CCSI
Carbon Capture Simulation Initiative

Predictive Dynamic Model of a Carbon Capture System: Pilot Scale Validation at National Carbon Capture Center

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CMTC 2015

For Accelerating Technology Development

Rapidly synthesize optimized processes to identify promising concepts → **Better understand internal behavior to reduce time for troubleshooting** → **Quantify sources and effects of uncertainty to guide testing & reach larger scales faster** → **Stabilize the cost during commercial deployment**

National Labs

- Berkeley Lab
- Pacific Northwest National Laboratory
- NETL
- Los Alamos National Laboratory EST. 1943
- Lawrence Livermore National Laboratory

Academia

- Carnegie Mellon
- Princeton University
- West Virginia University
- Boston University
- The University of Texas at Austin

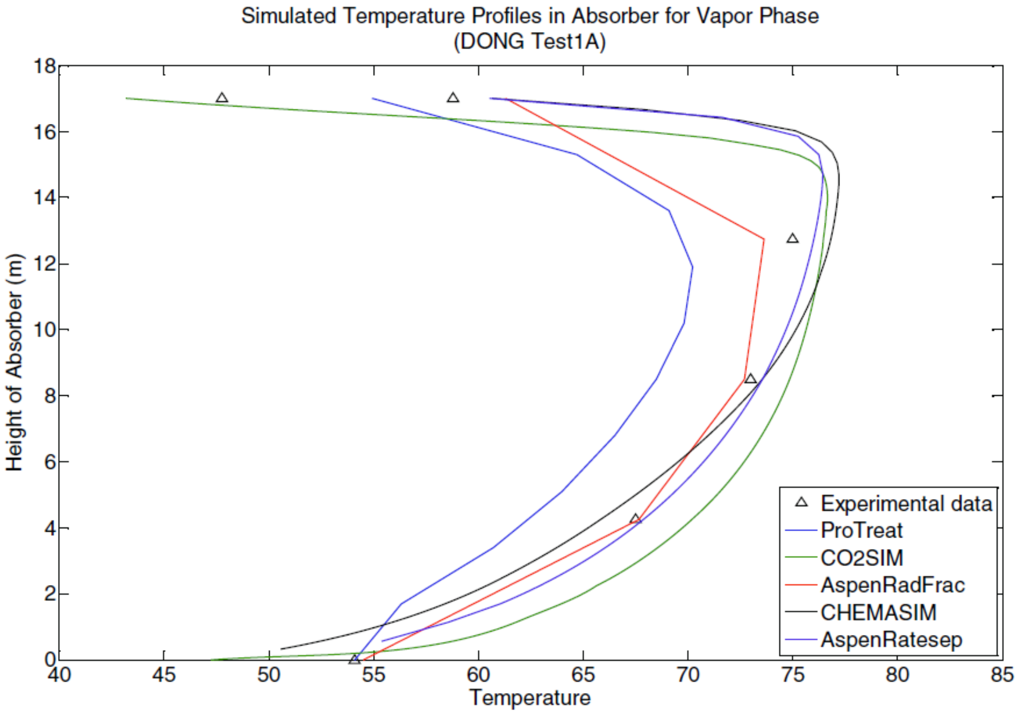
Industry

- ADA Environmental Solutions
- ALSTOM
- B&W thebabcock&wilcoxcompany
- GE
- EPRI Electric Power Research Institute
- FLUOR
- Phillips 66
- AEP American Electric Power
- Southern California Edison An EDISON INTERNATIONAL Company San Onofre Nuclear Generating Station
- Southern Company
- ExxonMobil
- Chevron
- URS
- Air Products
- EASTMAN
- aspentech
- ANSYS
- Schneider Electric
- PSE

Motivation

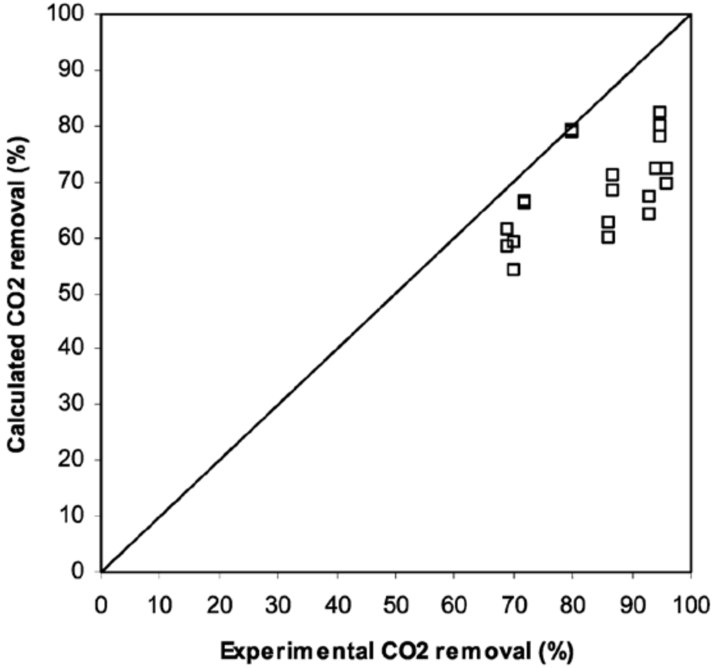
- Development of a Gold Standard baseline MEA model
  - Open source
  - Validation framework
  - Well documented
  - Uncertainties quantified
- Demonstrate as a Framework for proprietary systems
  - Methodology for robust, predictive models
- Steady state validation
- **Dynamic validation**

Deficiencies in Existing Steady State Models



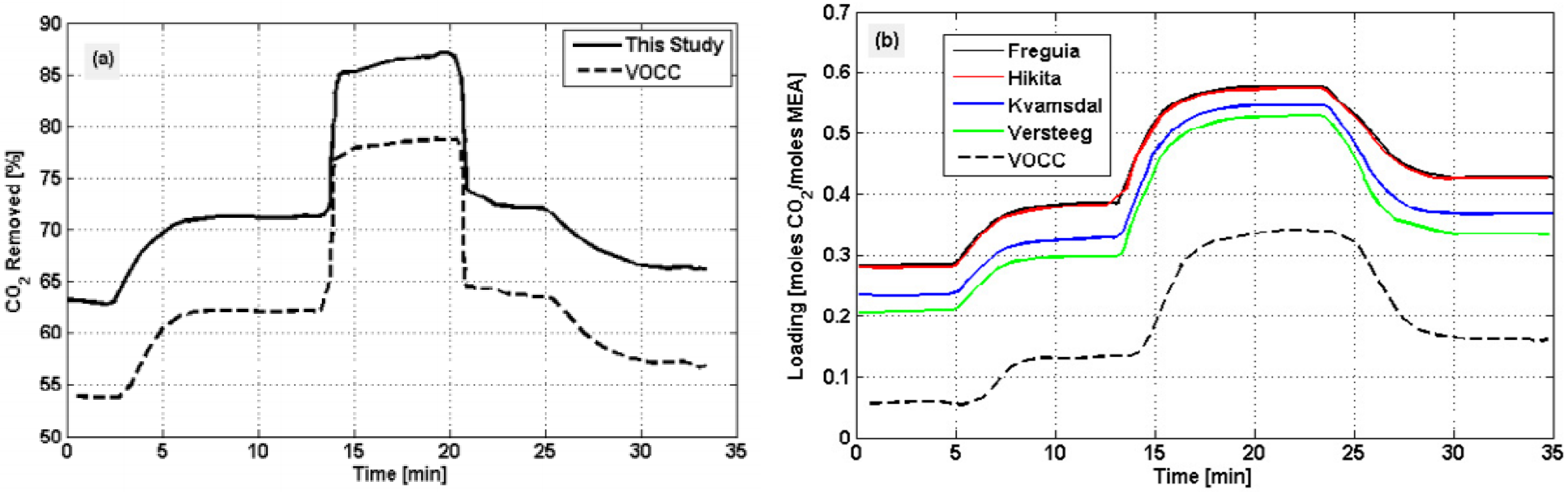
ProTreat-Optimized Gas Treating, Inc.; CO2SIM-NTNU/SINTEF CHEMASIM-BASF SE; AspenRatesep-modified by IFP

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



Zhang, et al., Rate-Based Process Modeling Study of CO_2 Capture with Aqueous Monoethanolamine Solution, Ind. Eng. Chem Res., 48, 9233-9246, 2009

Deficiencies in Existing Dynamic Models



***Data from NTNU/SINTEF**

Hanne M. Kvamsdal, Actor Chikukwa, Magne Hillestad, Ali Zakeri, Aslak Einbu, A comparison of different parameter correlation models and the validation of an MEA-based absorber model, Energy Procedia, 4, 1526-1533, 2011

Outline

- Steady state model
- Dynamic model using Aspen Dynamics
- Test conditions
- Dynamic data reconciliation
- Results
- Conclusion

How to Develop a Gold Standard Model

- Property models
  - Valid for absorber and stripper operating conditions
- Hydraulic and mass transfer models
  - Developed simultaneously with relevant properties models using both WWC and packing data
- Steady State Validation
- Dynamic Validation

