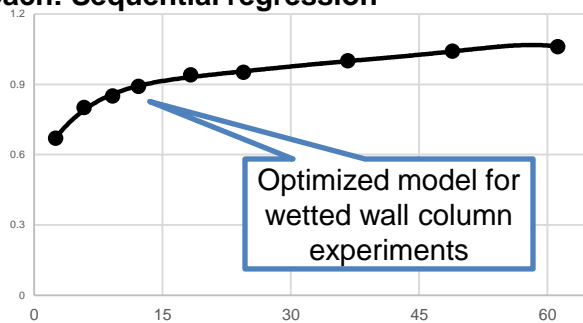
Physical Property Model Development

- Independent property models
 - Viscosity
 - Density/Molar Volume
 - Surface Tension
- Thermodynamic framework
 - Electrolyte-NRTL
 - Binary MEA-H₂O system
 - Ternary MEA-H₂O-CO₂ system
 - Vapor-Liquid Equilibrium
 - Heat Capacity
 - Heat of Absorption
 - Reaction Kinetics
 - Consistency with reaction equilibrium constants

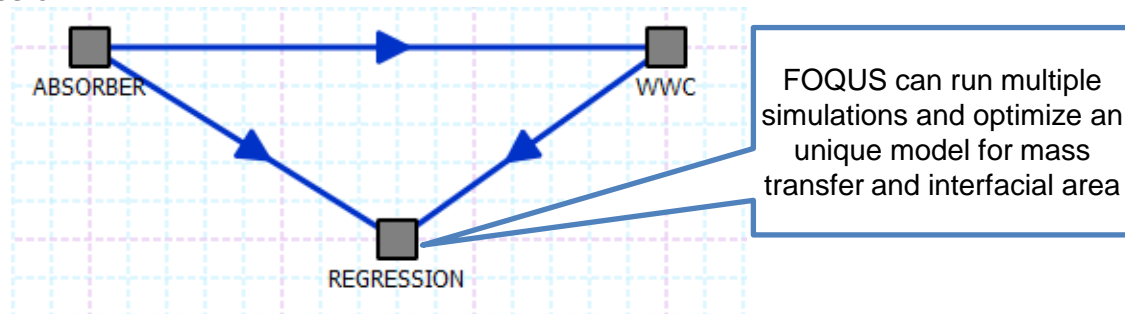
Integrated Mass Transfer Model Development

- Properties (diffusivity, viscosity, surface tension), interfacial area, mass transfer coefficients, and reaction kinetics all affect mass transfer
- Use data from both wetted wall column and packed column
- Simultaneous regression not possible in Aspen Plus
 - solution can be sub-optimal
- FOQUS enables simultaneous regression of multiple models

Usual approach: Sequential regression



FOQUS capability: Simultaneous regression



Validation with the Pilot Plant Data: State-of-the-Art in the Open Literature

Steady-State

- Existing data in the literature do not encompass wide variations in operating conditions
 - Solvent flowrate, flue gas flowrate and composition, lean loading, no. of beds, and presence/absence of intercooler

Dynamic

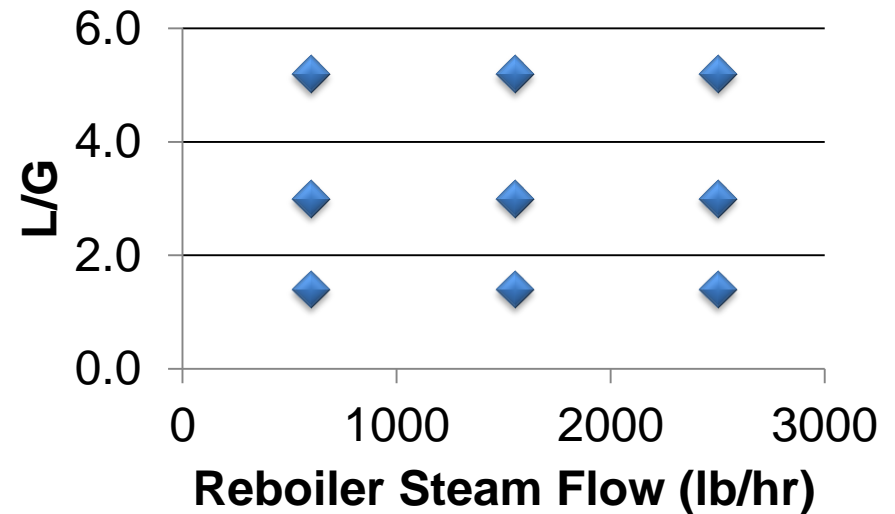
- Existing test runs do not ensure persistence of excitation nor the variability in operating conditions to capture the nonlinearities
 - Steps in all important manipulated and disturbance variables
 - Magnitude and directionality of steps
 - Conditions at which steps are introduced
- Existing dynamic test runs do not record/report transients in all key output variables (e.g. liquid sample analysis)

Validation of Model with Pilot Plant Data



Operating Conditions	Range
Solvent Flow (lb/hr)	7,000-26,000
Inlet Flue Gas (lb/hr)	5,000-6,500
Reboiler Steam Flow (lb/hr)	600-2,500
Inlet FG CO ₂ vol%	9-11%
# of beds	1-3
Intercooler	no - yes

