Modeling of MEA-based CO2 Capture Process with Uncertainty Quantification andValidationwithSteady-State and Dynamic Data from Pilot Plant

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Modeling of MEA-based CO_2 Capture Process with Uncertainty Quantification and Validation with Steady-State and Dynamic Data from Pilot Plant

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Post-Combustion Capture Conference
8-11th September, 2015
Regina, Canada

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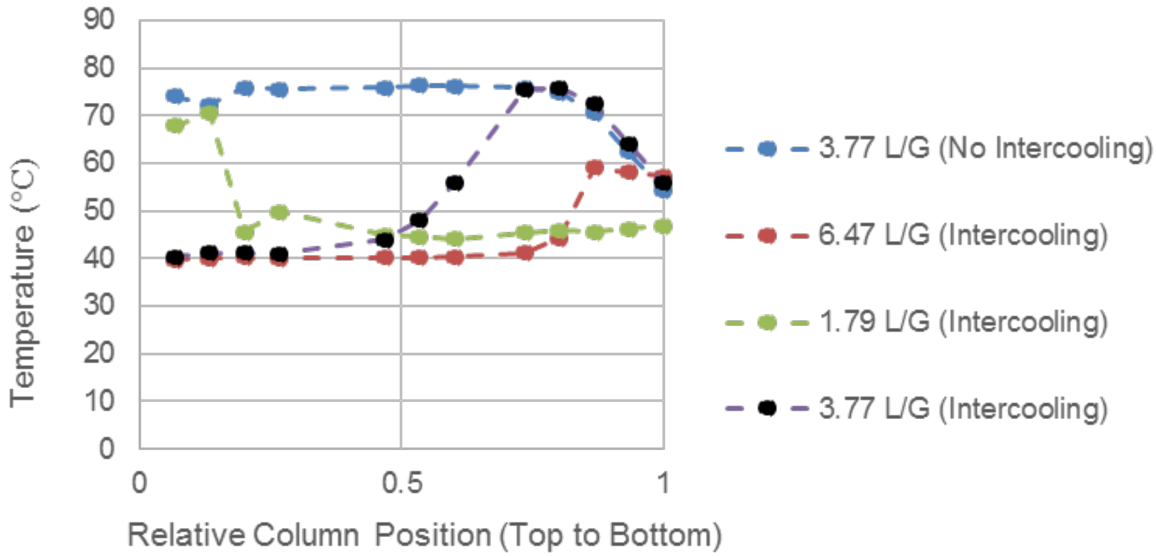
Gold Standard Solvent Model

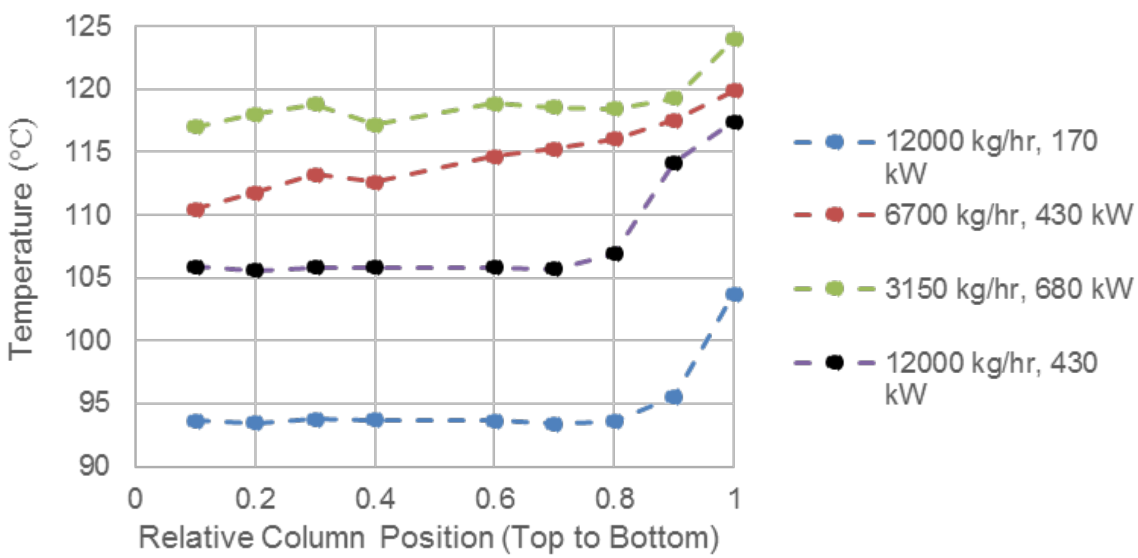
- Gold Standard model for comparing different proposals for advanced solvent-based capture technologies
  - Open source
  - Validated framework
  - Well documented
  - Uncertainties quantified

Challenges for a Gold Standard Model

Temperature Profile in the Absorber



Temperature Profile in the Regenerator



Our Approach to Developing a gold standard model?

- **Properties models**
  - All properties models must be valid for absorber and stripper operating conditions

- **Hydraulic and mass transfer models**
  - Mass transfer models should be developed simultaneously with *relevant* properties models using both WWC and packing data

- **Steady state model validation**

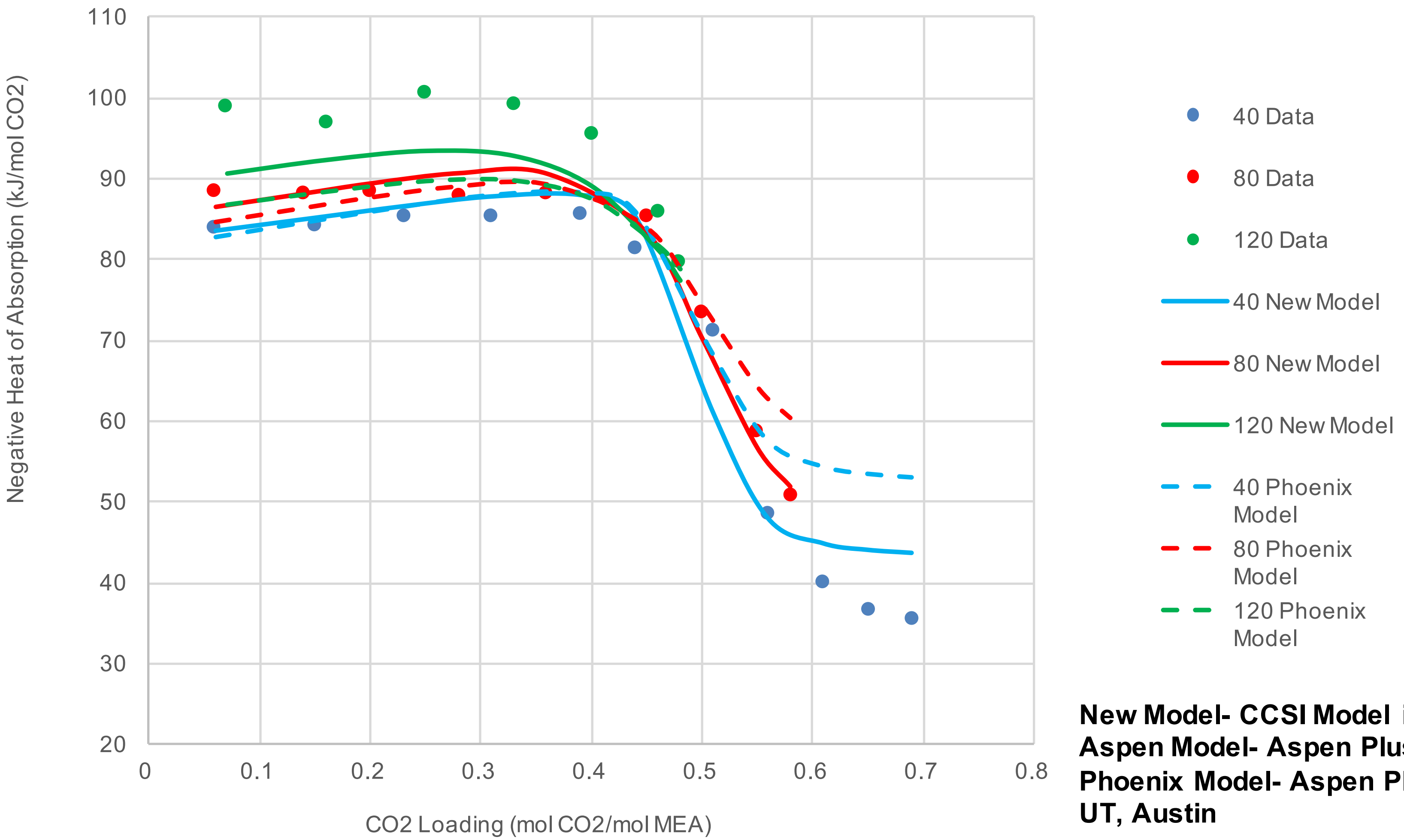
- **Dynamic model validation**

Properties Models

Physical Property Model Development

- Independent property models
  - Viscosity
  - Density/Molar Volume
  - Surface Tension
- Thermodynamic framework
  - Vapor-Liquid Equilibrium
    - Binary MEA-H_2O system
    - Ternary MEA-H_2O-CO_2 system
  - Heat Capacity
  - Heat of Absorption
  - Reaction Kinetics
    - Model developed for consistency with reaction equilibrium constants