Physical Property Model Development

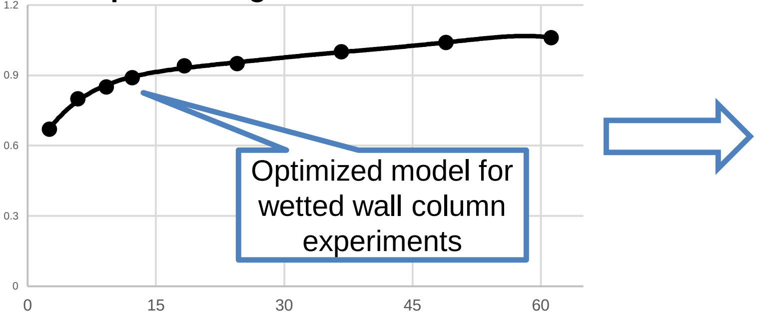
- Initial framework based upon the “Phoenix” model*
  - Developed by Prof. Rochelle’s Group at UT, Austin
- Independent property models
  - Viscosity
  - Density/Molar Volume
  - Surface Tension
- Thermodynamic framework
  - Vapor-Liquid Equilibrium
    - Binary MEA-H_2O system
    - Ternary MEA-H_2O-CO_2 system
  - Heat Capacity
  - Heat of Absorption
  - Reaction Kinetics
    - Model developed for consistency with reaction equilibrium constants

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

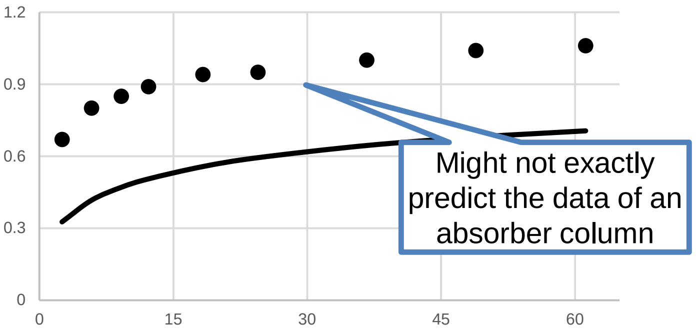
Integrated Mass Transfer Model Development

- Properties (such as diffusivity, viscosity, surface tension) as well as interfacial area, and mass transfer coefficients all affect mass transfer
- Data from both wetted wall column and packed column considered
- In Aspen Plus, simultaneous regression of these models not possible; thus solution can be sub-optimal
- FOQUS has the capability of simultaneous regression

Usual approach: Sequential regression

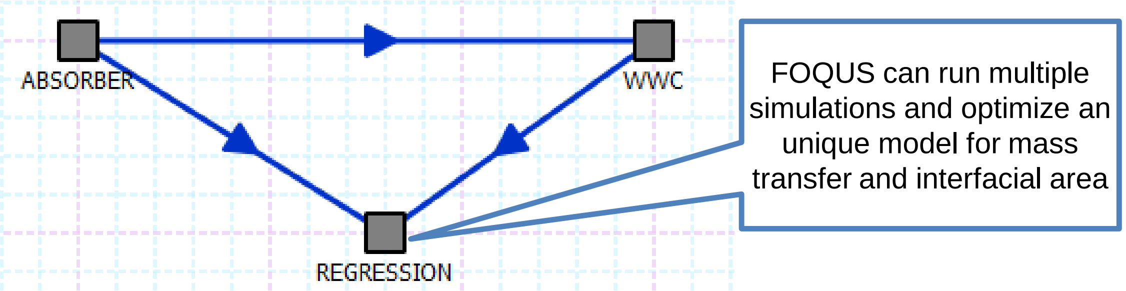


Optimized model for wetted wall column experiments



Might not exactly predict the data of an absorber column

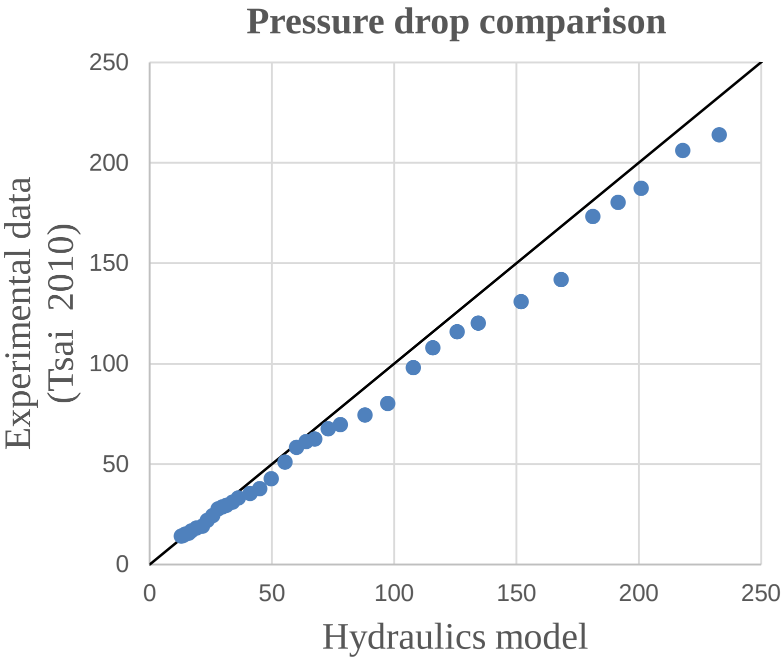
FOQUS capability: Simultaneous regression

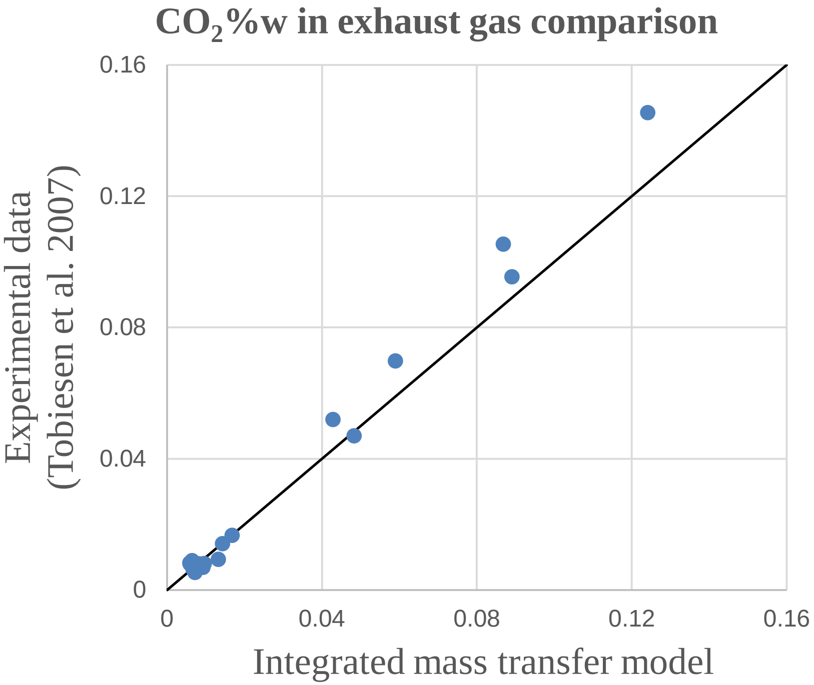


FOQUS can run multiple simulations and optimize an unique model for mass transfer and interfacial area