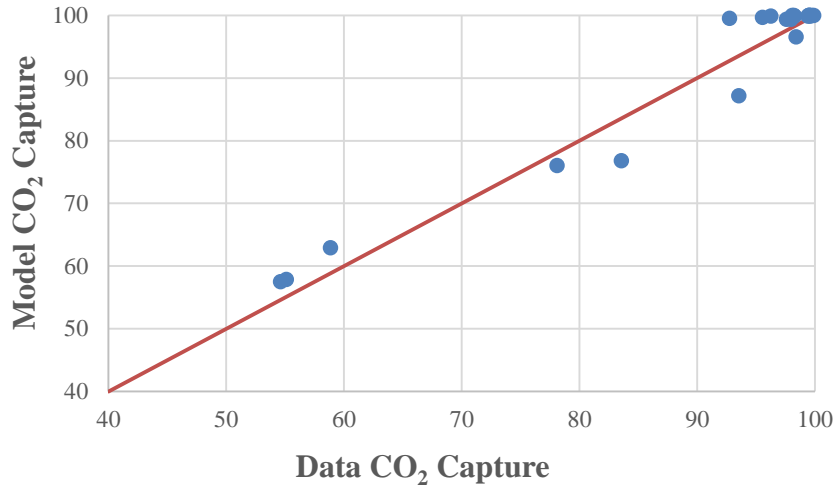
Steady-State Test Matrix



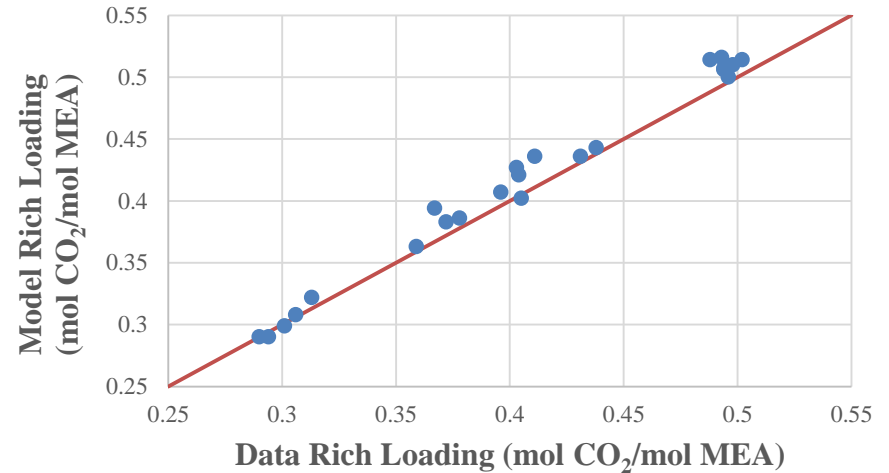
Steady State Absorber Validation

No parameter tuned

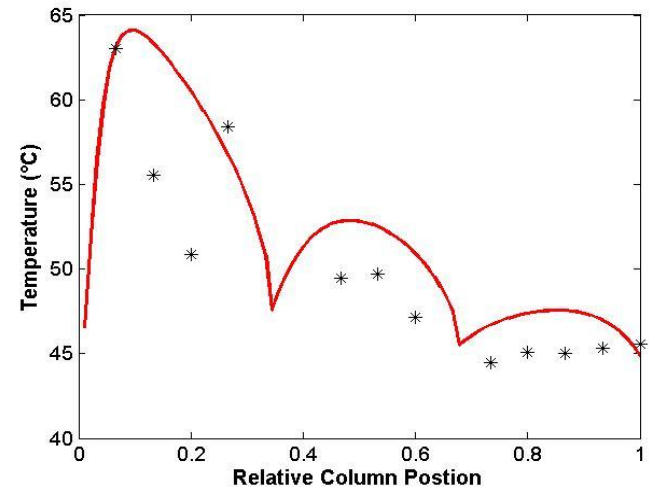
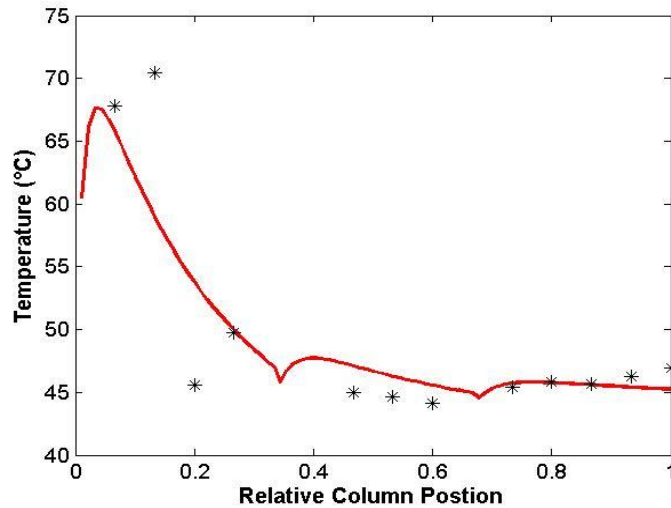
CO₂ Capture Prediction



