Modeling the Advanced Flash Stripper

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Primary Objective: Interpret & extrapolate NCCC data

- Present Work:
  - Data reconciliation
  - Empirical models of absorber and stripper data
  - Adjust and Validate Aspen Independence Model
  - Develop improved thermo for Aspen
- Future Work
  - Develop improved kinetics for Aspen
  - Validate Improved model
  - Optimize AFS with PZ
  - Optimize AFS with MEA and other solvents

NCCC Absorber Modeling

- Data reconciliation – get loading and [PZ] from density & viscosity
- Removal as a function of rich loading
- Removal predicted by Aspen Independence model
- Absorber pinched at long-term conditions

Calculate PZ and Loading from Density and Viscosity

- Density correlation
  - Freeman, 2011

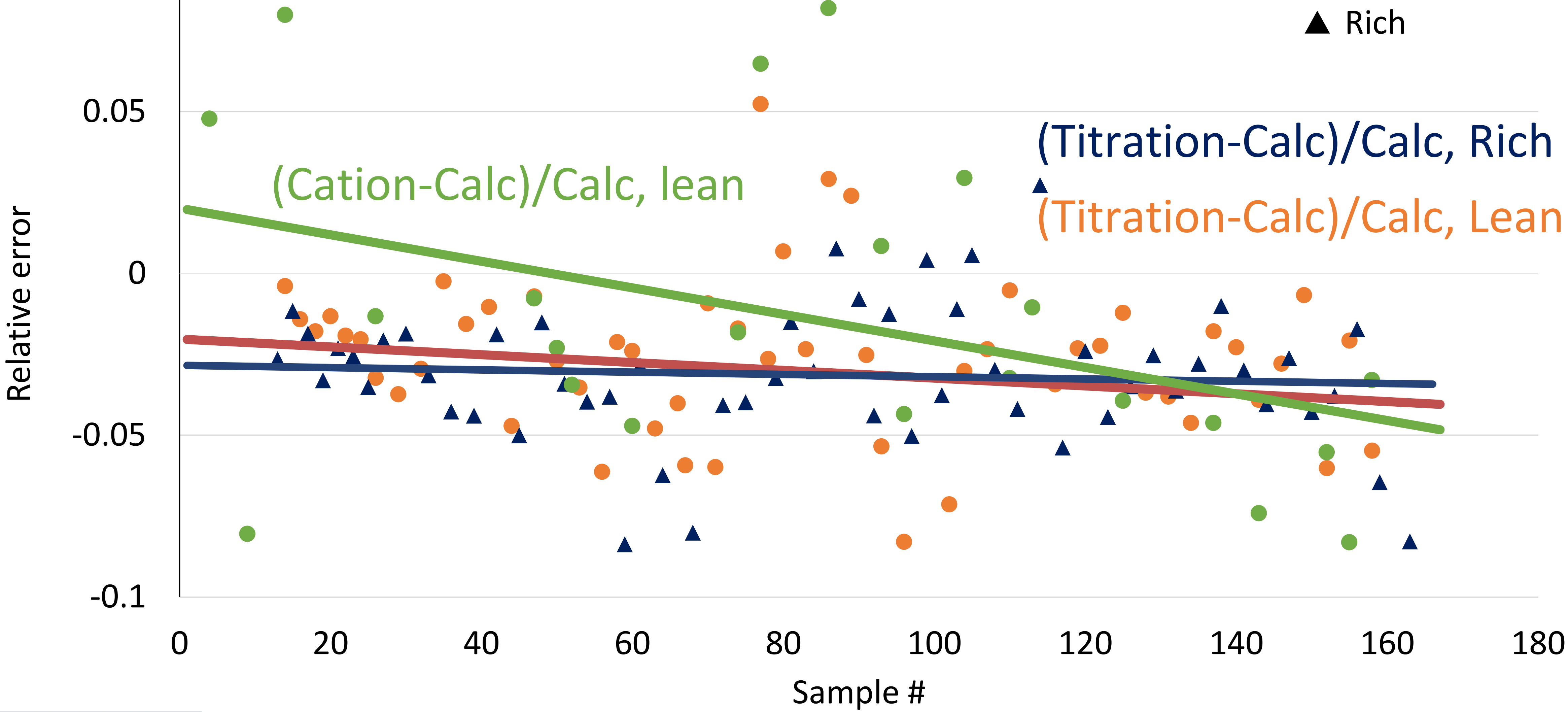
$$\rho_{PZ} = \rho_w \cdot (0.0407 \cdot C_{CO2} + 0.008 \cdot C_{PZ} + 0.991)$$