New VLE model better at capturing the trend in heat of absorption



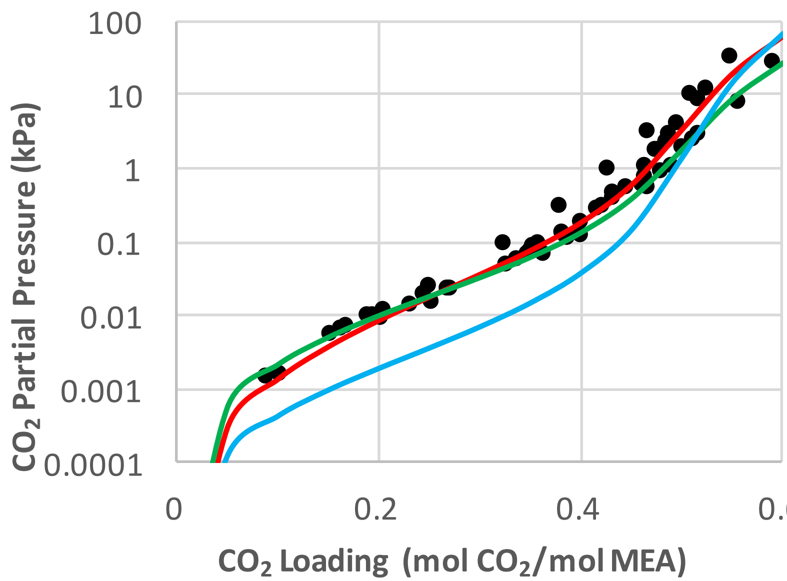
New Model- CCSI Model in Aspen Plus
Aspen Model- Aspen Plus Example Model
Phoenix Model- Aspen Plus Model from UT, Austin

Heat of Absorption Data* (30 wt% MEA and 40,80, and 120°C)

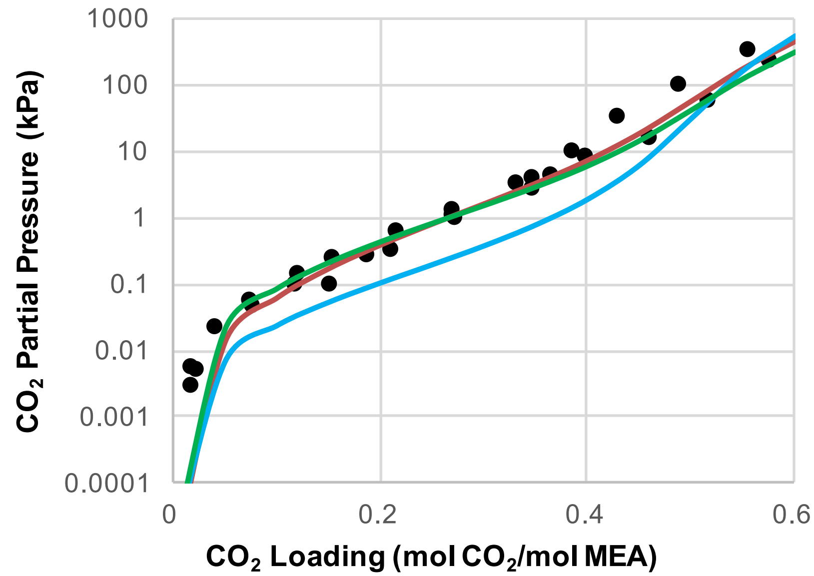
***Kim, Hoff, and Mejdell, Heat of Absorption of CO_2 with Aqueous Solution of MEA: New Experimental Data, GHGT-12, Austin, TX, 6-9th Oct, 2014**

New model agrees well with the VLE data

40°C, 30 wt% MEA

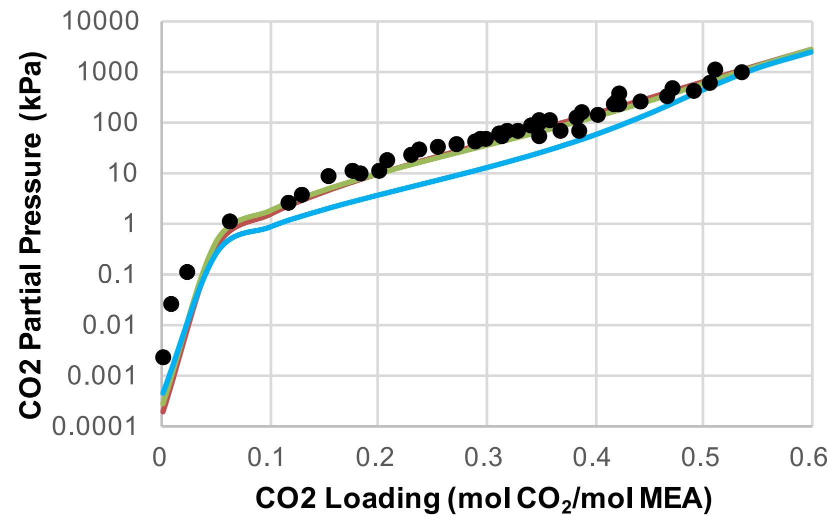


80°C, 30 wt% MEA



- Data
- New Model
- Aspen Model
- Phoenix Model

120°C, 30 wt% MEA

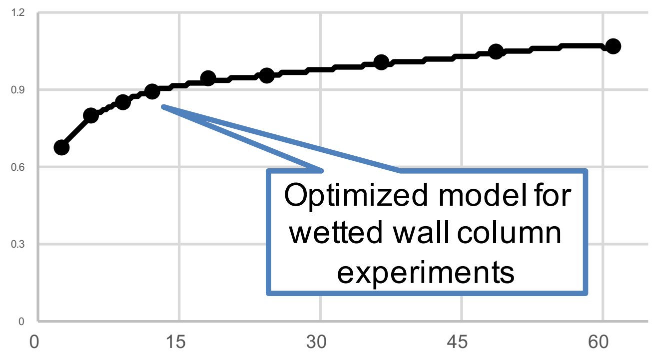


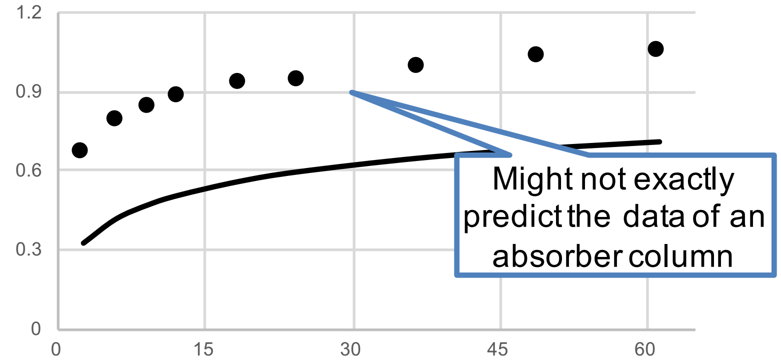
New Model- CCSI Model in Aspen Plus
Aspen Model- Aspen Plus Example Model
Phoenix Model- Aspen Plus Model Developed at UT, Austin

Hydraulic and Mass Transfer Models

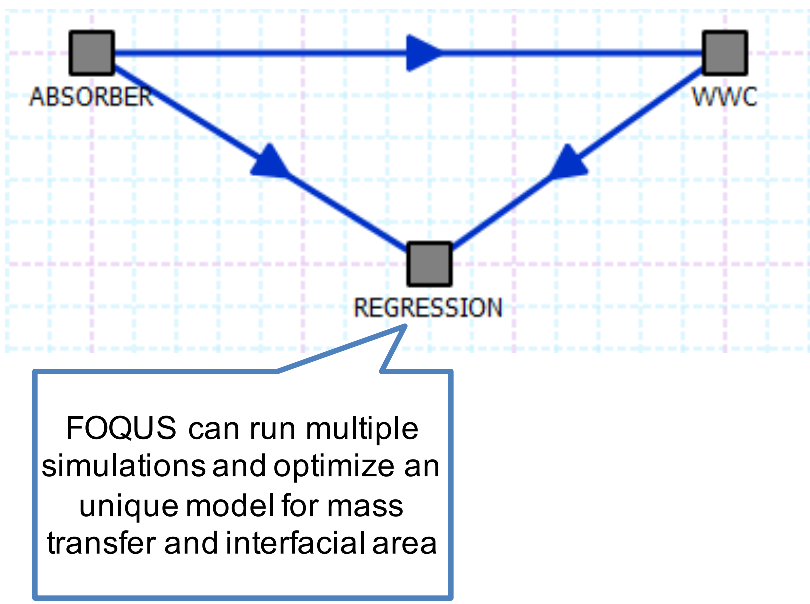
Integrated Mass Transfer Model Development