Rich Loading Comparison



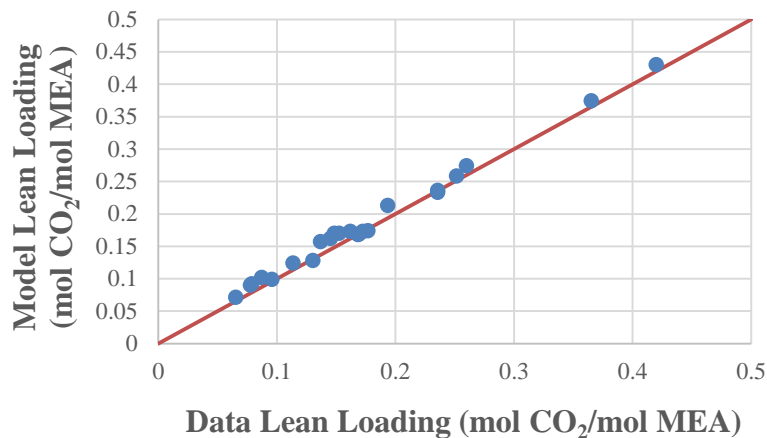
Sample Temperature Profiles



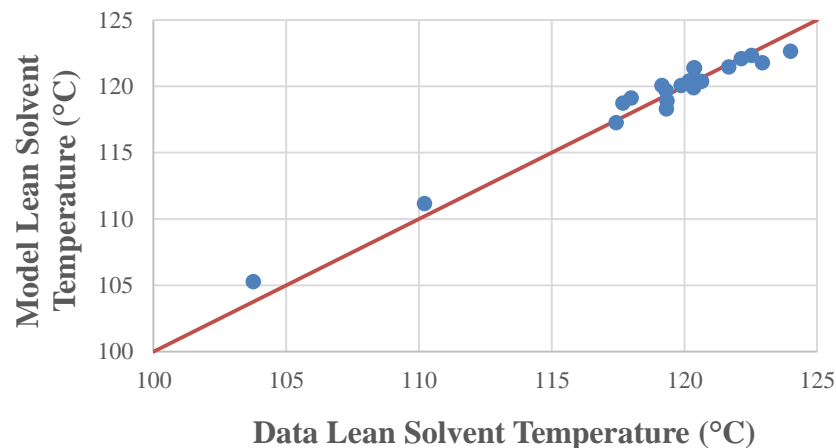
Steady State Regenerator Validation

No parameter tuned

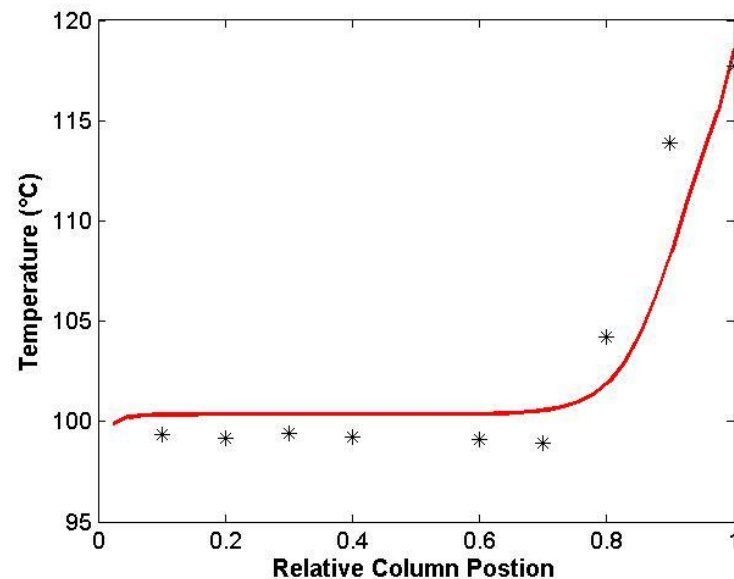
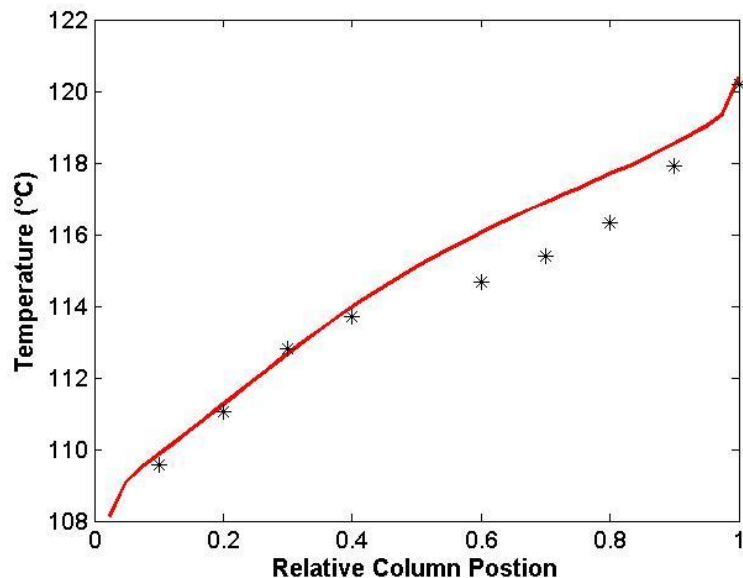
Lean Loading Comparison



Lean Solvent Temperature Comparison



Sample Temperature Profiles



Dynamic Data Reconciliation

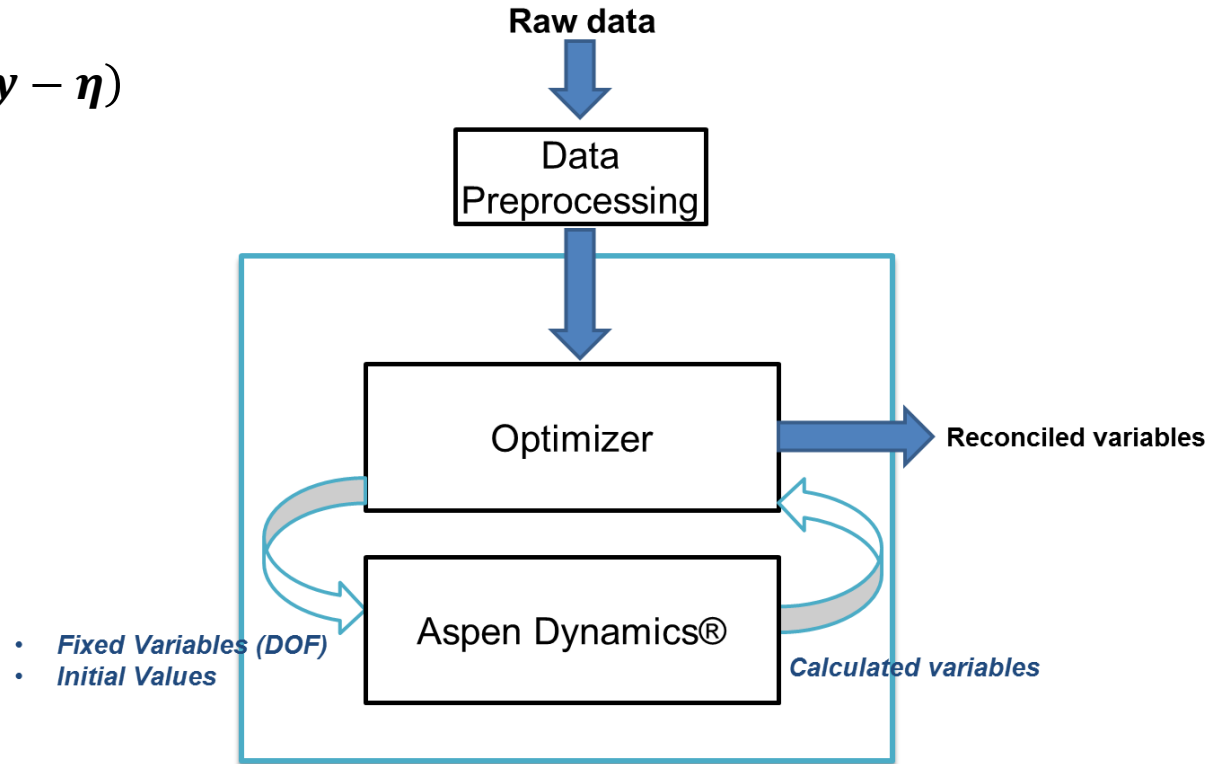
- Measurement noise, sensor bias, and unmeasured data
- Data reconciliation guarantees mass and energy conservation in the dynamic data

$$\min (\mathbf{y} - \boldsymbol{\eta})' \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\eta})$$