- Viscosity correlation
  - From 2, 5, 7, 9 m PZ viscosity measured by Freeman

$$\mu = \mu_w \cdot exp\left[\left(\frac{A}{T} - B\right) \cdot (C \cdot C_{PZ} + D \cdot C_{CO2} + E \cdot C_{PZ} \cdot C_{CO2})\right]$$

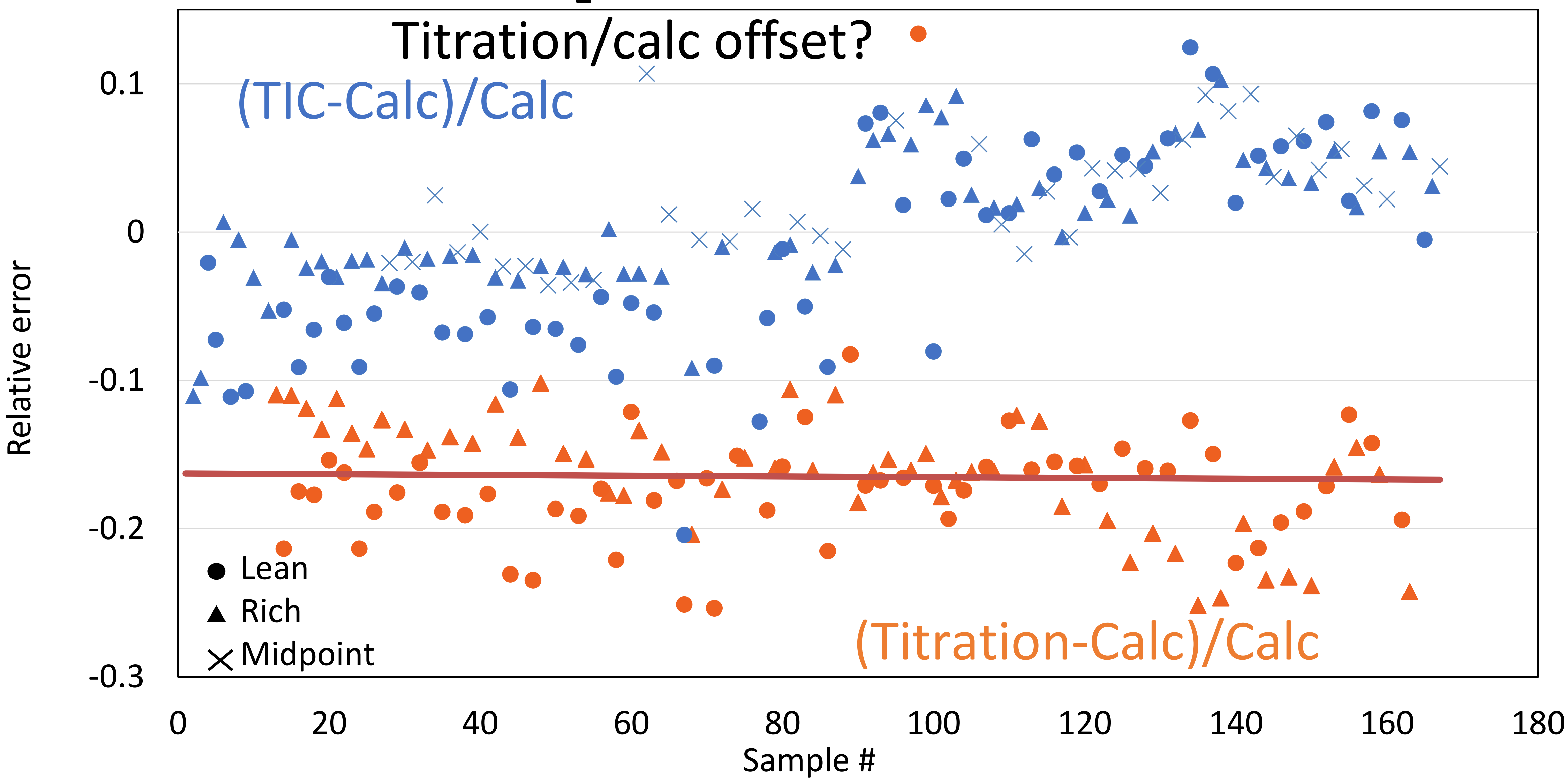
$$\mu_w = A' \cdot 10^{B'/(T-C')}$$

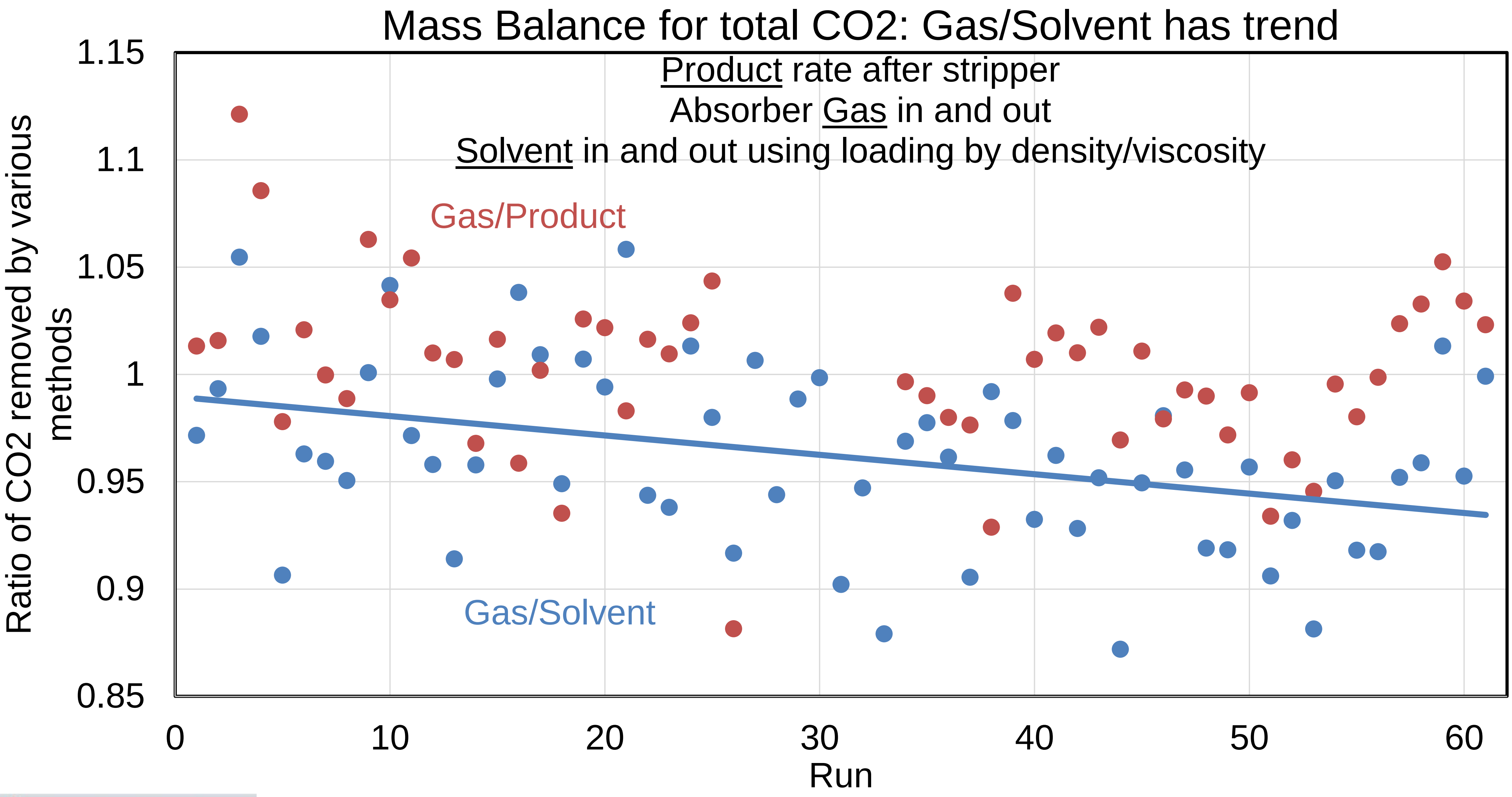
Data Reconciliation: PZ (wt %)
Cation, Titration, & Calc are reliable