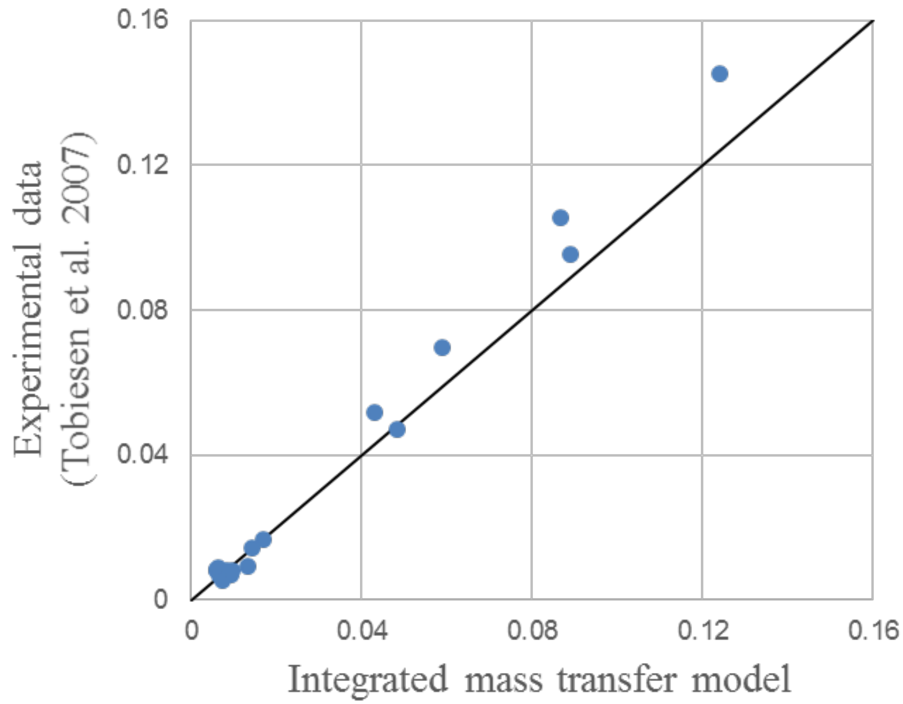
Usual approach: Sequential regression





FOQUS capability: Simultaneous regression





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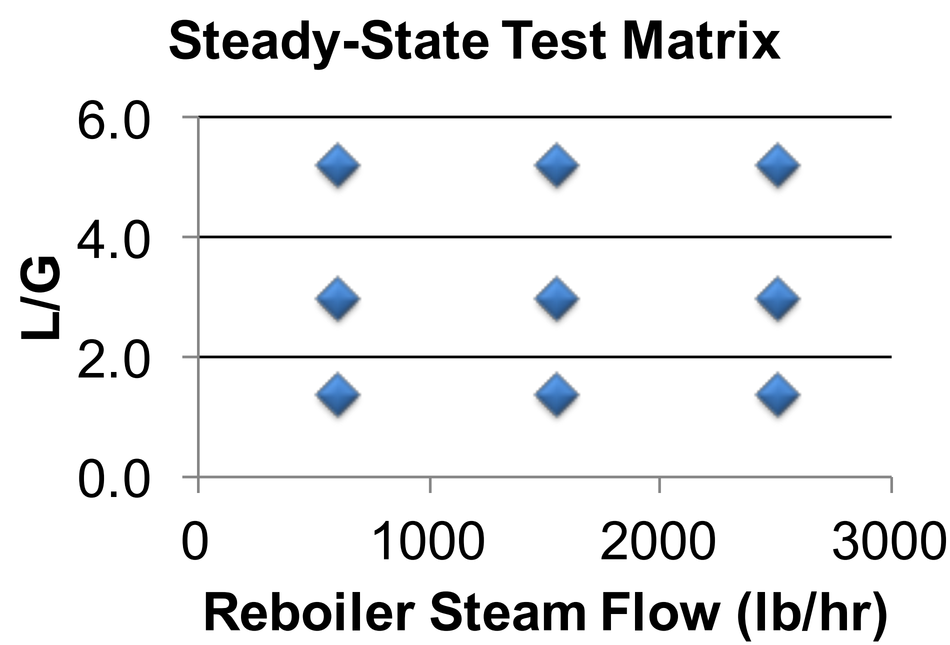
Test Runs at National Carbon Capture Center, Al: Steady-State Runs

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

- **All possible combinations of different operating conditions tested**

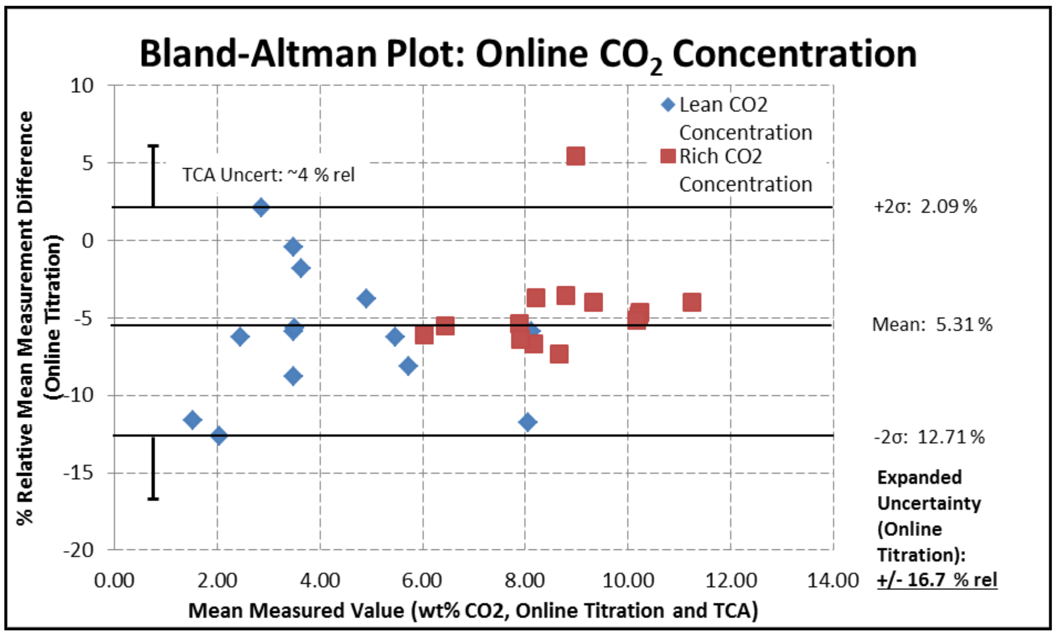


Uncertainty of the Measurement Techniques

- **Dynamic Test Runs**: Gas Chromatography (GC) for Amine Concentration and Bench Equivalence Point (EQP) Base Titration (CO_2 Concentration)
- **Steady State Runs**: Online EQP Acid Titration (Amine Concentration) and Online EQP Base Titration (CO_2 Concentration)

➢ Analysis Techniques Repeatability Evaluation

➢ Analysis Techniques Uncertainty Evaluation



Critical Model Parameters:

Portion of Campaign	Dynamic	Steady State
Amine Concentration (wt% MEA Nominal) % rel expanded uncertainty (k=2)	4.9%	7.3%
CO_2 Loading (mol CO_2 / mol MEA) % rel expanded uncertainty (k=2)	7.4%	10.7%

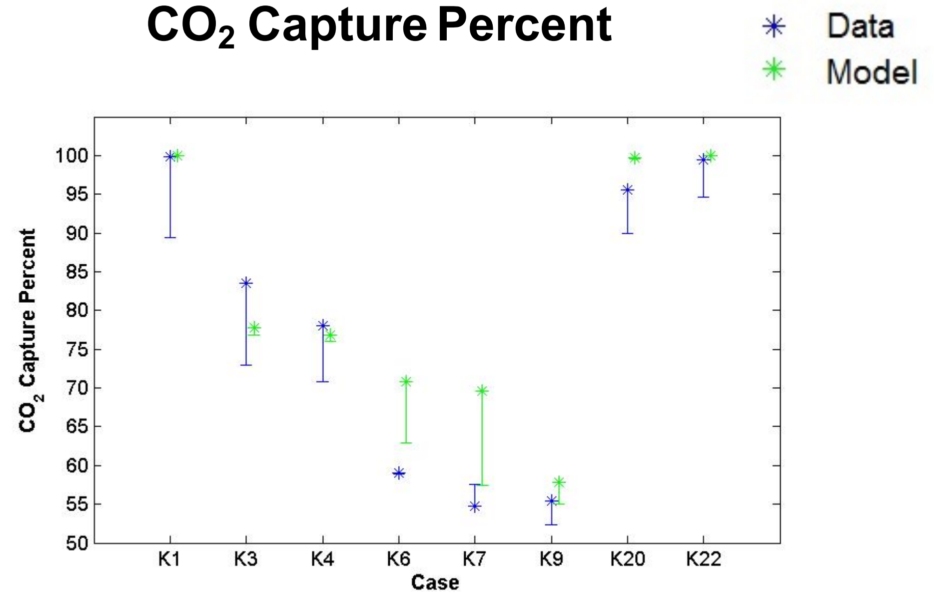
Steady State Absorber Validation

No parameter tuned

Input Variables

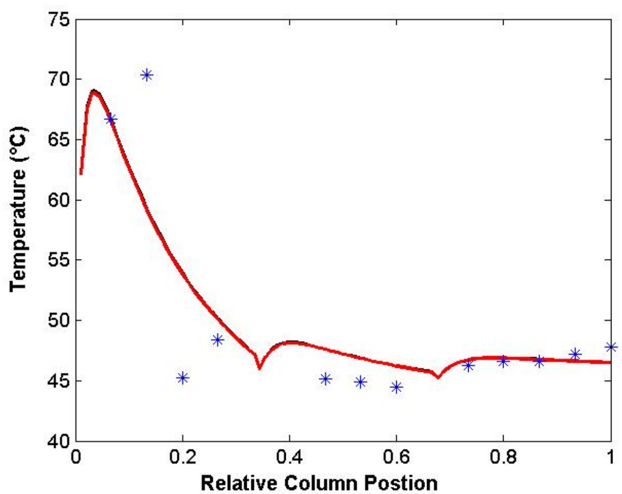
Case	L/G (mass)	Beds/ Intercooling	Lean Loading (mol CO_2/mol MEA)
K1	3.00	3/Yes	0.145
K3	1.41	3/Yes	0.091
K4	1.40	3/Yes	0.083
K6	3.02	3/Yes	0.347
K7	5.24	3/Yes	0.399
K9	1.41	3/Yes	0.239
K20	2.38	1/No	0.075
K22	4.89	2/Yes	0.130