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^{TM} 252Y

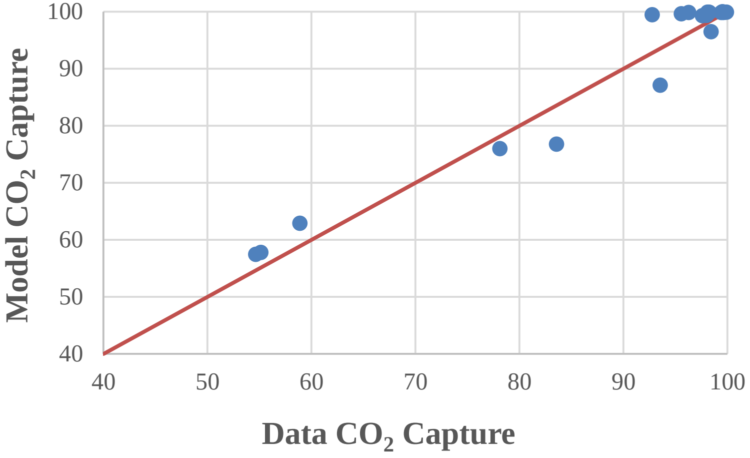




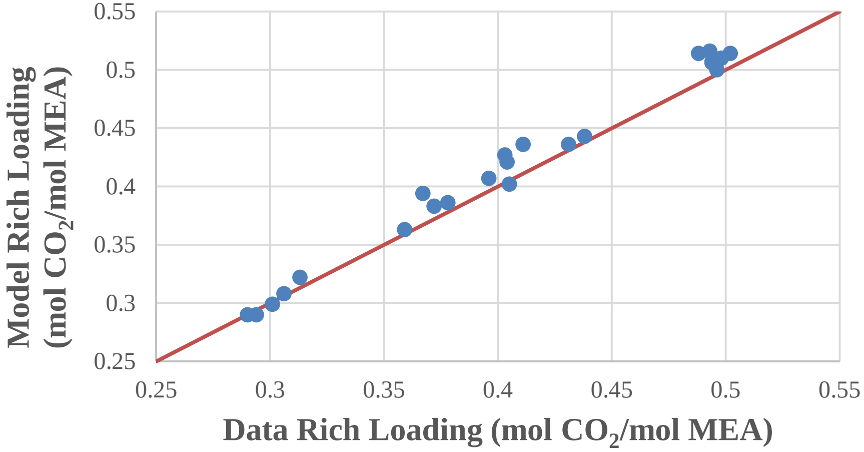
Steady State Validation

Absorber Validation

CO_2 Capture Prediction

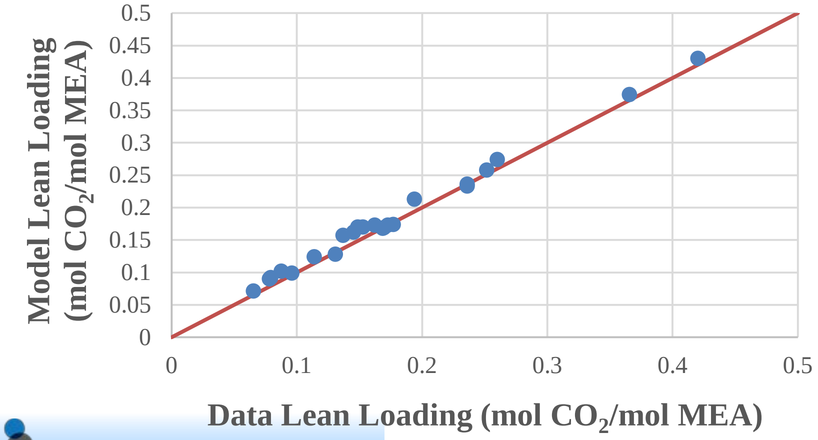


Rich Loading Comparison

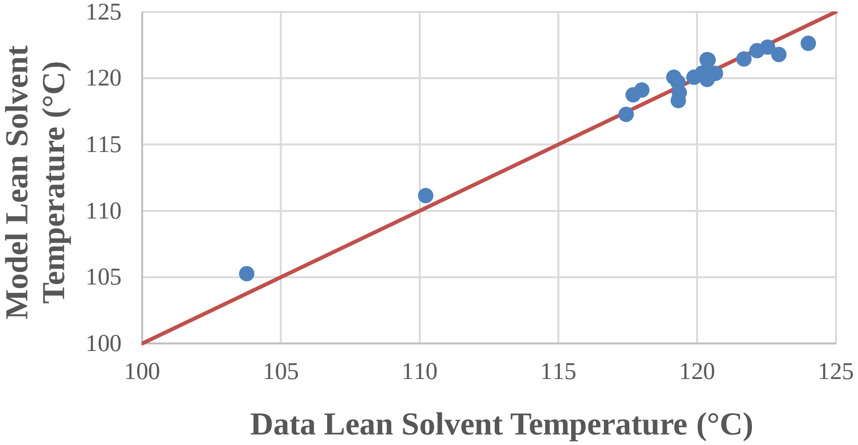


Regenerator Validation

Lean Loading Comparison

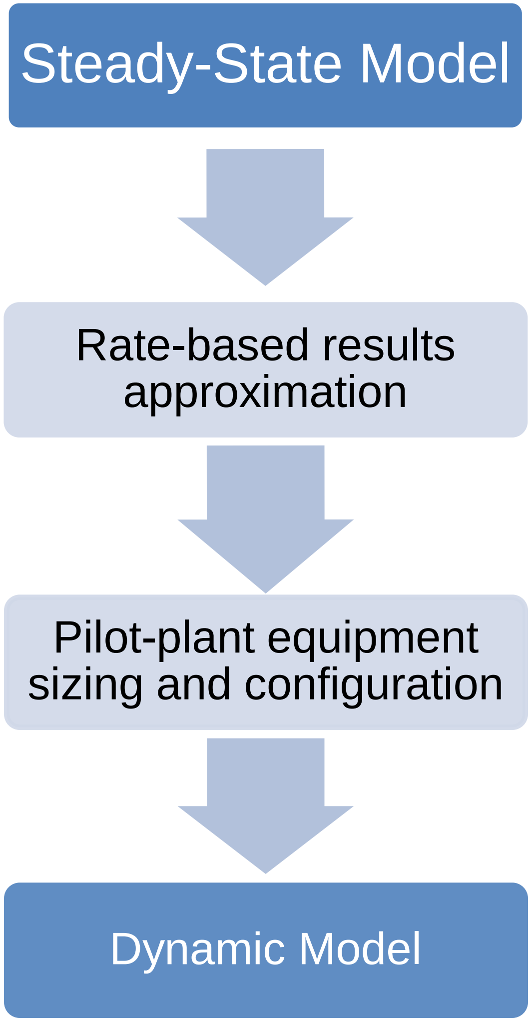


Lean Solvent Temperature Comparison



Aspen Dynamics

- **Capability of using a steady-state model to generate a dynamic model**
- Properties model are shared, including user models
- Absorber and regenerator can only be solved using an equilibrium assumption
- Rate-based results can be approximated by Murphree efficiencies*



Steady-State Model

Rate-based results approximation

Pilot-plant equipment sizing and configuration

Dynamic Model

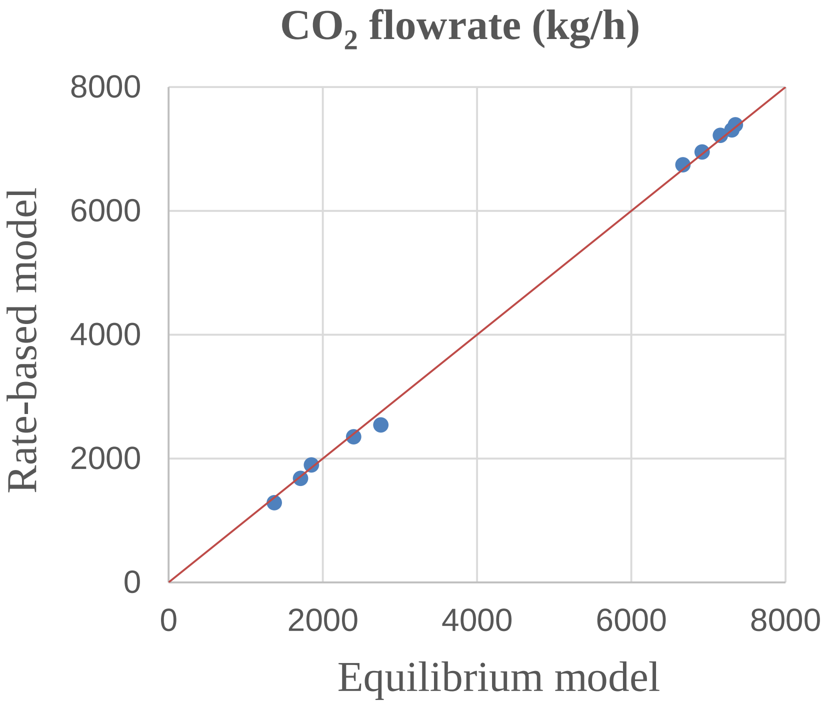
*Zhang et al. “Modeling and model predictive control of a MEA-based post-combustion CO_2 capture process”. Industrial Engineering Chemistry Research 2015.

Dynamic Model Development

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		Regenerator	
	Max	Min	Max	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



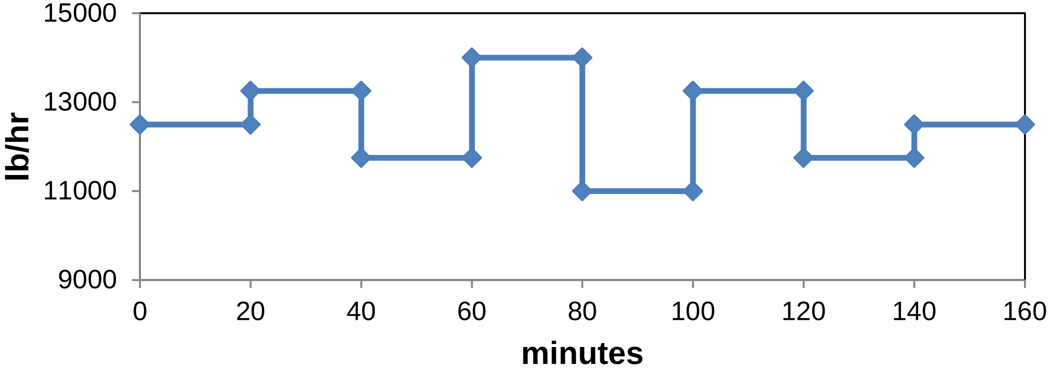
Correlated component efficiency implemented in Aspen Dynamics