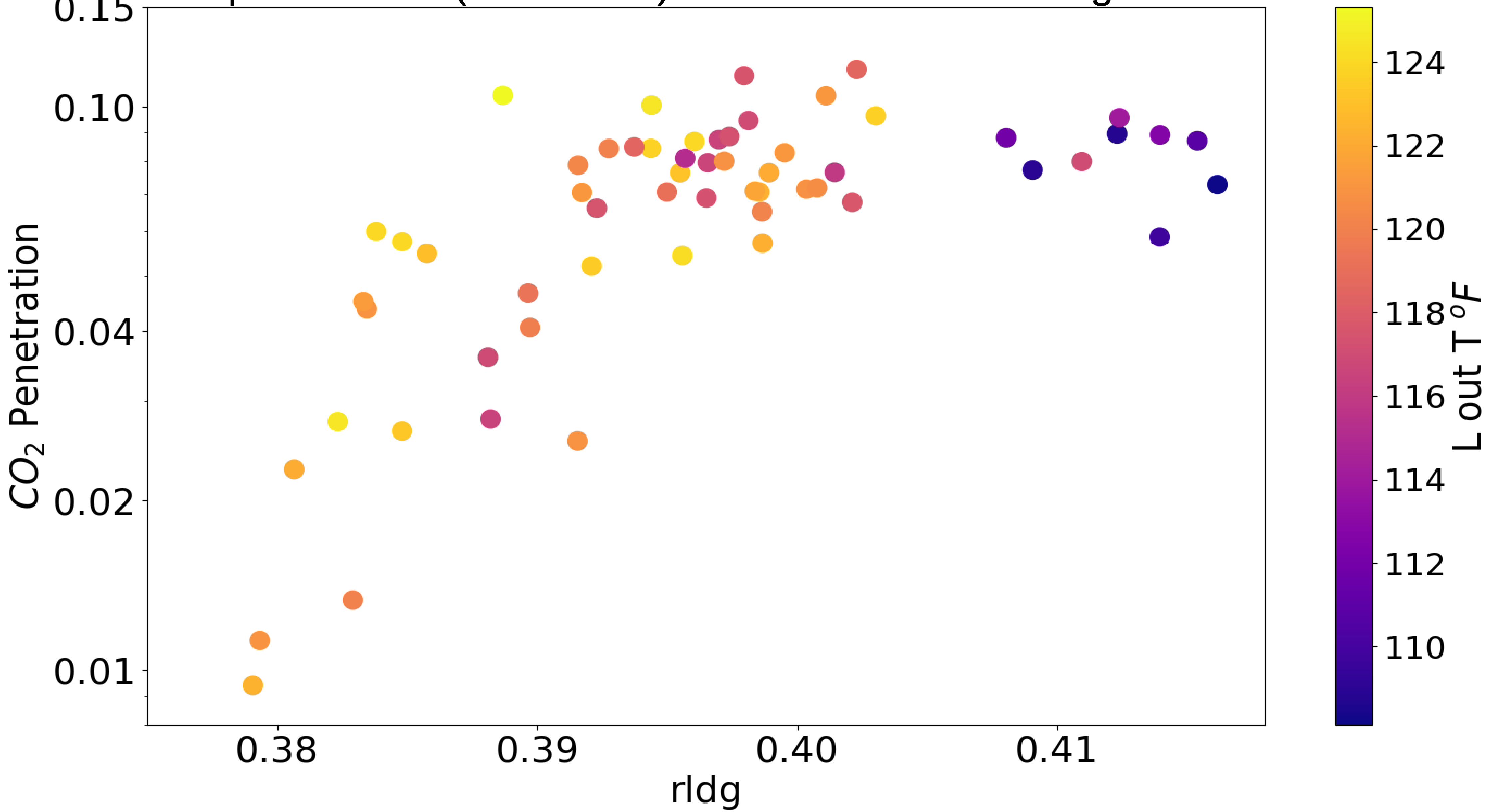
CCSI² Carbon Capture Simulation for Industry Impact | NATIONAL ENERGY TECHNOLOGY LABORATORY | BERKELEY LAB | Lawrence Livermore National Laboratory | Los Alamos NATIONAL LABORATORY EST.1943 | Pacific Northwest NATIONAL LABORATORY | WestVirginiaUniversity | THE UNIVERSITY OF TEXAS AT AUSTIN | U.S. DEPARTMENT OF ENERGY

Reconciliation: CO_2 (wt %) TIC unreliable?