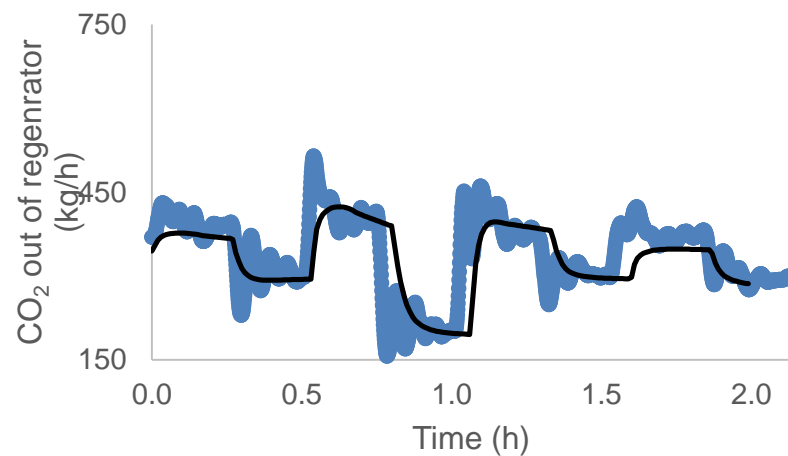
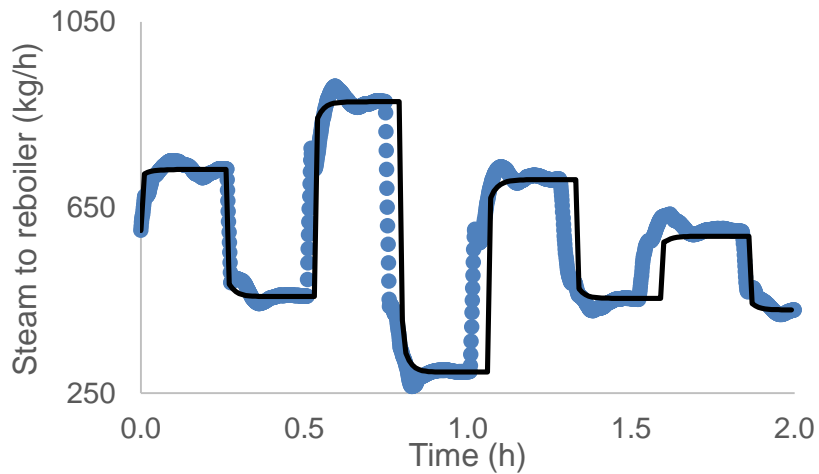
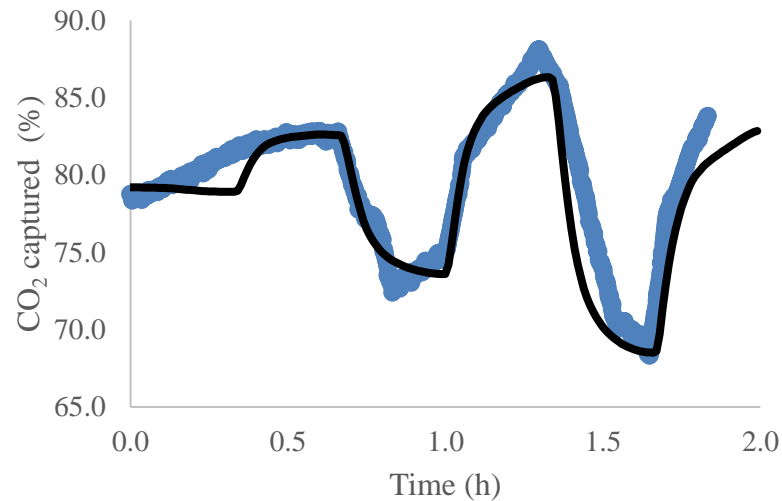
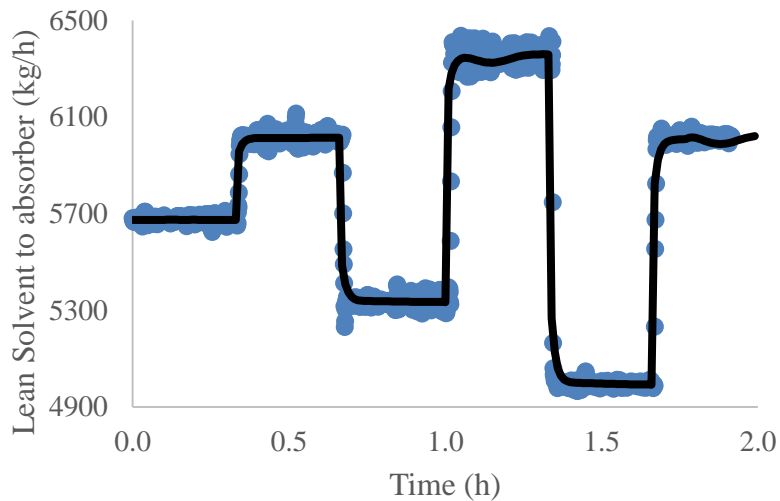
s.t.

$$\dot{\boldsymbol{\eta}} = \mathbf{f}(\boldsymbol{\eta}, \mathbf{u}, \boldsymbol{\theta})$$

$$\mathbf{g}(\boldsymbol{\eta}, \mathbf{u}, \boldsymbol{\theta}) \leq \mathbf{0}$$



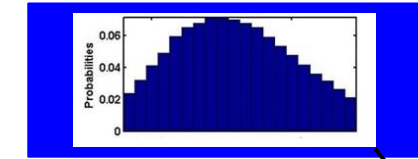
Absorber Validation with DDR



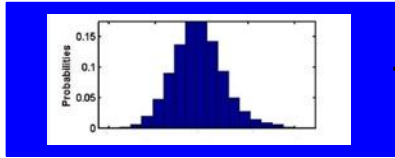
● Data

— Model

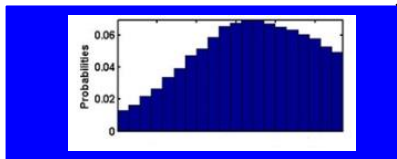
Propagate input uncertainties to quantify the uncertainty in predictions



Uncertainty in Properties Models

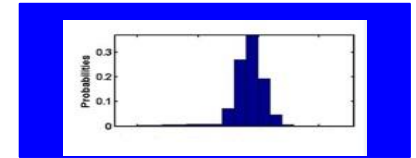
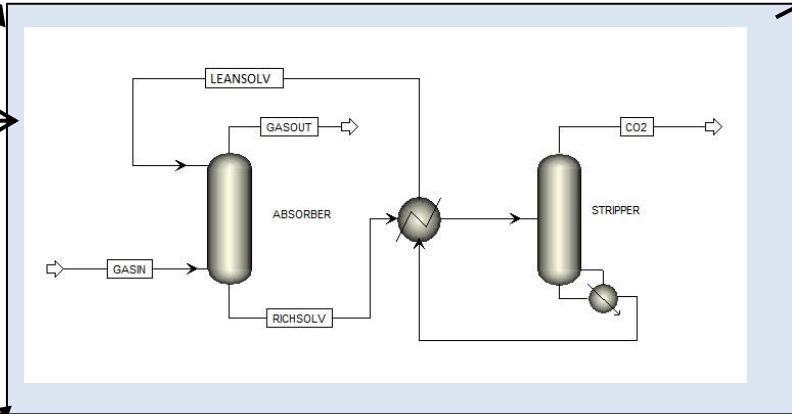


Uncertainty in Hydraulic Models, Mass and Heat Transfer Models



Uncertainty in Kinetic Models

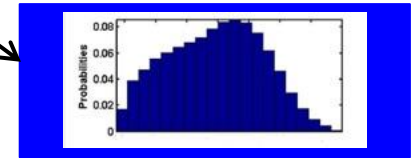
Process Simulation



Uncertainty in % CO₂ Capture



Uncertainty in Energy Requirement



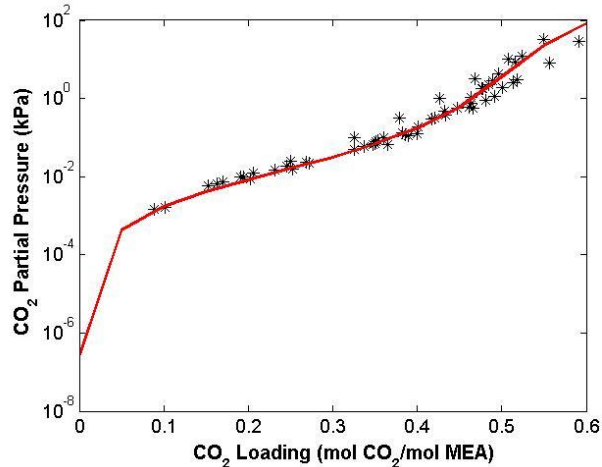
Uncertainty in Estimation of Other Key Variables