CO_2 Capture Percent

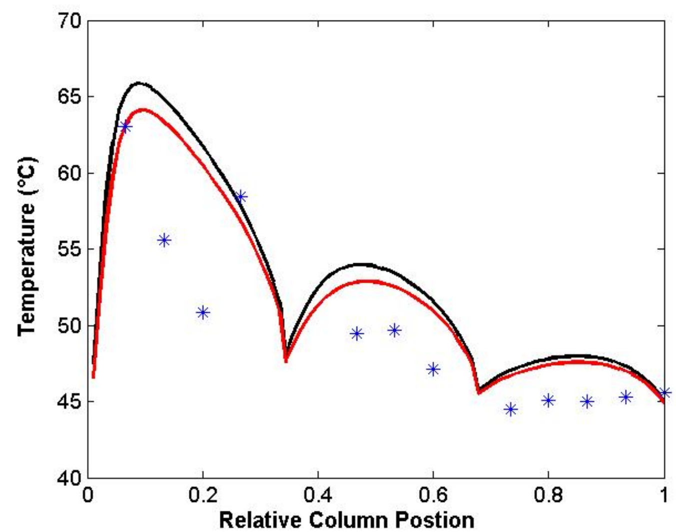


Sample Temperature Profiles

Case K4



Case K6



Model
Model (Loading Discrepancy Included)
Data

* Relative positions of 0 and 1 represent top and bottom of column, respectively

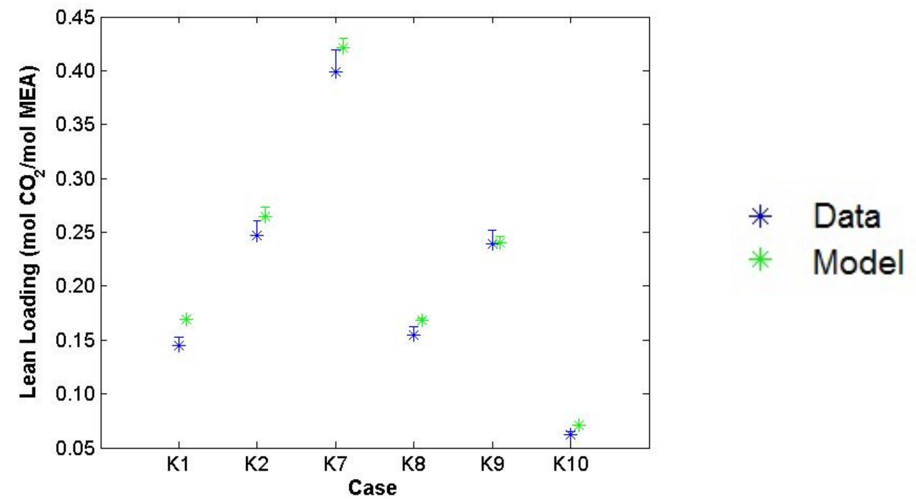
Regenerator Validation

No parameters tuned

Input Variables

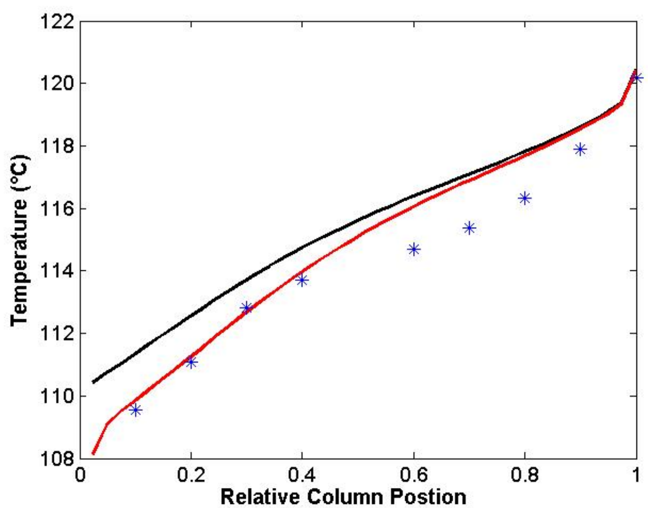
Case	Rich Solvent Flow (kg/hr)	Reboiler Duty (kW)	Rich Loading (mol CO_2/mol MEA)
K1	7242	430.61	0.384
K2	12284	429.54	0.385
K7	12092	169.63	0.471
K8	12042	676.79	0.275
K9	3337	165.74	0.474
K10	3358	670.62	0.477

Lean Loading Prediction

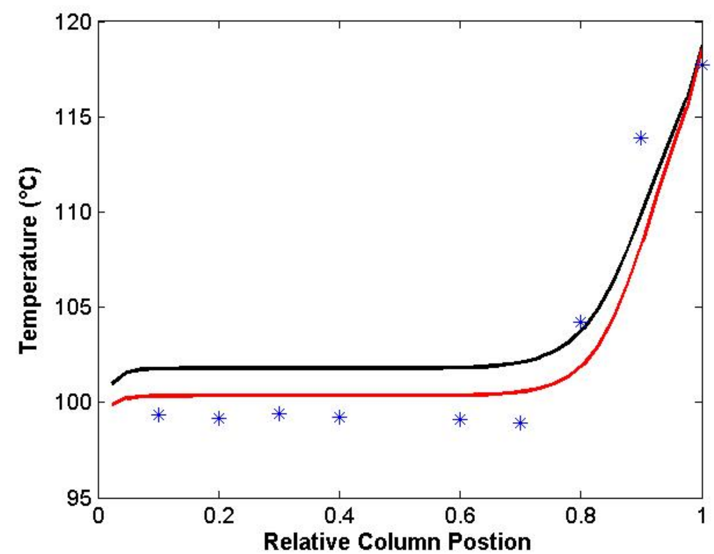


Sample Temperature Profiles

Case K1



Case K9



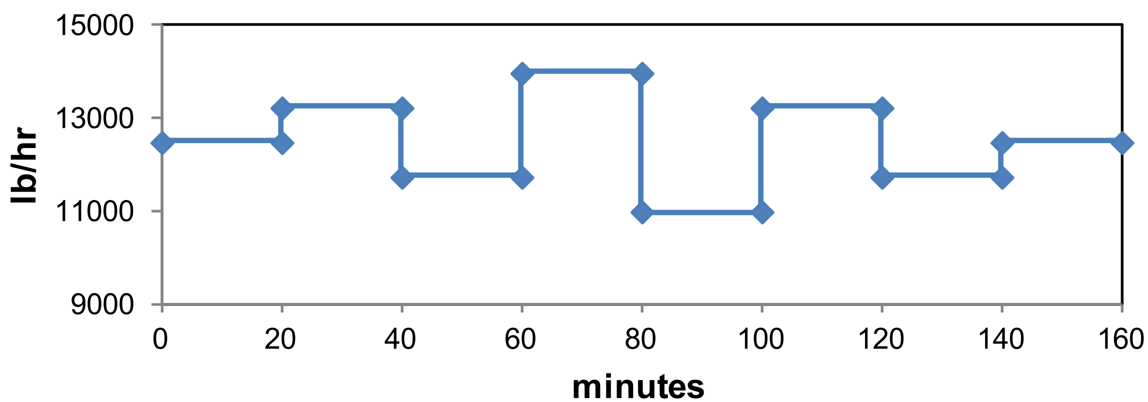
Model
Model (Loading Discrepancy Included)
Data

Dynamic Model Validation

Dynamic Test Conditions

- Dynamic tests capture nonlinearity
- Persistence of excitation
- Step test conducted
  - Solvent flow (lb/hr); x_1=6, datum= 12,500
  - Inlet flue gas(lb/hr); x_2=10, datum= 5,000
  - Reboiler Steam Flow(lb/hr); x_3=6, datum = 5,000

Test#	Test Condition
1	datum
2	+x% of datum
3	-x% of datum
4	+2x% of datum
5	-2x% of datum
6	+x% of datum
7	-x% of datum
8	datum



Time periods as well as x_1, x_2, and x_3 determined by conducting initial step tests and recording sensitivities in outputs

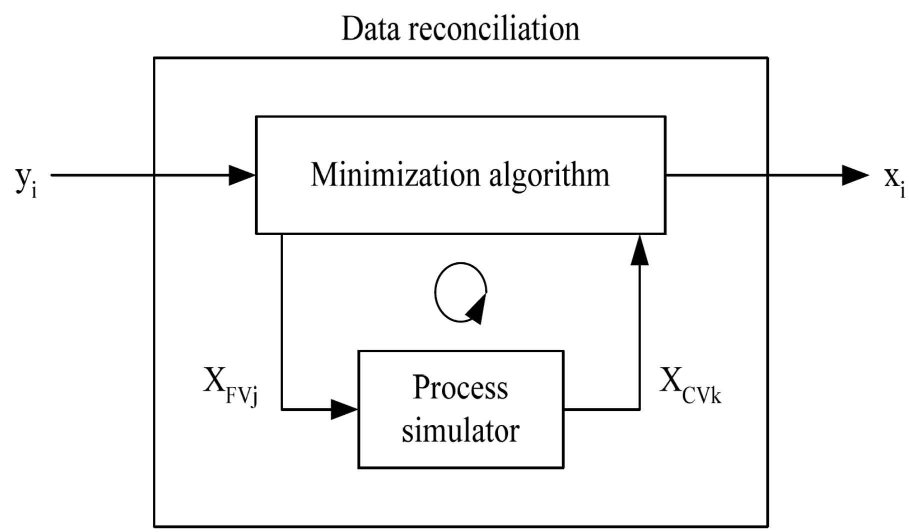
Dynamic data reconciliation

- Noisy, inaccurate, and missing measurements
- Noisy data are preprocessed using a filter
- Filtered data used for data reconciliation that guarantees mass and energy conservation during dynamic run

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

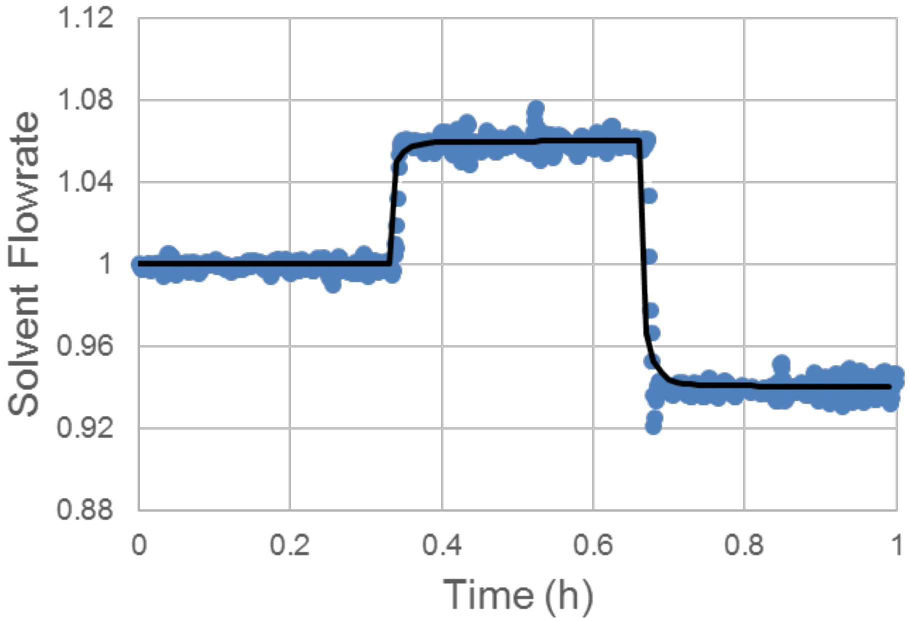
s.t.