Mass Balance for total CO2: Gas/Solvent has trend
Product rate after stripper
Absorber Gas in and out
Solvent in and out using loading by density/viscosity
Gas/Product
Gas/Solvent
Ratio of CO2 removed by various methods
Run
1.15
1.1
1.05
1
0.95
0.9
0.85
0
10
20
30
40
50
60

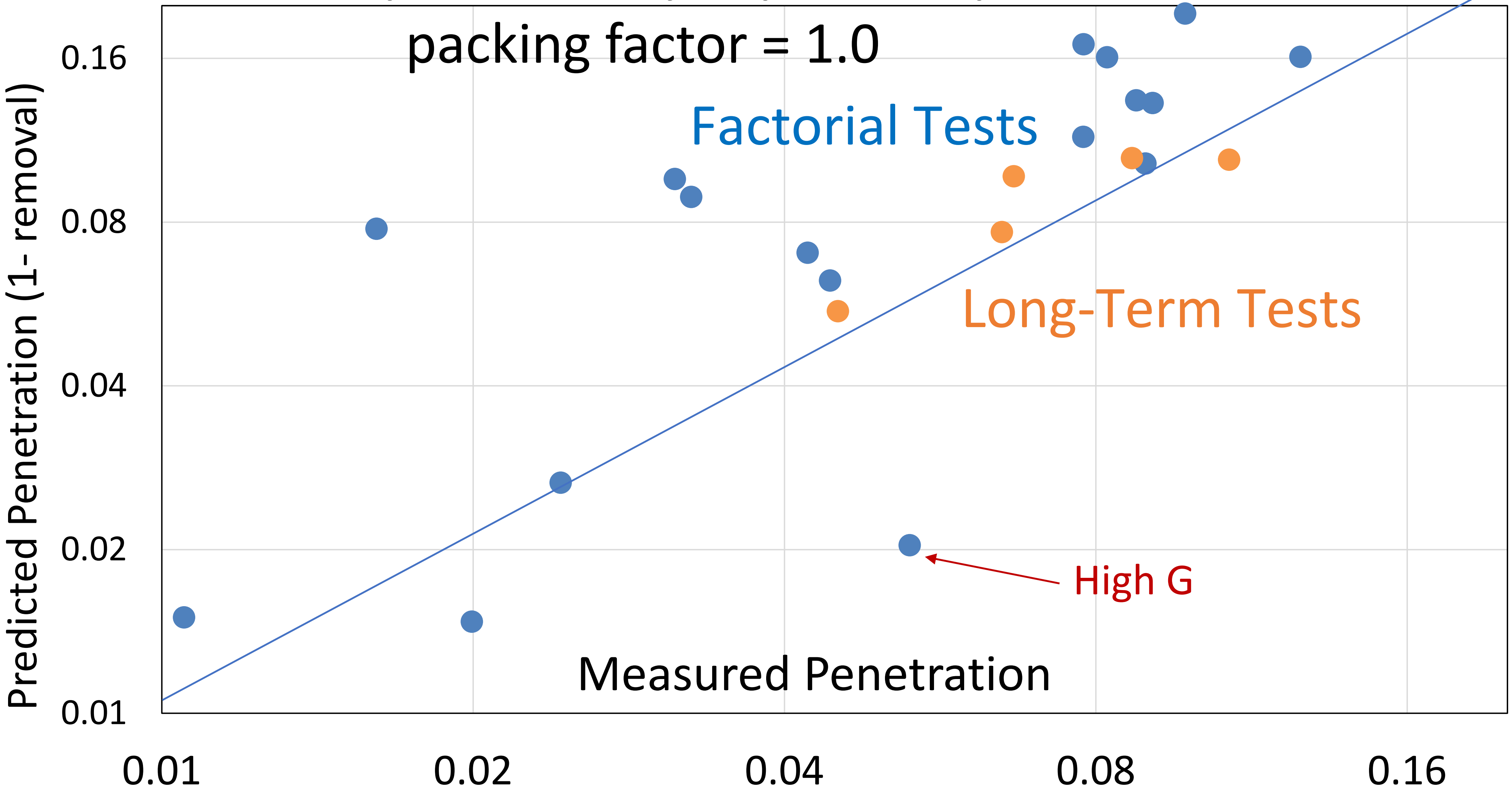
CO2 penetration (1-removal) varies with rich loading and Rich T