CCSI team conducted tests at NCCC

Dynamic Test Conditions

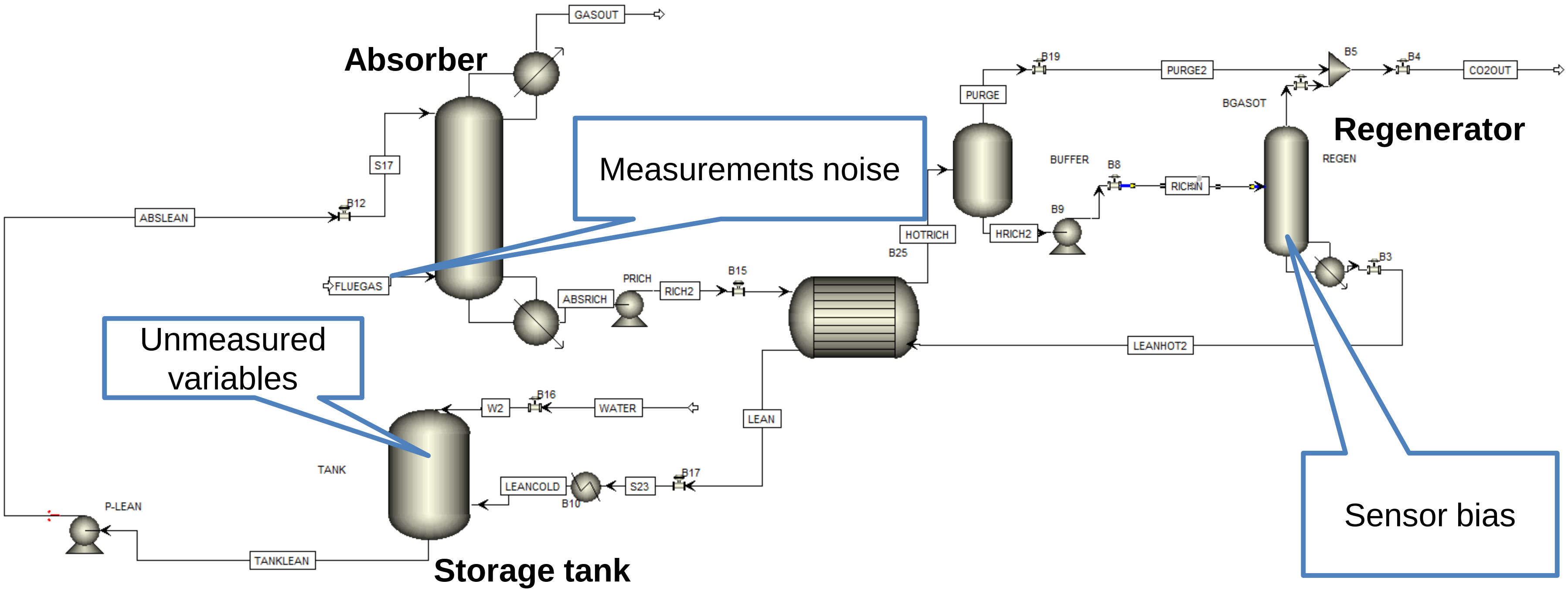
- Dynamic tests capture nonlinearity
- Persistence of excitation
- Step test conducted
  - Solvent flow (lb/hr); x_1=6, datum= 12,500
  - Inlet flue gas(lb/hr); x_2=10, datum= 5,000
  - Reboiler Steam Flow(lb/hr); x_3=6, datum = 5,000

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

Challenges of Dynamic Validation



Absorber

Regenerator

Storage tank

Measurements noise

Unmeasured variables

Sensor bias

Dynamic data can contain noisy, inaccurate and missing measurements

Dynamic Data Reconciliation

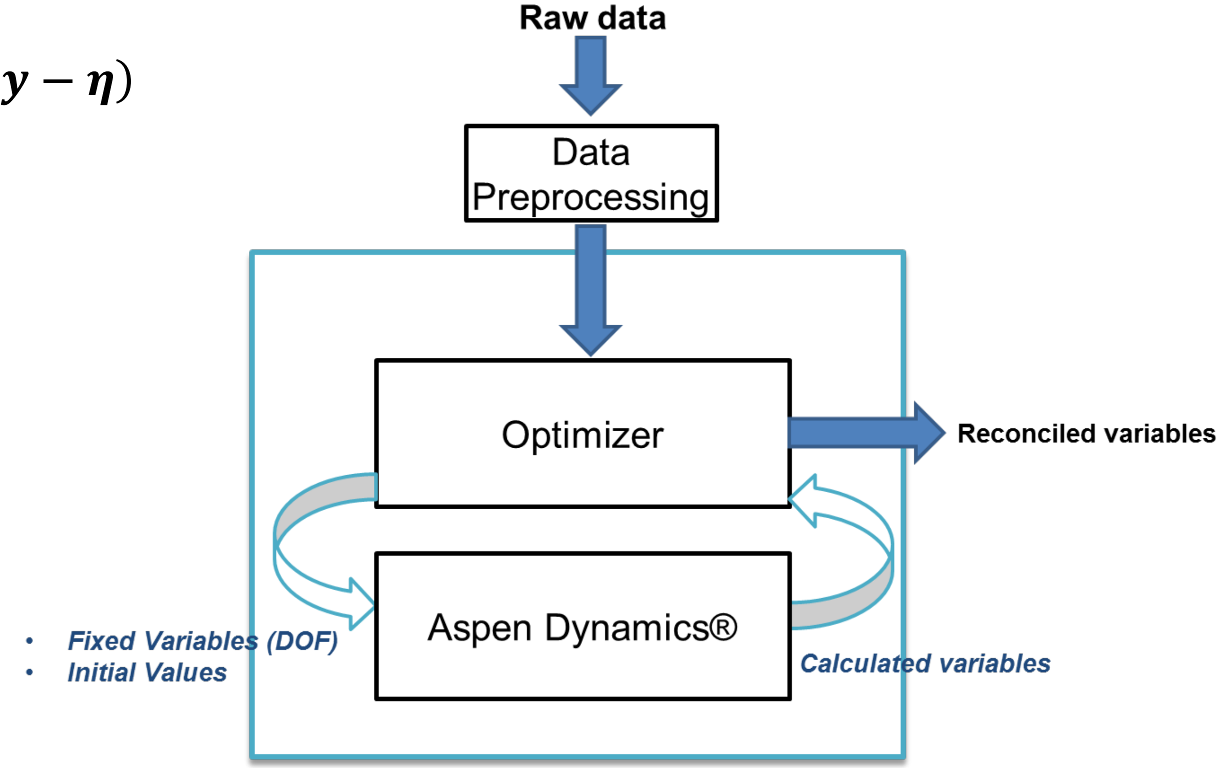
- Noisy, inaccurate, and missing measurements
- Data reconciliation guarantees mass and energy conservation in the dynamic data

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

s.t.