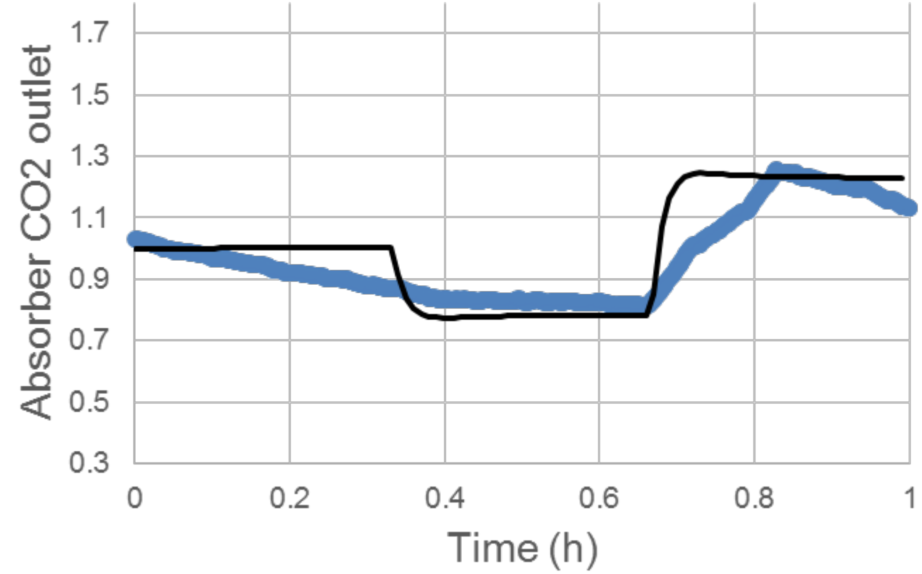
$$\dot{\boldsymbol{\eta}} = \boldsymbol{f}(\boldsymbol{\eta}, \boldsymbol{u}, \boldsymbol{\theta})$$
$$\mathbf{g}(\boldsymbol{\eta}, \boldsymbol{u}, \boldsymbol{\theta}) \leq \mathbf{0}$$

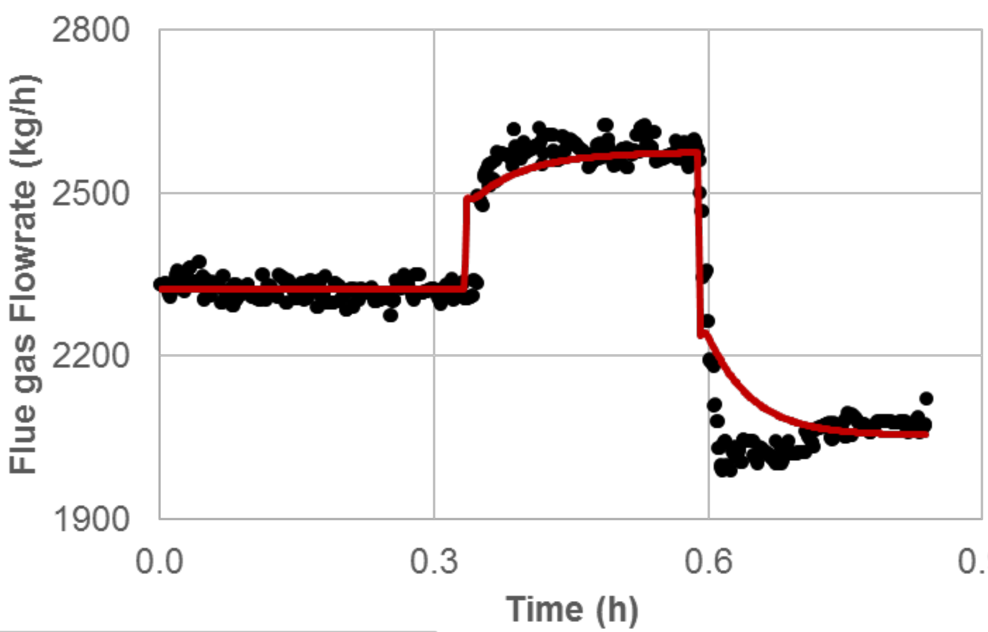


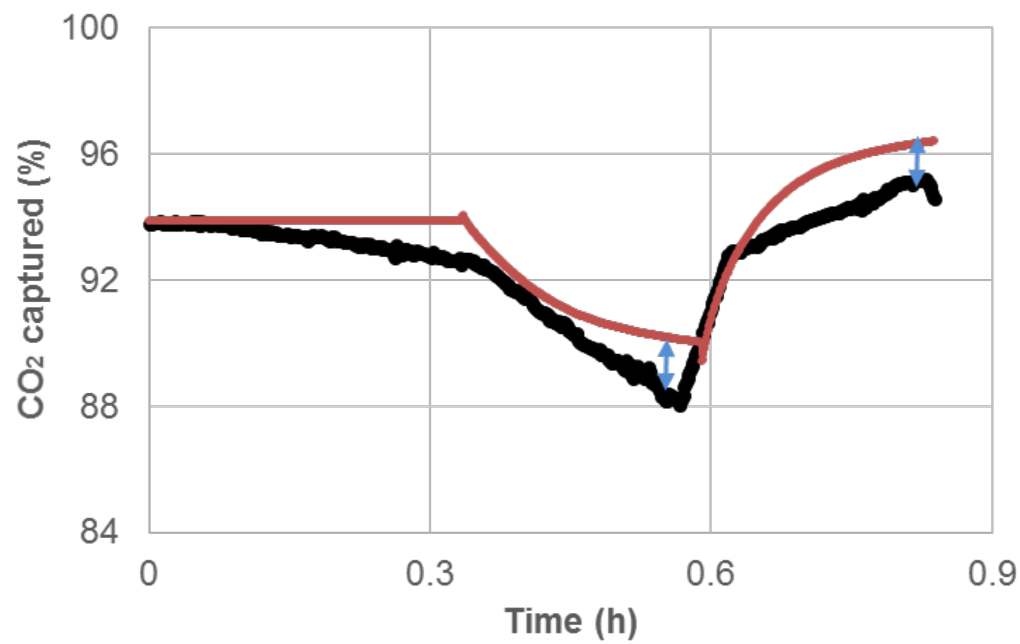
Needs to redraw the fig

Results (figures would be updated)









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Conclusions

- Steady state model is validated with pilot plant data over wide range- both in mass-transfer limited as well as reactions-limited regions. Consideration of the measurement discrepancy in liquid loading improves model prediction.
- A dynamic data reconciliation approach is developed to account for the noisy, incorrect, and missing data.
- Dynamic model estimates both the gain as well as the time constant of the process reasonably well.

Thank you!

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Current Status

- Initial framework based upon the "Phoenix" model* (Rochelle Group at UT-Austin)
  - e-NRTL thermodynamic framework
- Updated models
  - All physical property models
  - Hydrodynamic models
  - New VLE model- New data for VLE, heat of absorption, and heat capacity
  - Simultaneous regression of wetted wall column and packed column data for mass transfer correlations along with diffusivity and interfacial area
  - Steady state validation
  - Initial dynamic validation
- Uncertainty quantification of numerous sub-models

***Jorge Mario Plaza, Ph.D. Dissertation, UT Austin, May 2012**

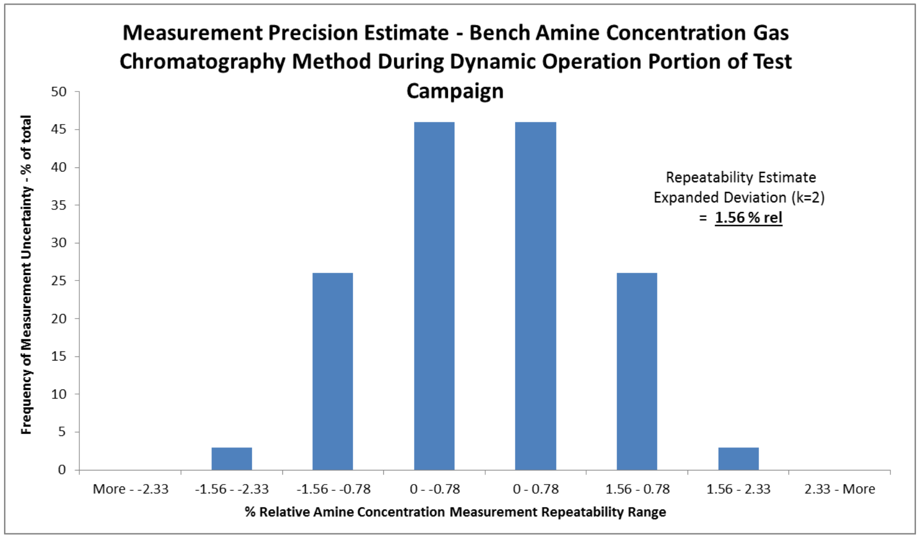
NCCC vs Other Pilot Plants

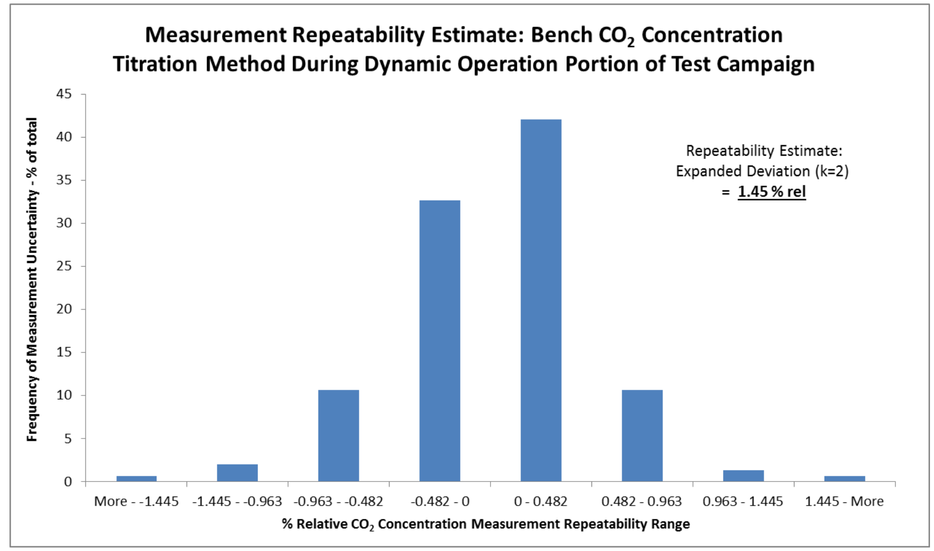
	CO_2 Capacity (tpd)	Source of Flue Gas	Absorber		Regenerator	
			Diameter (cm)	Height (m)	Diameter (cm)	Height (m)
UT, Austin	3.0	Non-coal	42.7	6.1	42.7	6.1
NTNU/ SINTEF	0.3	Non-coal	15.0	4.4	10.0	3.9
ITC, Regina	1.0	Non-coal	33.0	7.1	33.0	10.0
ITT, Stuttgart	0.3	Non-coal	12.5	4.2	12.5	2.5
Esbjerg CASTOR	24.0	Coal	110.0	17.0	110.0	10.0
NCCC (PSTU)	10.0	Coal	64.1	18.5	59.1	12.1