Uncertainty Quantification of Process models

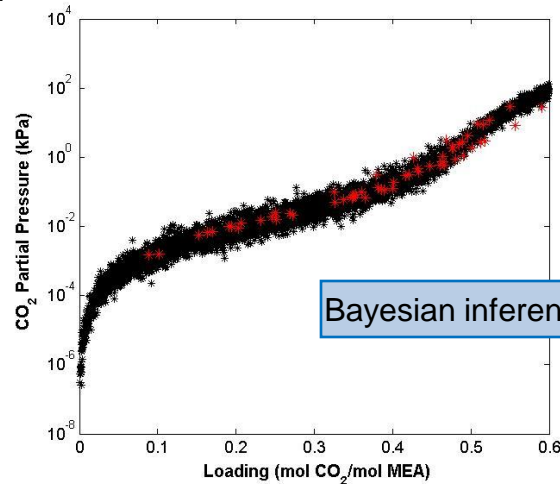
VLE Data/Model Comparison at 40°C

* Model
* Data

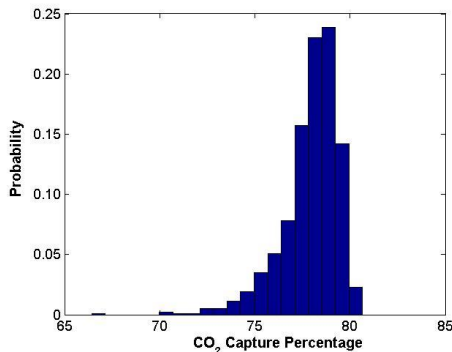
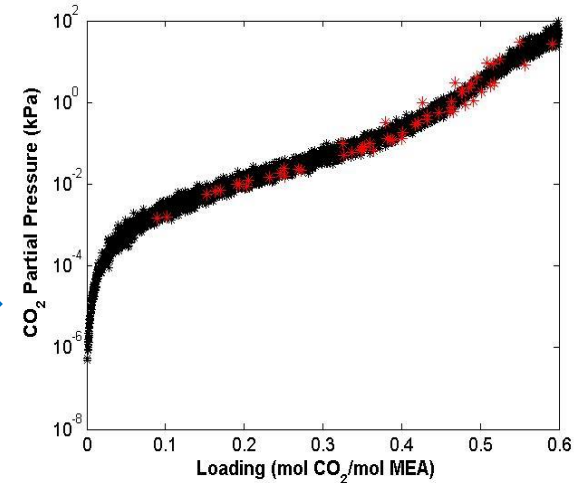
Deterministic Model



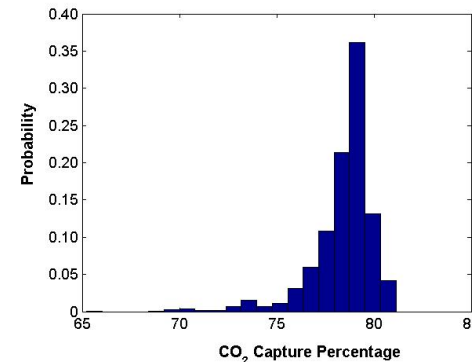
Stochastic Model (Prior Parameter Distribution)