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

$$g(\eta, u, \theta) \leq 0$$



Raw data

Data Preprocessing

Optimizer

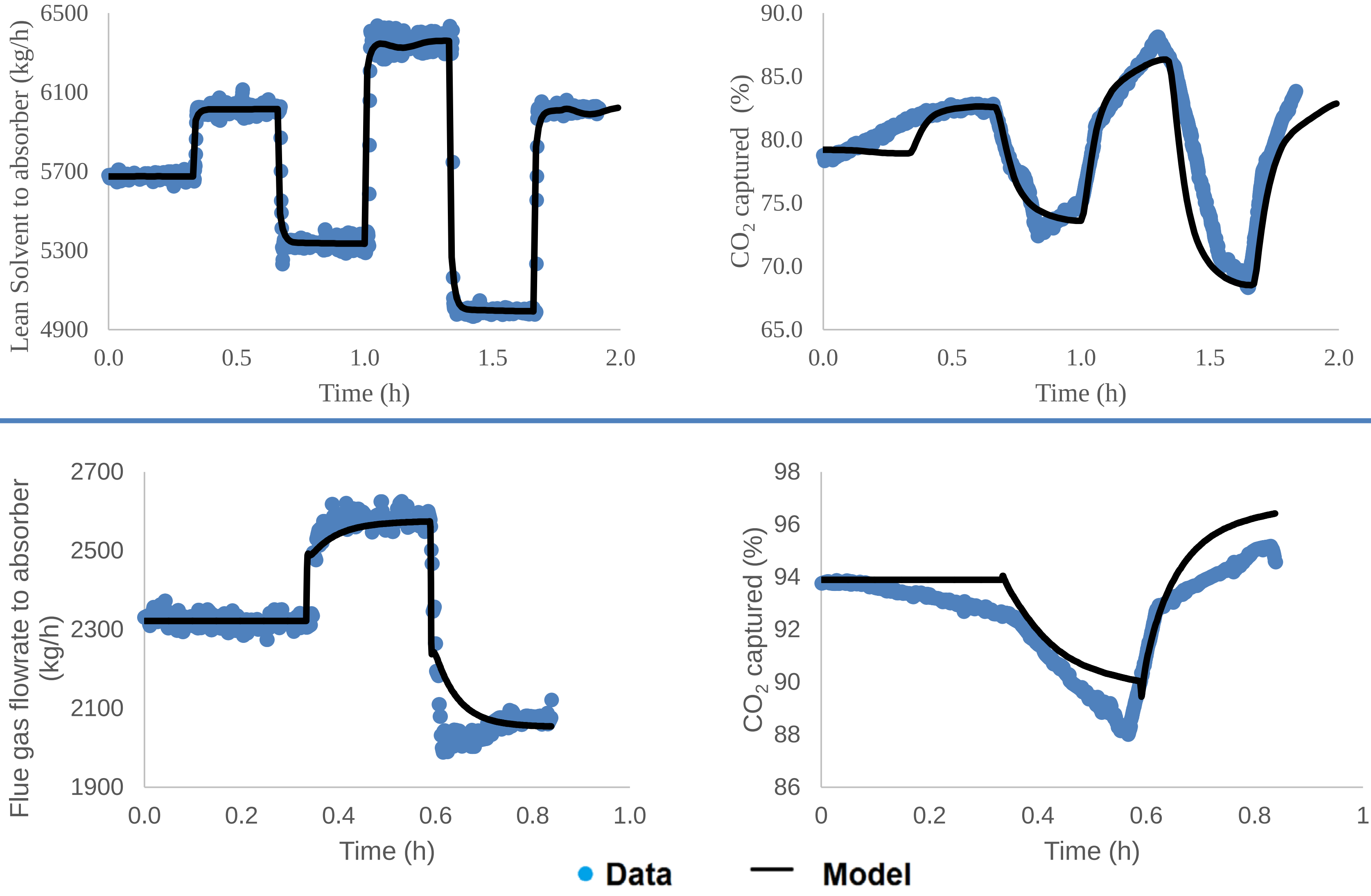
Reconciled variables

Aspen Dynamics®

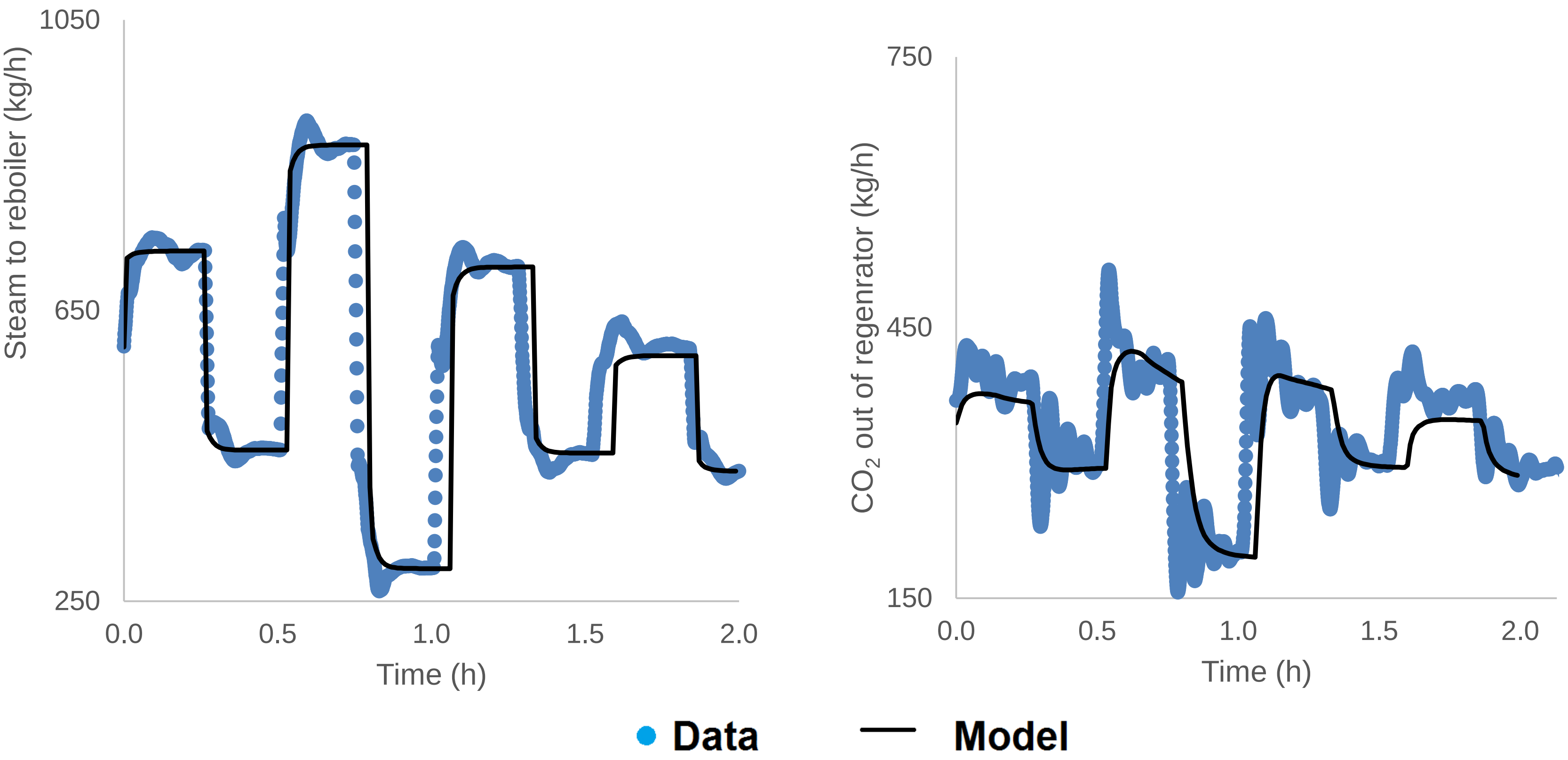
- *Fixed Variables (DOF)*
- *Initial Values*

Calculated variables

Absorber Validation with DDR



Regenerator Validation with DDR



Conclusions

- Efficiency-based dynamic model captures most of behavior in steady state rate-based model
- Dynamic data reconciliation enables best use of noisy inaccurate, and missing data
- Dynamic model predicts gain & time constant of process
- Demonstrates how dynamic data can be used for model validation
- Accuracy of dynamic model might allow its use for control applications

Thank you!

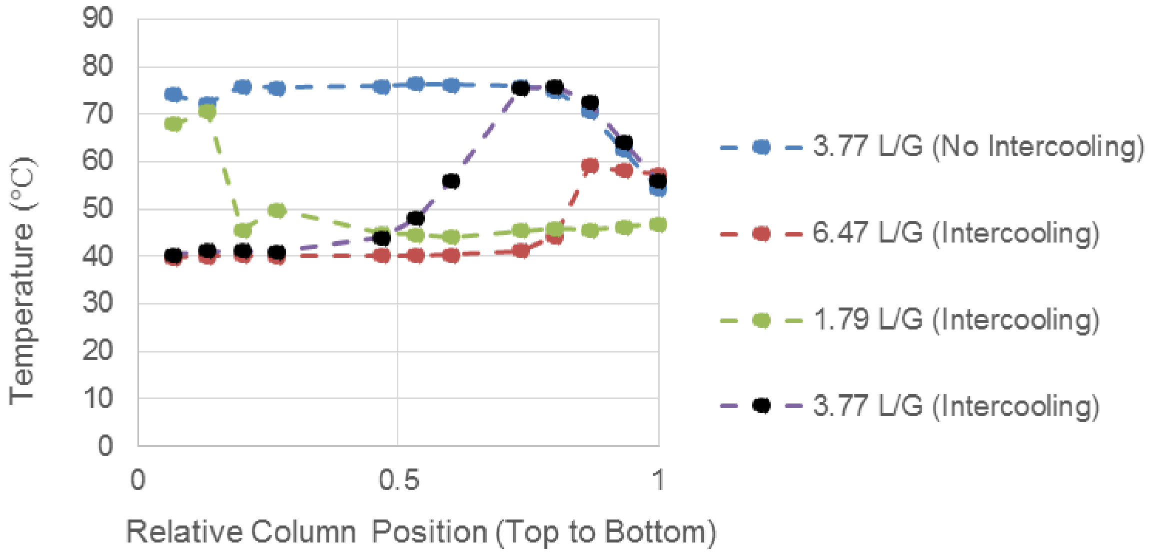
Acknowledgements

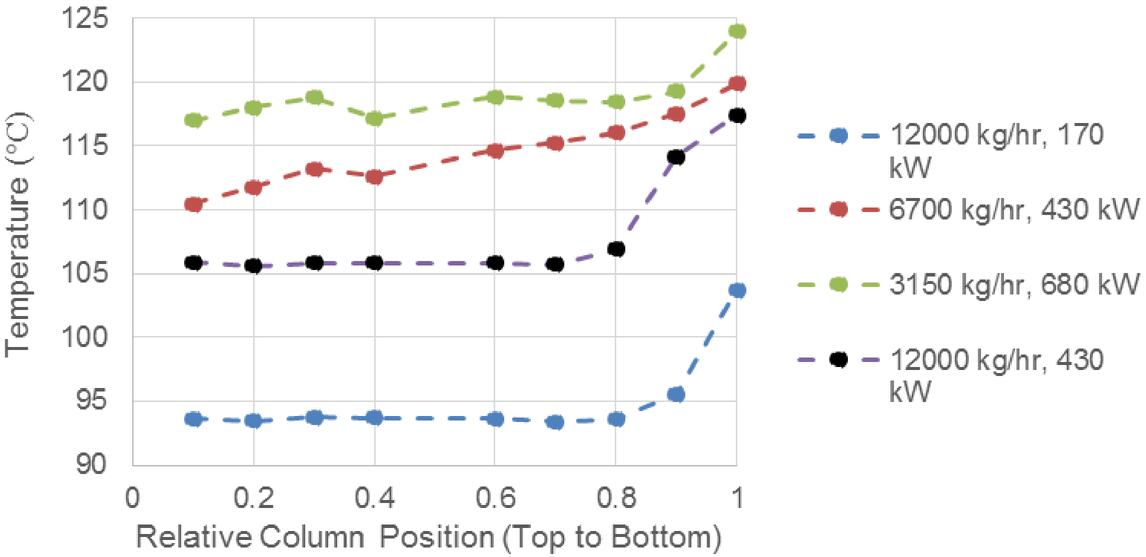
This research was conducted through the Carbon Capture Simulation Initiative (CCSI), funded through the U.S. DOE Office of Fossil Energy.