Intercooler and flexibility of number of beds also differ

Repeatability Estimation Results

Repeatability:



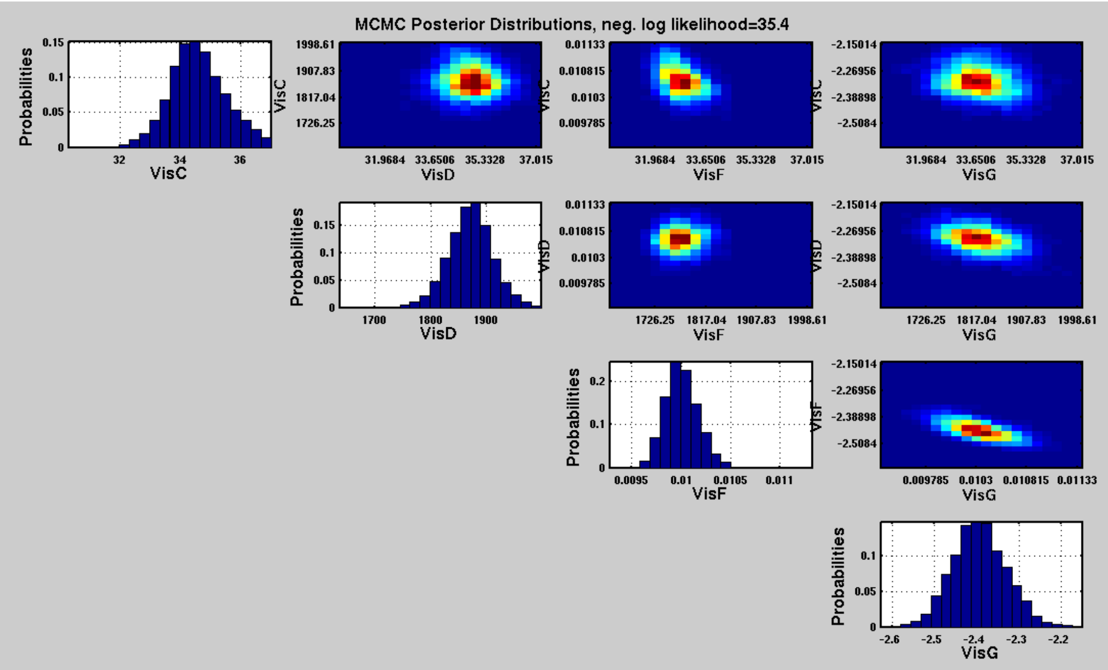


Bench GC repeatability:
1.56 % rel (k=2)

Bench EQP base titration repeatability: 1.45 % rel (k=2), other titrations assumed similar

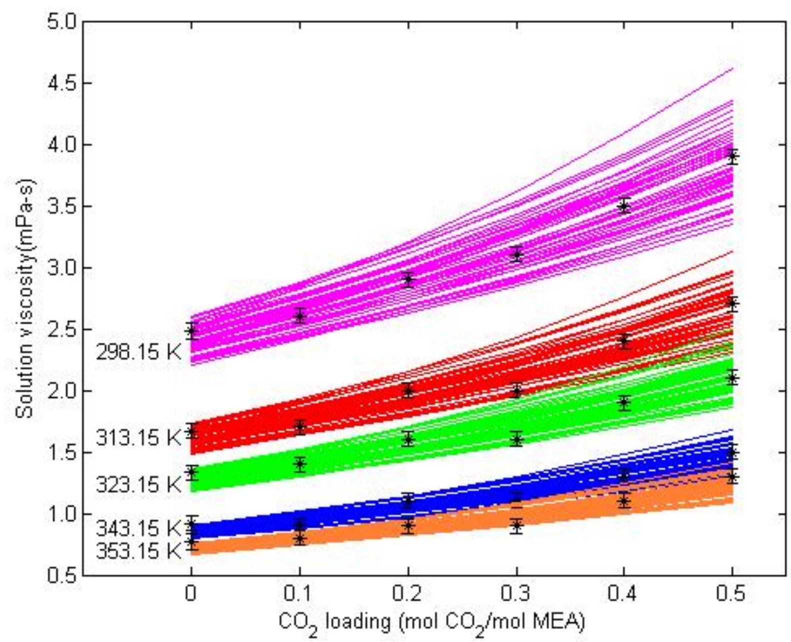
Based on this analysis it is assumed that all methods used during the test campaign exhibit good repeatability, ~1.5 % rel expanded repeatability (k=2)

Stochastic Viscosity Model Results



Posterior Distributions of Parameters for Viscosity Model

Sample stochastic data/model comparison (X_{MEA}=20%)
Sample size of 100 drawn from posterior distributions



Data points from Amundsen et al., Journal of Chemical & Engineering Data, 2009, 54, 3096-3100

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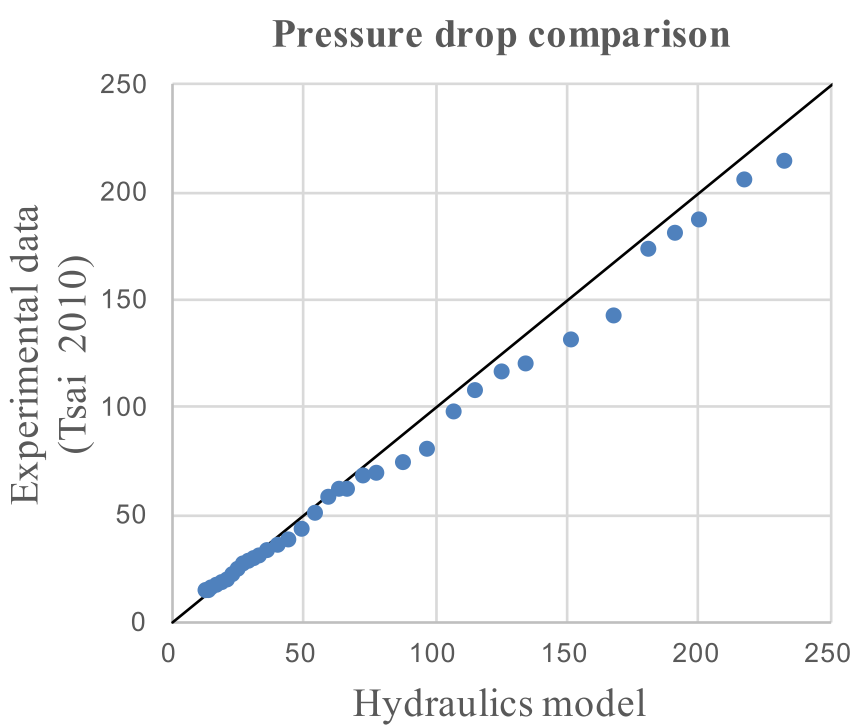
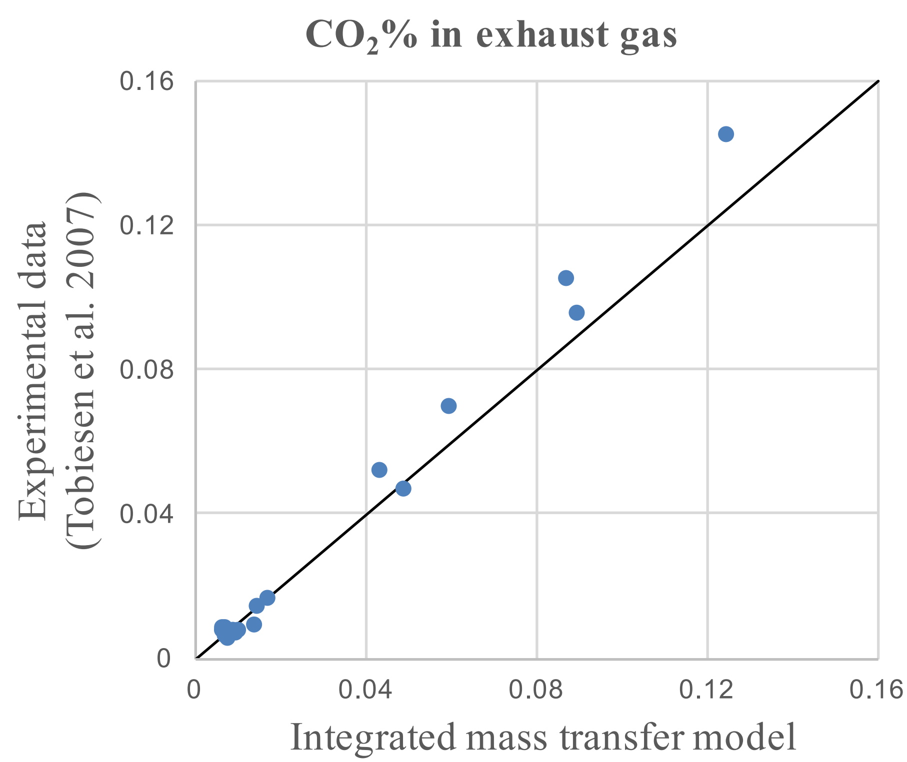
Integrated Mass Transfer Model Results

- Final model form for hydraulics and mass transfer models:
  - Pressure drop: Billet and Schultes (1999)
  - Holdup: Tsai (2011)
  - Mass transfer coefficients: Billet and Schultes (1993)
  - Interfacial area: Tsai et al. (2012)
- Model parameters regressed for Mellapak plus™ 252Y