Posterior Parameter Distribution

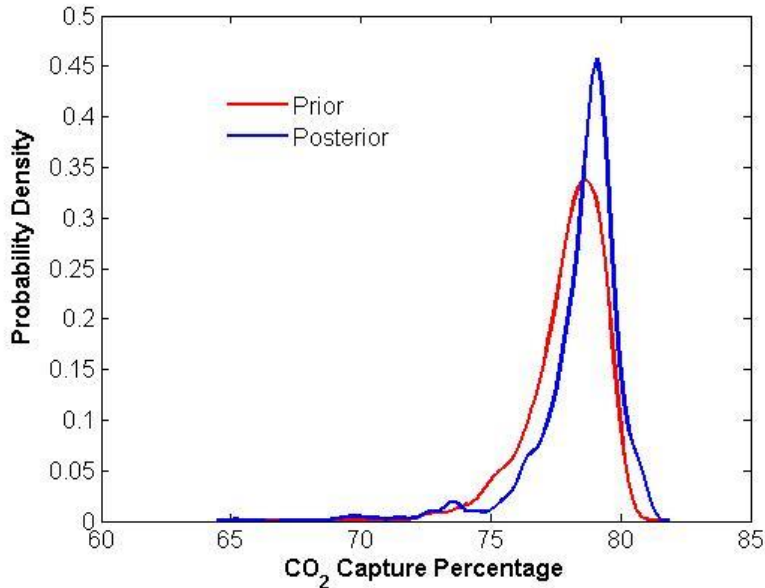


Process Model



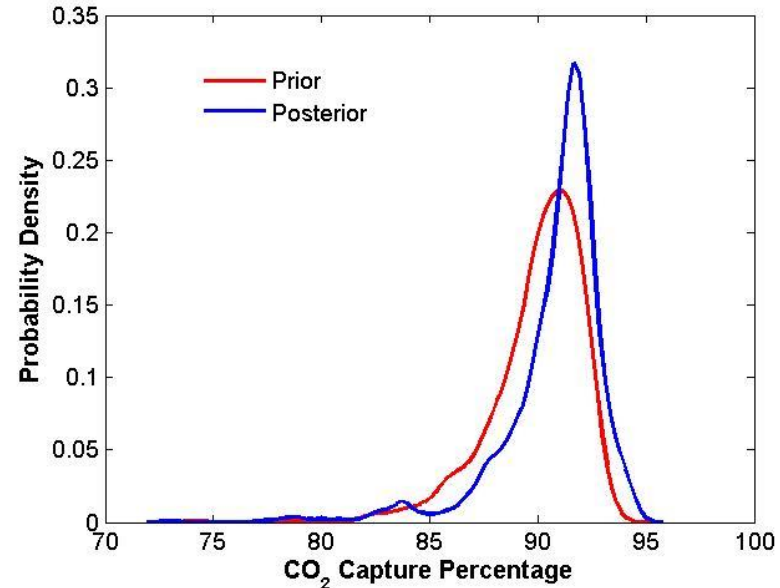
Process Model

Absorber Uncertainty Quantification



Case 1

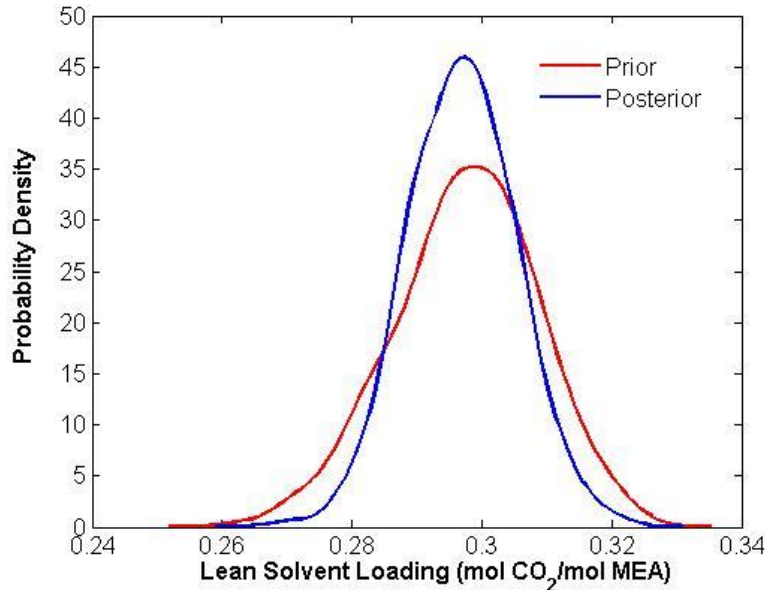
Liquid Flowrate: 3000 kg/hr
Vapor Flowrate: 680 kg/hr
Lean Loading: 0.35 mol CO₂/MEA



Case 2

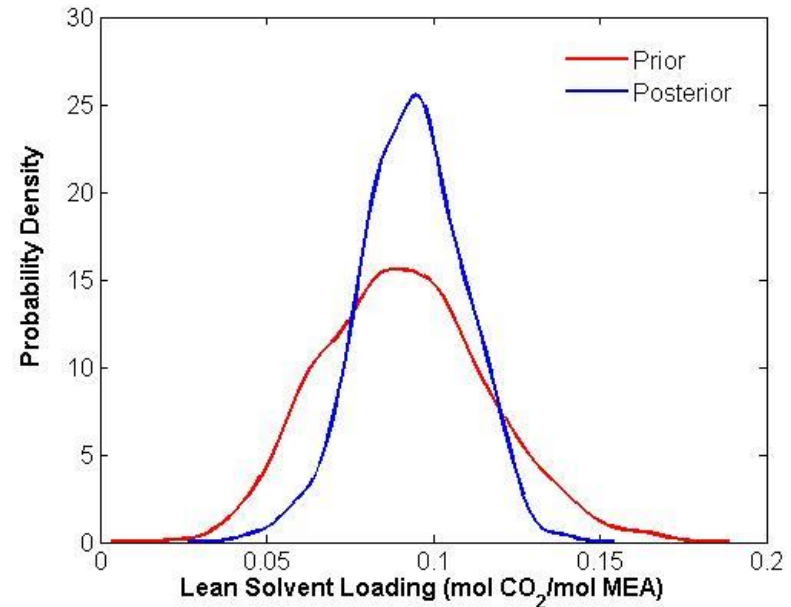
Liquid Flowrate: 3600 kg/hr
Vapor Flowrate: 680 kg/hr
Lean Loading: 0.35 mol CO₂/MEA

Stripper Uncertainty Quantification



Case 1

Solvent Flowrate: 3100 kg/hr
Reboiler Duty: 140 kW
Rich Loading: 0.5 mol CO₂/MEA



Case 2

Solvent Flowrate: 3100 kg/hr
Reboiler Duty: 400 kW
Rich Loading: 0.3 mol CO₂/MEA

High-Viscosity Solvent

- A novel solvent designed by GE is being investigated by the CCSI team. Some features of this solvent are:
 - High-viscosity and its strong dependence on the CO₂ loading
 - Low vapor-pressure
 - Higher degradation temperature leading to high-pressure operation of the desorber thus reducing the CO₂ compression penalty
- Experimental data including VLE and heat of absorption data were obtained for developing thermodynamic and transport properties model.
- Experiments were also conducted at a bench-scale system as well as on a wetted wall column apparatus. The experimental data were utilized to develop models for the interfacial area, mass transfer coefficients and holdup, that are directly affected by the viscosity.

Viscosity Model

Andrade Model in Aspen Plus

$$\ln(\mu_{mix}) = \sum_i w_i \ln(\mu_i) + \sum_i \sum_j (k_{ij} w_i w_j + m_{ij} w_i^2 w_j^2)$$

$$k_{ij} = a_{ij} + \frac{b_{ij}}{T}$$

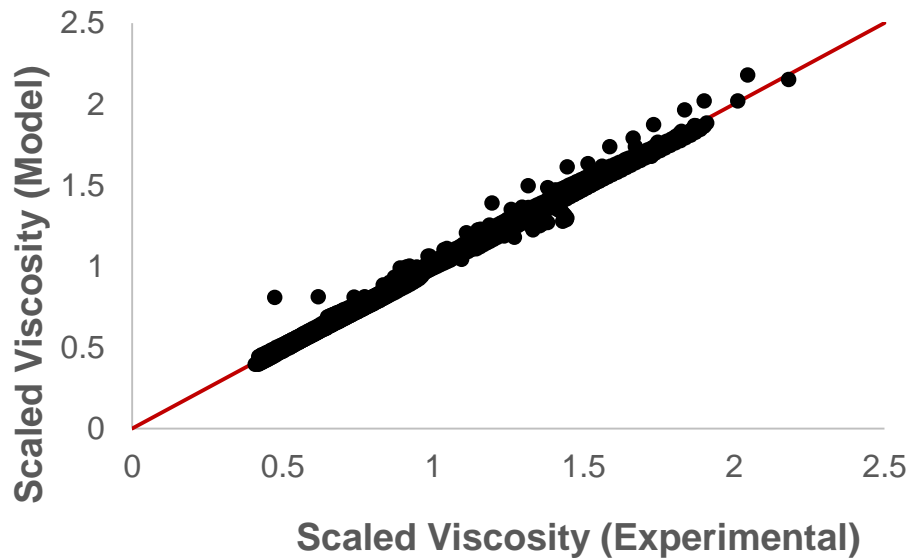
$$m_{ij} = c_{ij} + \frac{d_{ij}}{T}$$

$$\ln(\mu_i) = a_i + \frac{b_i}{T} + c_i \ln(T)$$

Akaike Information Criterion (Parameter Selection)

$$AIC = N \ln\left(\frac{SSE}{N}\right) + 2k$$

k = Number of Parameters
N = Number of Data
SSE = Sum of Square Error



* Data and Model predictions given in terms of $\ln(\mu_{mix})$.