A portion of this work was conducted as part of the National Energy Technology Laboratory's Regional University Alliance (NETL-RUA), a collaborative initiative of the NETL; this technical effort was performed under the RES contract DE-FE0004000.

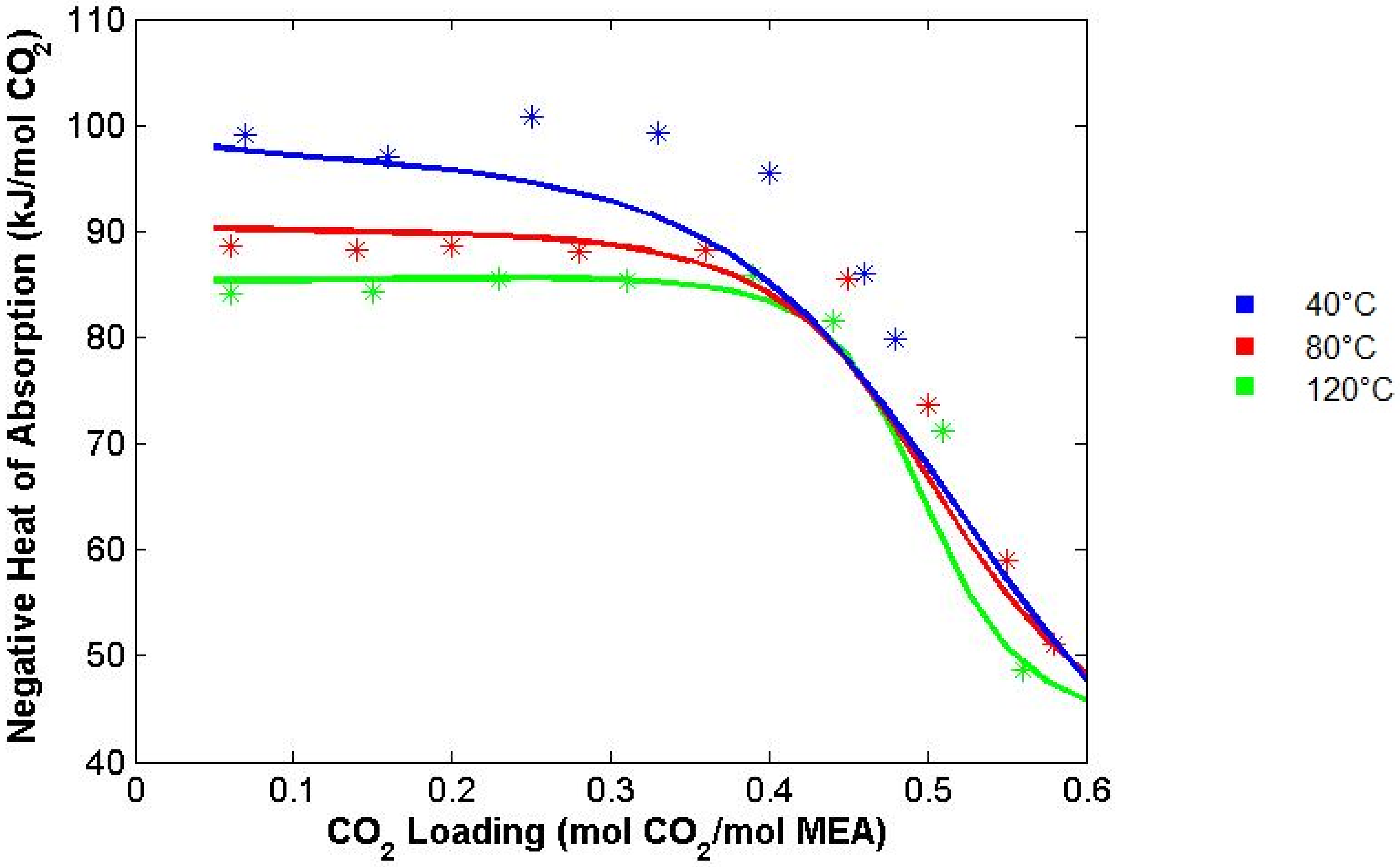
Disclaimer

Challenges for a Gold Standard Model





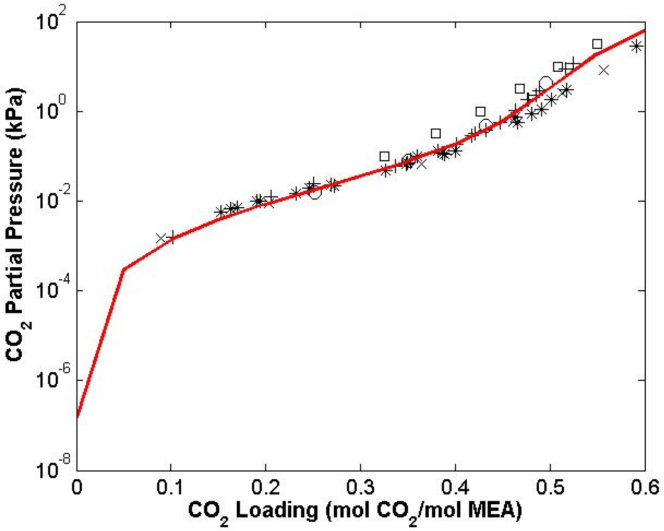
Heat of Absorption Comparison



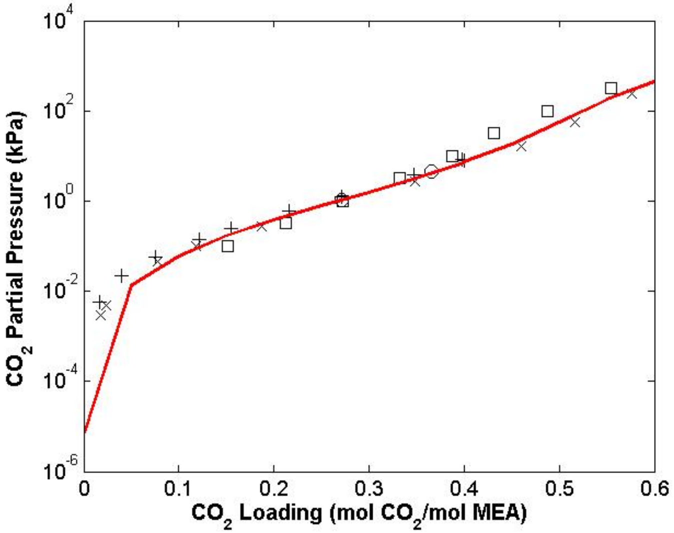
Data from: Kim et al., Energy Procedia,2014;63:1446-1455

VLE Ternary Data Model Fit (30 wt%)

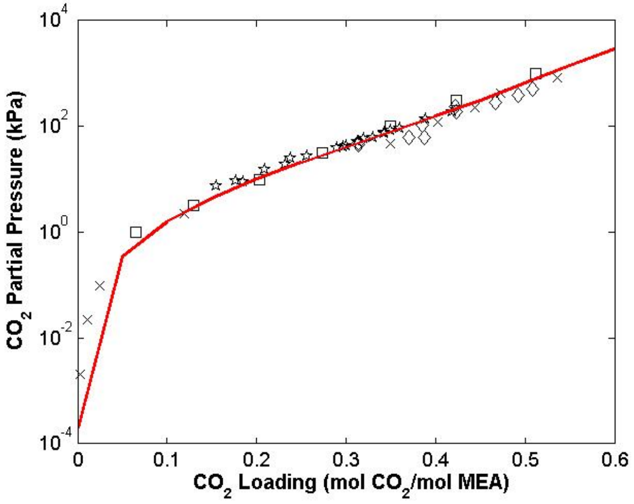
40°C



80°C



120°C



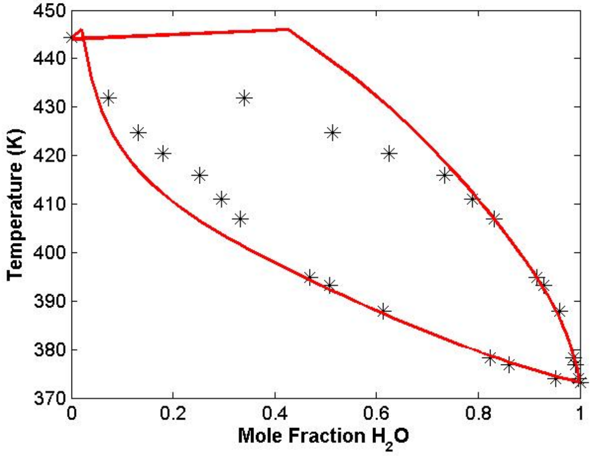
Data

+ Aronu et al.
✳ Hilliard
× Jou et al.
○ Dugas
□ Lee et al.
◇ Xu
☆ Ma'mun et al.