Repeatability and Uncertainty Estimation for Solvent Analysis Measurement Techniques

- Solvent Measurement Analysis Techniques Used During the Test Campaign:
- Dynamic Portion: Gas Chromatography (GC) for Amine Concentration and Bench Equivalence Point (EQP) Base Titration (CO_2 Concentration)
- Steady State Portion: Online EQP Acid Titration (Amine Concentration) and Online EQP Base Titration (CO_2 Concentration)

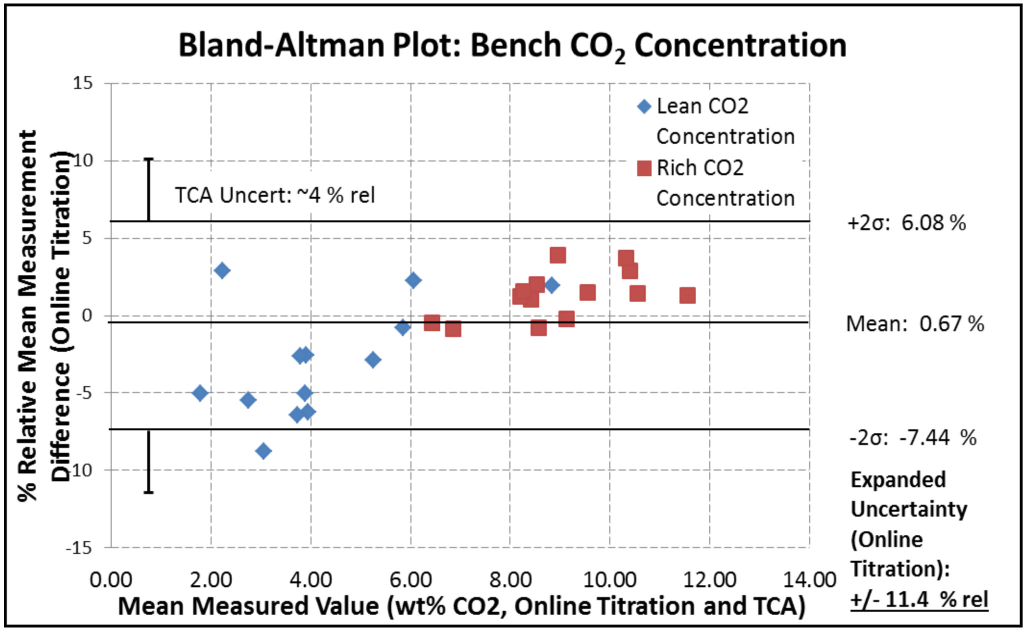
Analysis Techniques Repeatability Evaluation:

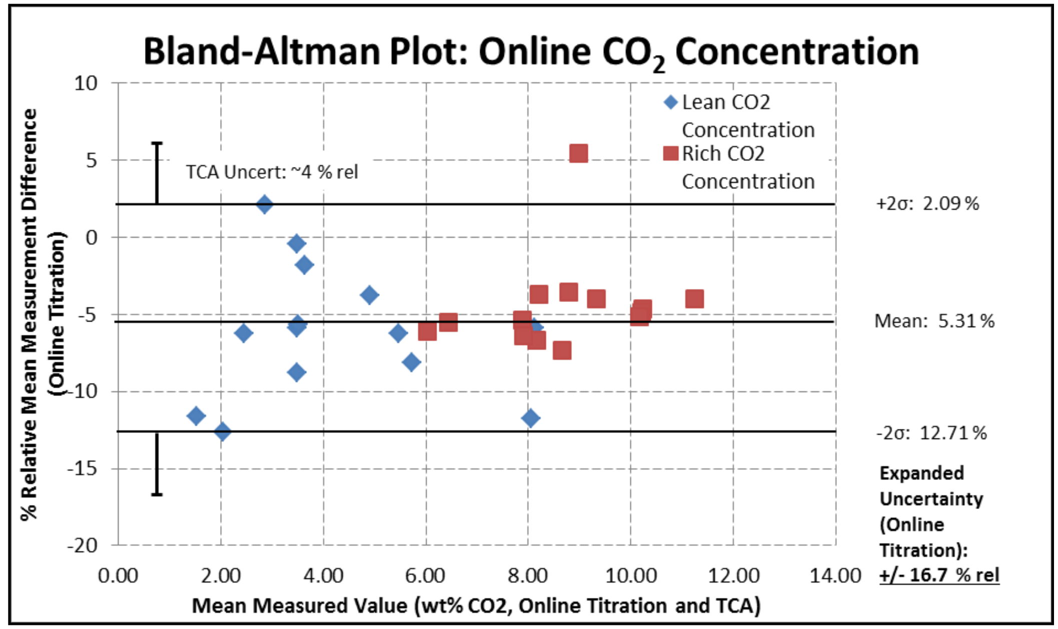
- Repeatability of Gas Chromatography and Bench Equivalence Point Base Titration evaluated statistically through repeated duplicated and triplicate measurement sets
- Repeatability of Online Equivalence Point Acid and Base Titrations assumed to be similar to Bench Titration because instruments use similar sampling equipment manufactured by the same provider (Metrohm AG)

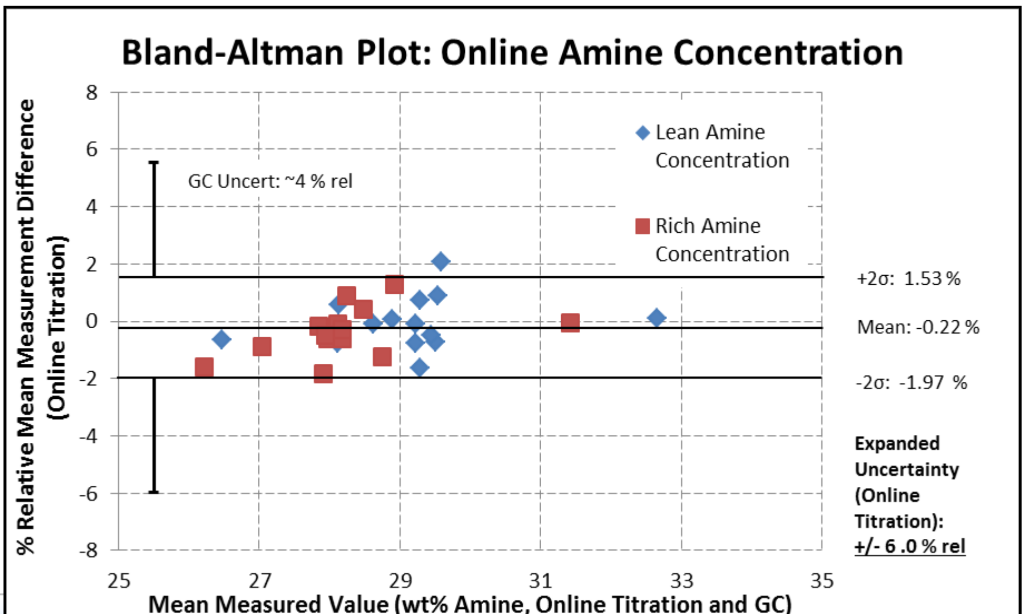
Analysis Techniques Uncertainty Evaluation:

- Uncertainty of Gas Chromatography evaluated by point checks with analytical standards
- Uncertainty of Online Acid Titration evaluated by repeated comparisons with Gas Chromatography
- Uncertainty of Bench and Online Base Titration evaluated by repeated comparisons with Total Inorganic Carbon.