Thermodynamic Framework

Physical Equilibrium

$$P_{CO_2} = H_{CO_2} x_{CO_2} \gamma_{CO_2}$$

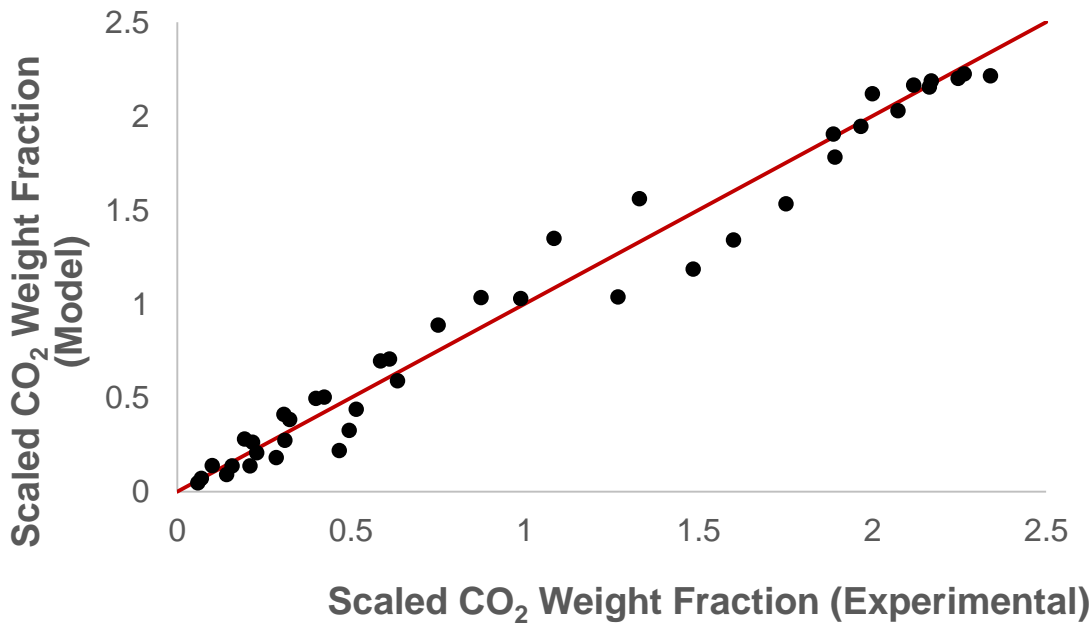
Chemical Equilibrium

$$K_{eq} = \frac{[Prod]}{[React][CO_2]}$$

Model parameters calibrated to optimize fit to VLE data:

$$H_{CO_2} = \exp\left(H_1 + \frac{H_2}{T}\right)$$

$$K_{eq} = \exp\left(K_1 + \frac{K_2}{T}\right)$$



Model Validation Using Bench Scale Data

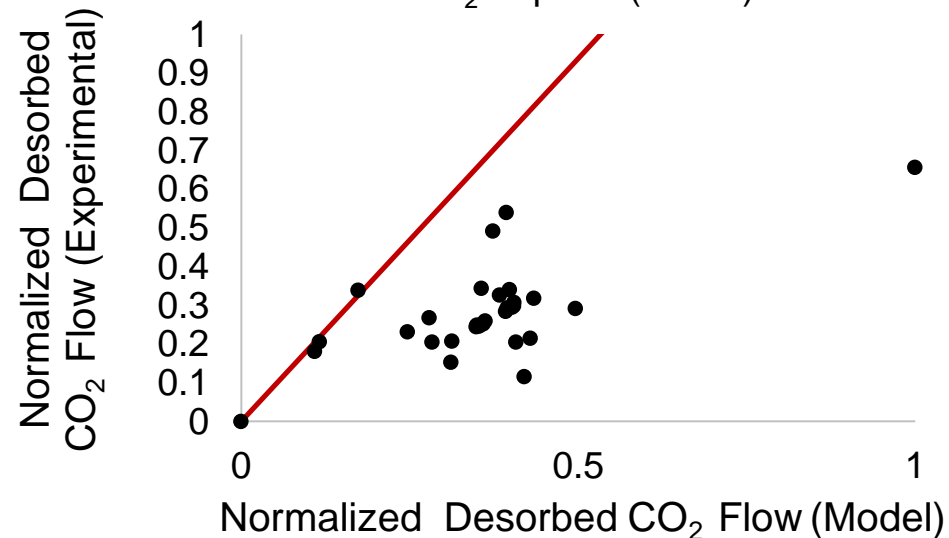
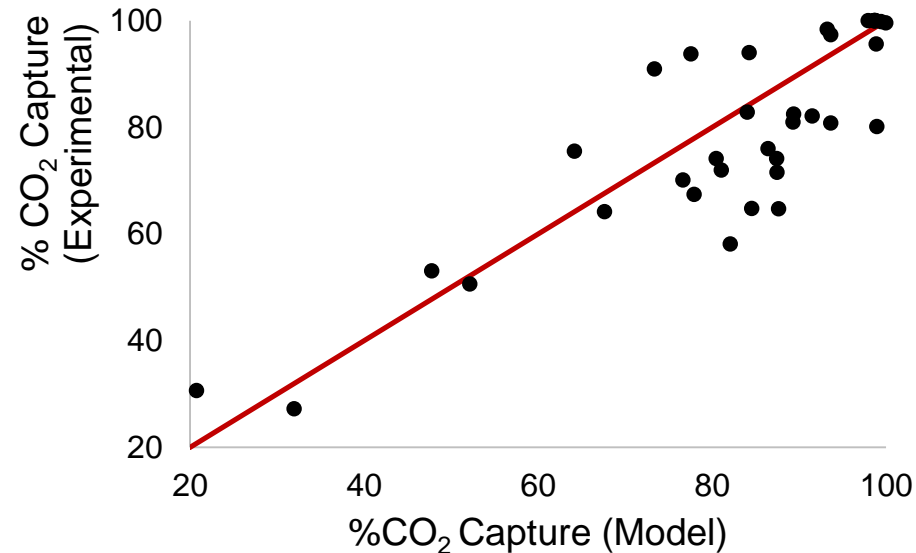
- Rate-based Aspen Plus™ model
 - Mass transfer coefficients: Modified Billet and Schultes model¹ (1993)
 - Interfacial area: Modified Tsai Model (2010)
 - Holdup: Modified Billet and Schultes model (1999)
- The pre-exponential factor and activation energy of the forward reaction were regressed