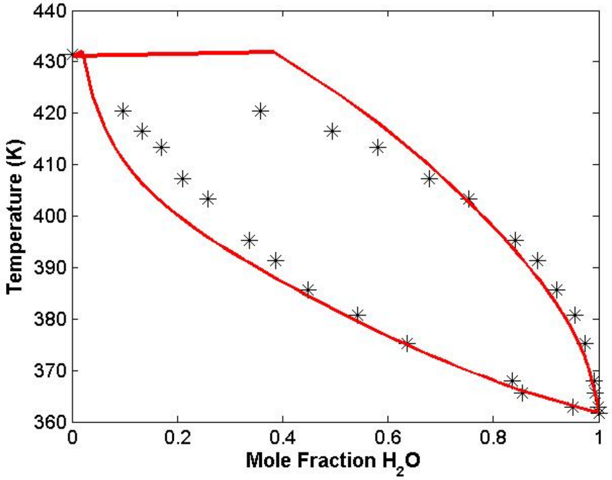
VLE Data Binary Data Model Fit

Txy Diagrams (data from Cai et al.)

P = 101.33 kPa

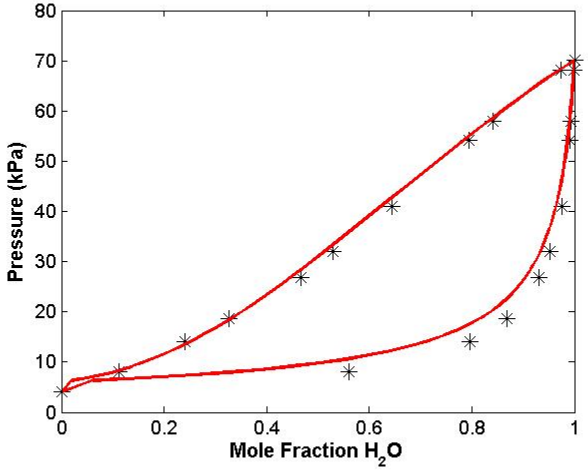


P = 66.66 kPa



Pxy Diagrams (data from Tochigi et al.)

T = 363.15 kPa



Cai et al., J Chem Eng Data,1996;41:1101-1103
Tochigi et al., J Chem Eng Data, 1999;44:588-590

NCCC vs Other Pilot Plants

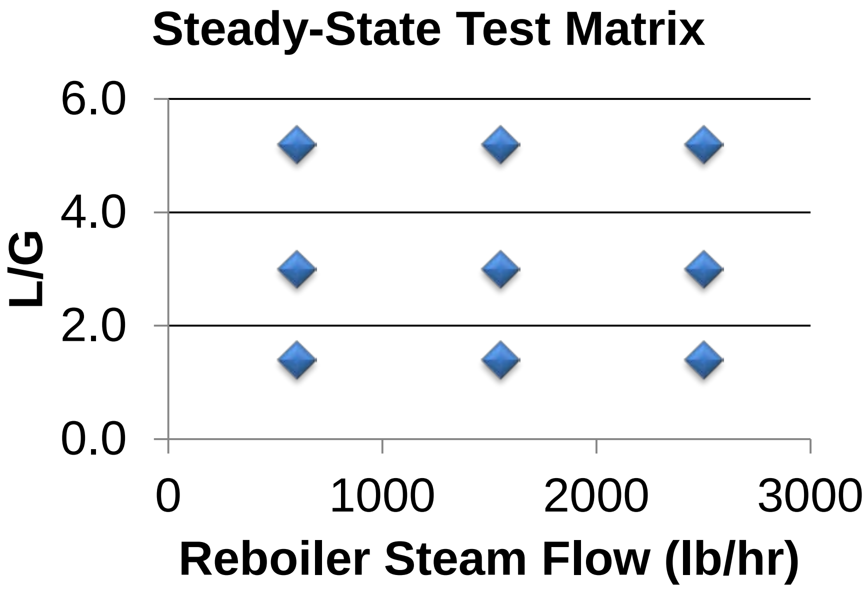
	CO_2 Capacity (tpd)	Source of Flue Gas	Absorber		Regenerator	
			Diameter (cm)	Height (m)	Diameter (cm)	Height (m)
UT, Austin	3.0	Non-coal	42.7	6.1	42.7	6.1
NTNU/ SINTEF	0.3	Non-coal	15.0	4.4	10.0	3.9
ITC, Regina	1.0	Non-coal	33.0	7.1	33.0	10.0
ITT, Stuttgart	0.3	Non-coal	12.5	4.2	12.5	2.5
Esbjerg CASTOR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

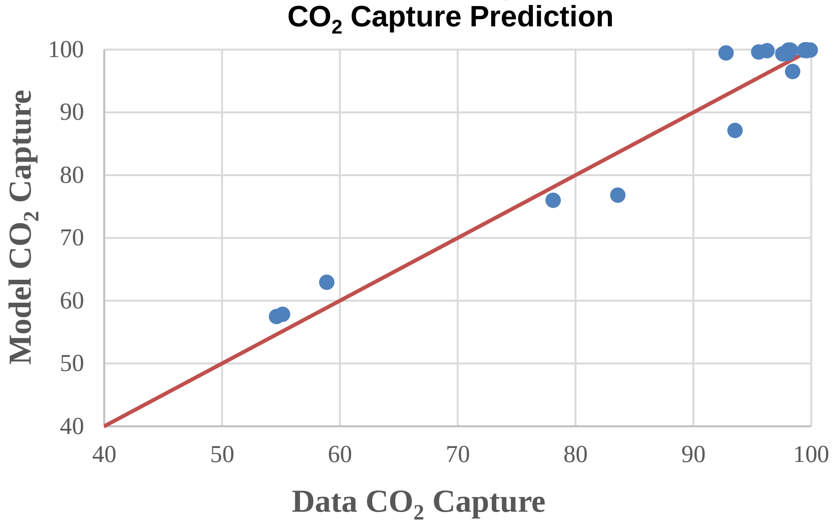
Steady-State Test Runs

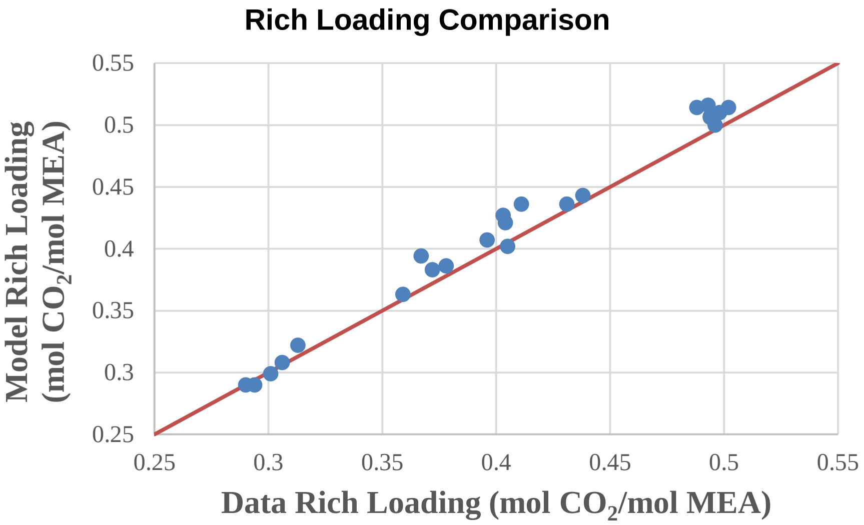
Operating Conditions	Range
Solvent Flow (lb/hr)	7,000-26,000
Inlet Flue Gas (lb/hr)	5,000-6,500
Reboiler Steam Flow (lb/hr)	600-2,500
Inlet FG CO_2 vol%	9-11%
# of beds	1-3
Intercooler	no - yes

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



Steady State Absorber Validation


CO_2 Capture Prediction


Rich Loading Comparison

Percent Deviation Between Data and Model Values (Summary)

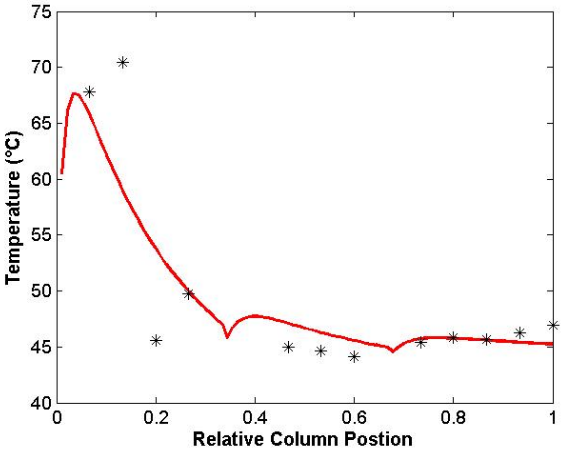
	Data CO_2 Capture-Liquid vs. Gas Discrepancy	CO_2 Capture-Gas Side	CO_2 Capture-Liquid Side	Rich Loading
Maximum	9.19	8.09	10.84	7.36
Average	3.62	2.69	3.97	2.69