Repeatability Estimation Results



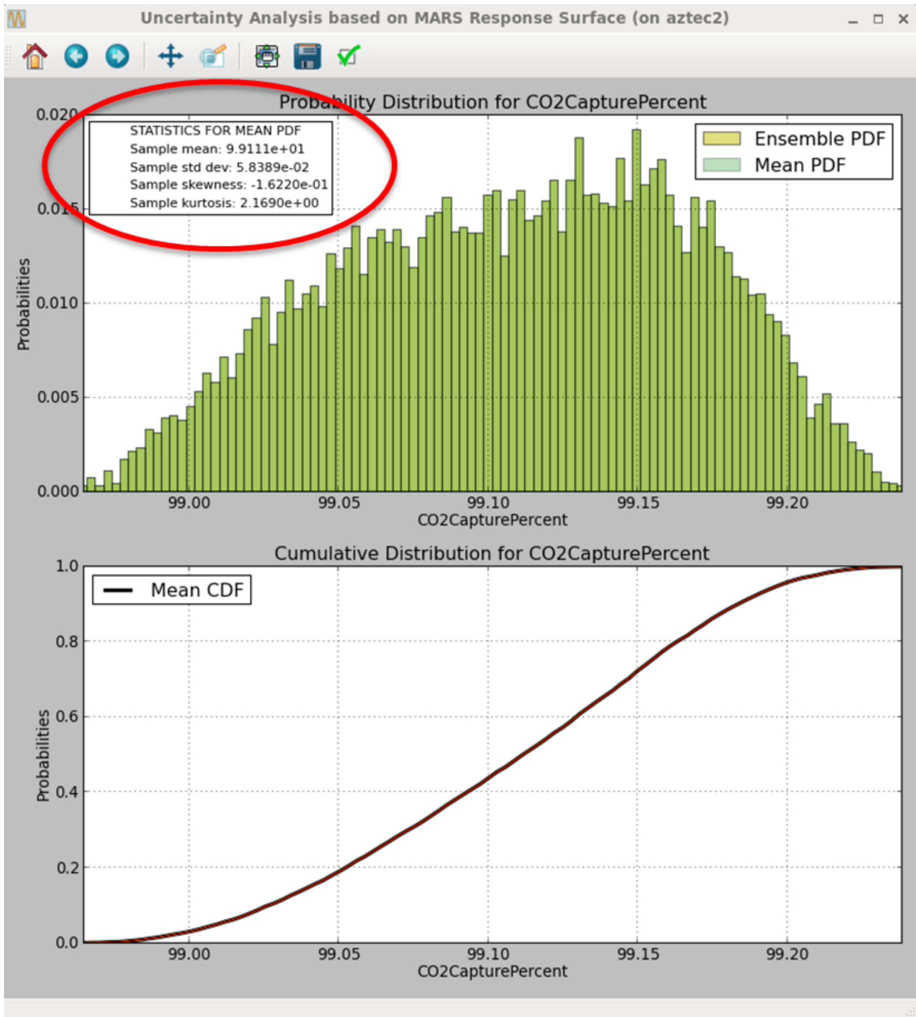




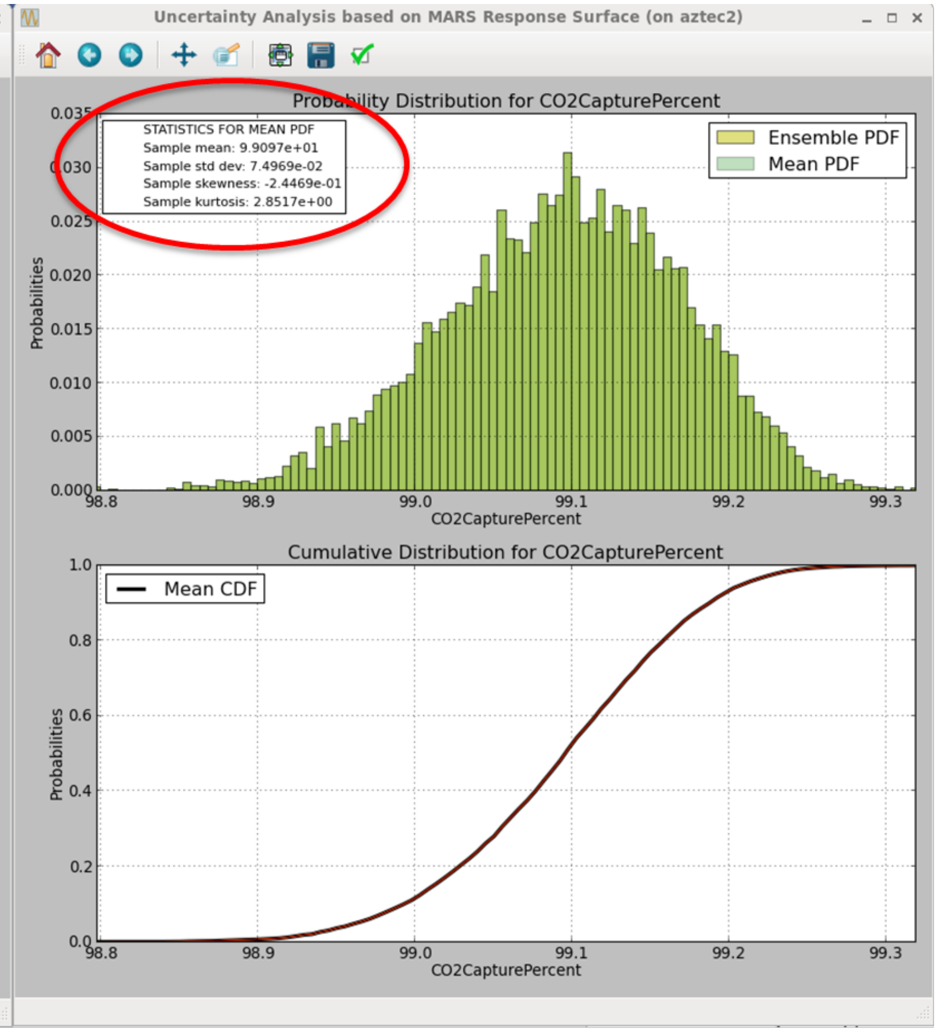
Critical Model Parameters:

Portion of Campaign	Dynamic	Steady State
Amine Concentration (wt% MEA Nominal) % rel expanded uncertainty (k=2)	4.9%	7.3%
CO_2 Loading (mol CO_2 / mol MEA) % rel expanded uncertainty (k=2)	7.4%	10.7%

UQ for the Entire Process Model

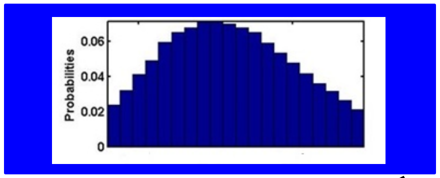


With properties model posteriors

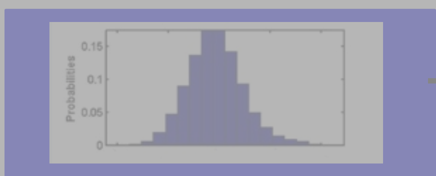


No properties model posteriors

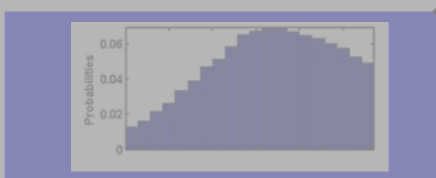
UQ for the Entire Process Model



Uncertainty in Properties Models (only viscosity, density, surface tension)

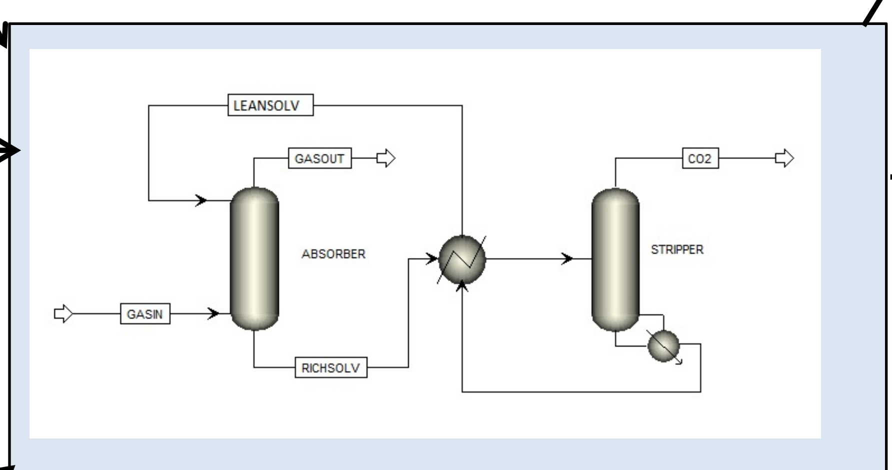


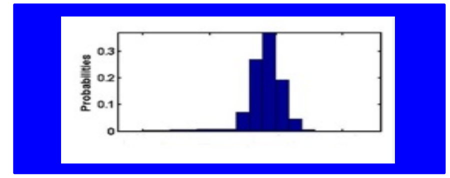
Uncertainty in Hydraulic Models, Mass and Heat Transfer Models



Uncertainty in Kinetic Models

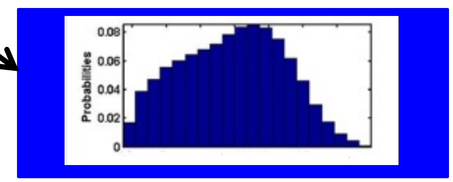
Process Simulation





Uncertainty in % CO_2 Capture

Uncertainty in Energy Requirement



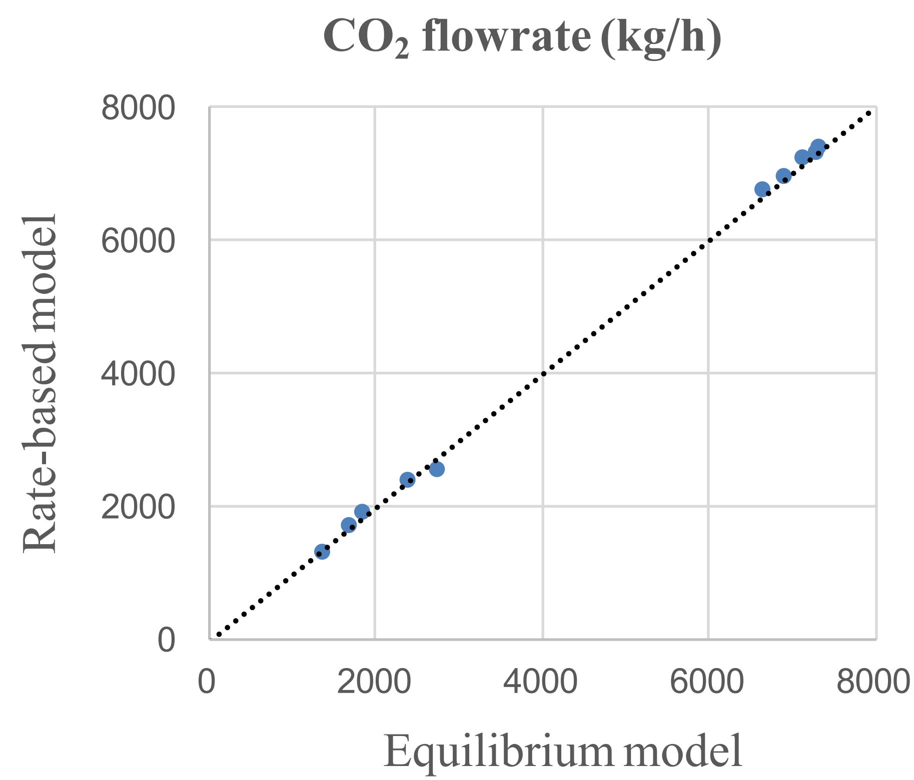
Uncertainty in Estimation of Other Key Variables

Dynamic Modeling using Aspen Dynamics

Efficiency Model

$$\varepsilon = A\left(\frac{F_L}{F_{Lo}}\right)^{B}\left(\frac{F_V}{F_{Vo}}\right)^{C}\left(\frac{CO_{2\,load}}{CO_{2\,load,o}}\right)^{D}\left(\frac{MEA}{MEA_o}\right)^{E}$$

Conditions	Absorber Max	Absorber Min	Regenerator Max	Regenerator Min
Liquid flowrate (kg/h)	12961	5390	6503	4981
Gas flowrate (kg/h)	2325	2133	623	441
MEA (%w)	25.41	11.92	0.27	0.24
CO_2 loading (mol/mol)	0.25	0.12	0.47	0.15



Correlated component efficiency implemented in Aspen Dynamics