$$r_{CO_2} = k_f \left([CO_2][Reac] - \frac{1}{K_{eq}} [Prod] \right)$$

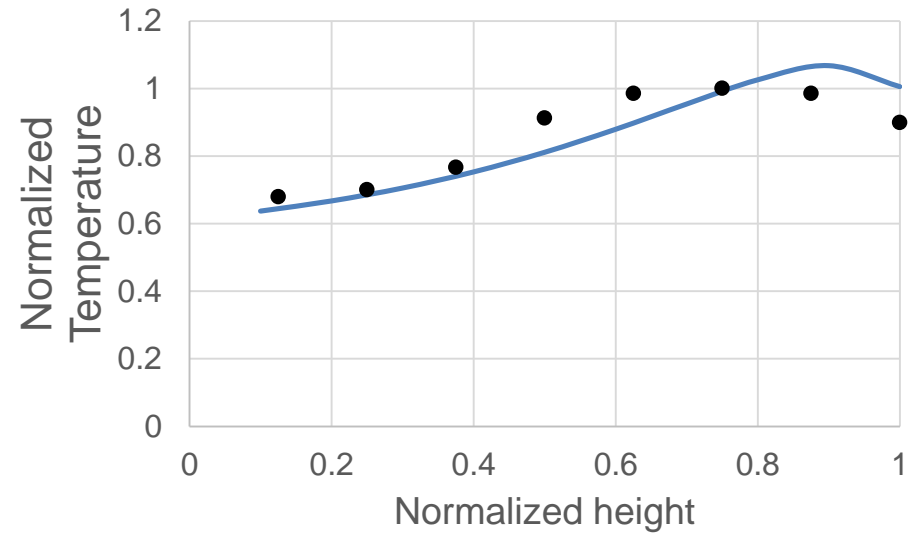
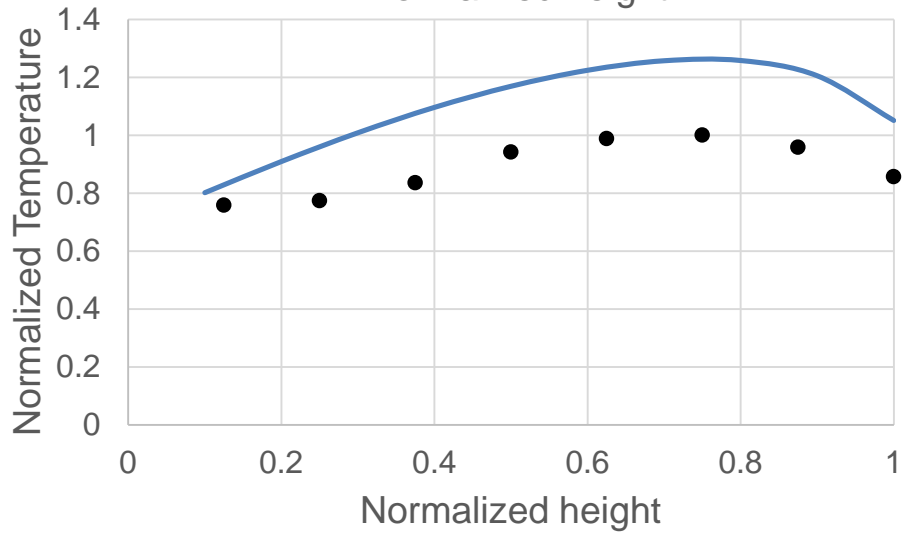
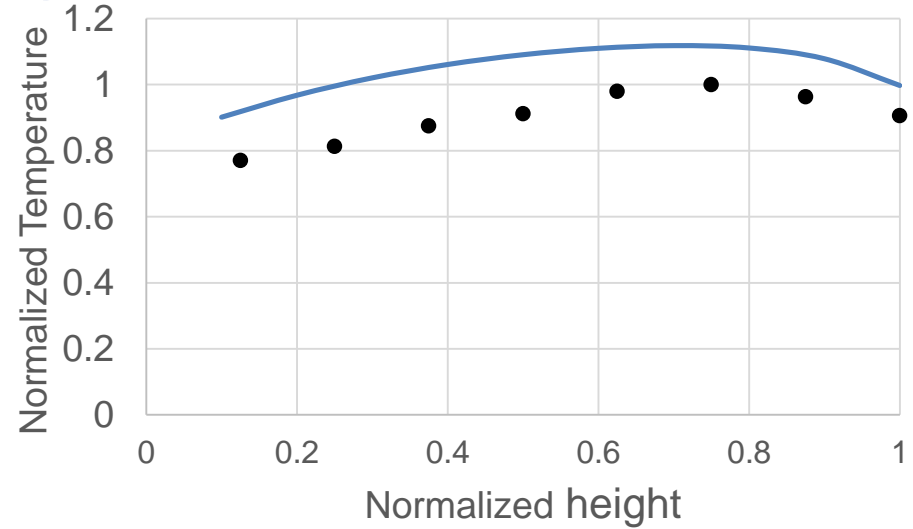
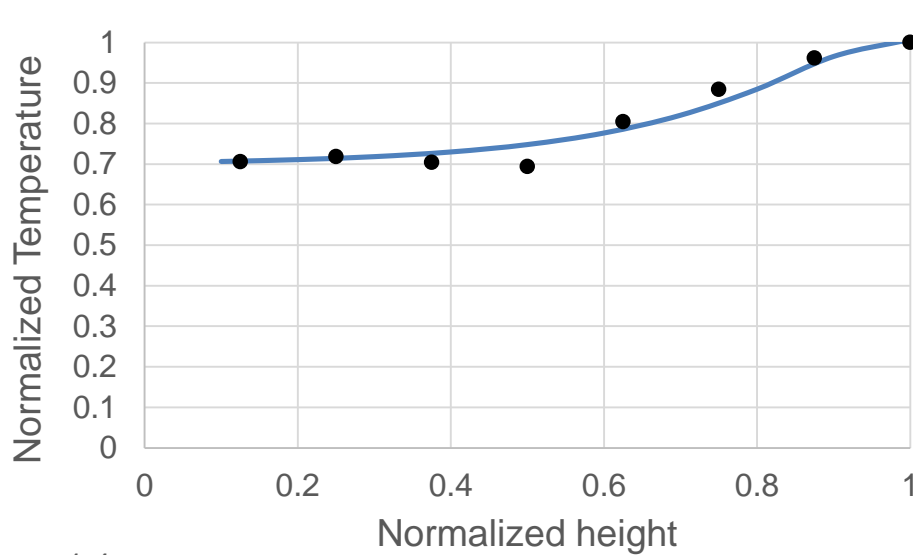
¹Billet R, Schultes M. Predicting Mass Transfer in Packed Columns. Chem. Eng. Technol. 1993;16(1):1-9.

²Tsai R.E. Mass Transfer Area of Structured Packing. Ph.D. Dissertation, UT, Austin, 2010

³Billet R, Schultes M. Prediction of Mass Transfer Columns with Dumped and Arranged Packings: Updated Summary of the Calculation Method of Billet and Schultes. Chem. Eng. Res. Des. 1999; 77(A6): 498-504.



Model Validation Using Bench Scale Data



• Experimental — Model

Conclusions

- Developed validated modeling framework with UQ capabilities for a **gold standard** model that is capable of accurate estimation in wide operating range both under steady-state and dynamic conditions
- Developed dynamic model validation protocol
- Model predicted the experimental data for the scaleup case satisfactorily
- Demonstrated how synergistic coupling between experimental protocol and modeling methodology be mutually beneficial and informative- highly useful for scale up

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Thank You