Steady State Absorber Validation

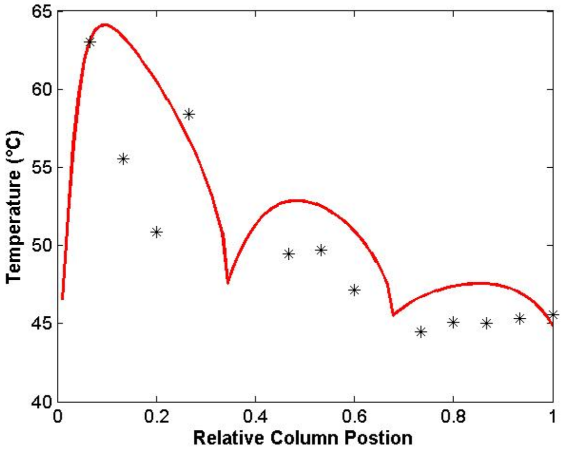
Sample Temperature Profiles

No parameter tuned

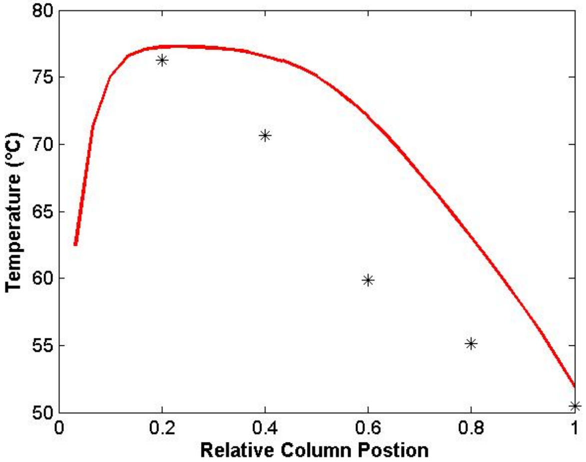
Case K3



Case K6



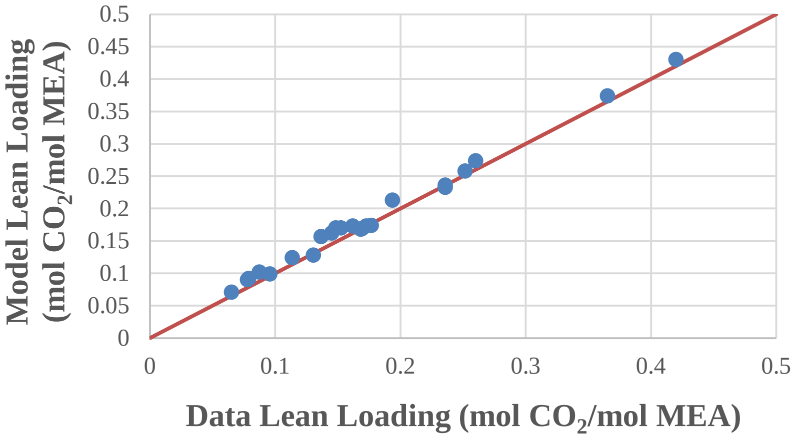
Case K20

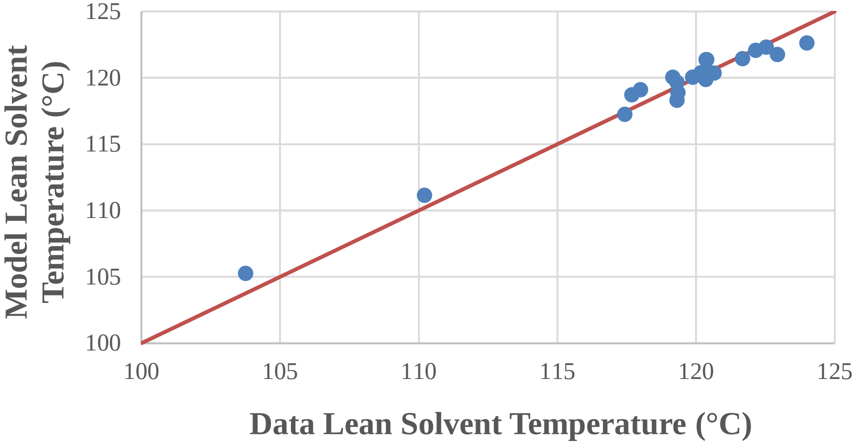


Relative column positions of 0 and 1 correspond to top and bottom of column, respectively

Case	L/G (mass)	Beds/Intercooling	Lean Loading (mol CO_2/mol MEA)
K3	1.41	3/Yes	0.091
K6	3.02	3/Yes	0.347
K20	2.38	1/No	0.075

Steady State Regenerator Validation


Lean Loading Comparison


Lean Solvent Temperature Comparison

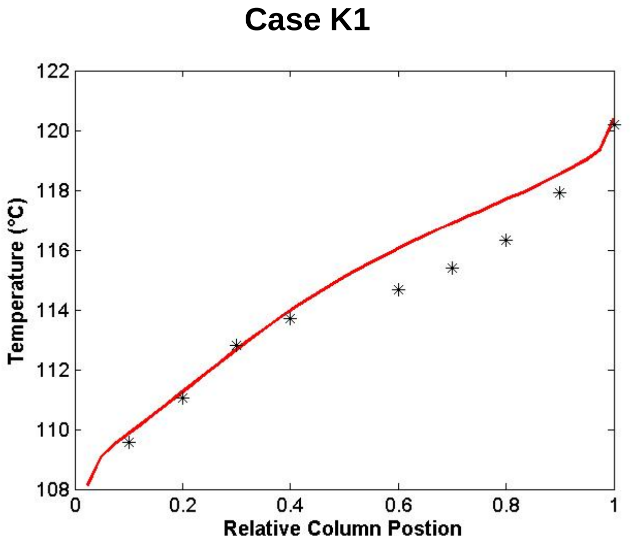
Percent Deviation Between Data and Model Values (Summary)

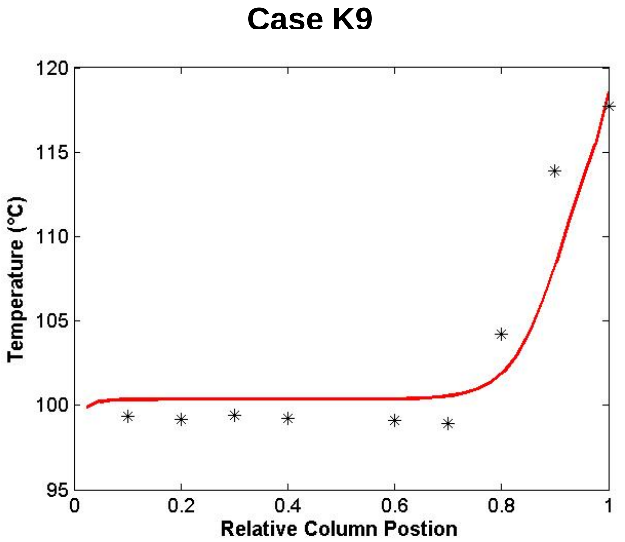
	Lean Loading	Lean Solvent Temperature
Maximum	**16.53**	**1.14**
Average	**6.39**	**0.48**

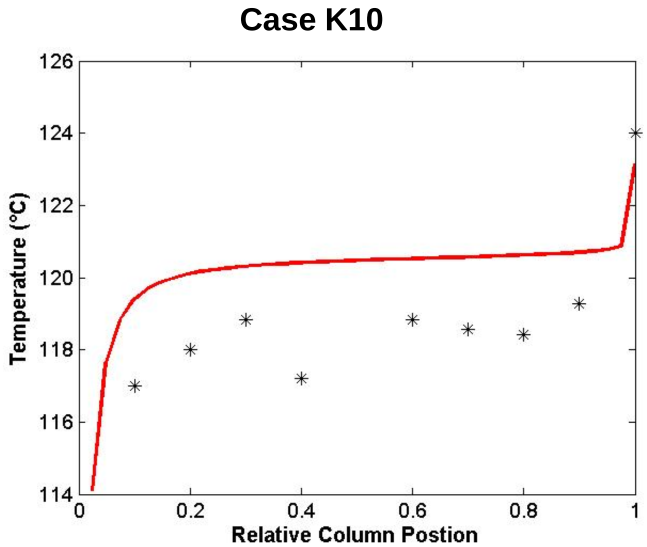
Regenerator Validation

No parameters tuned

Sample Temperature Profiles


Case K1


Case K9


Case K10

Case	Rich Solvent Flow (kg/hr)	Reboiler Duty (kW)	Rich Loading (mol CO_2/mol MEA)
K1	7242	430.61	0.384
K9	3337	165.74	0.474
K10	3358	670.62	0.477

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