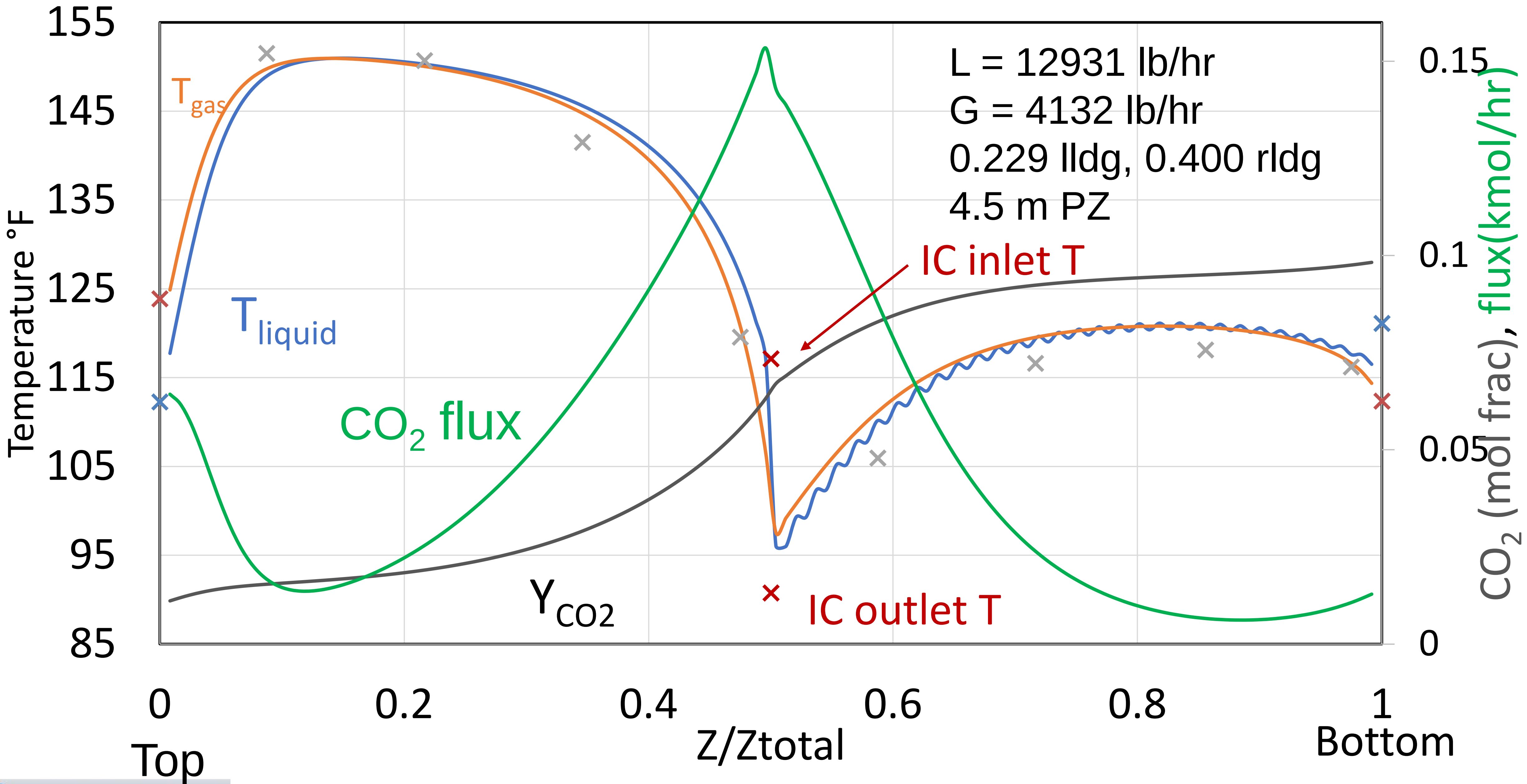


Independence model (by Frailie)

- CO_2 solubility, C_p, amine volatility by eNRTL
- Wetted wall column k_g' by diffusion with chemical kinetics
- Packing wetted area, k_l as measured by Song
- Rate-based absorption with reaction in the boundary layer

CO2 removal predicted by Aspen Independence, packing factor = 1.0

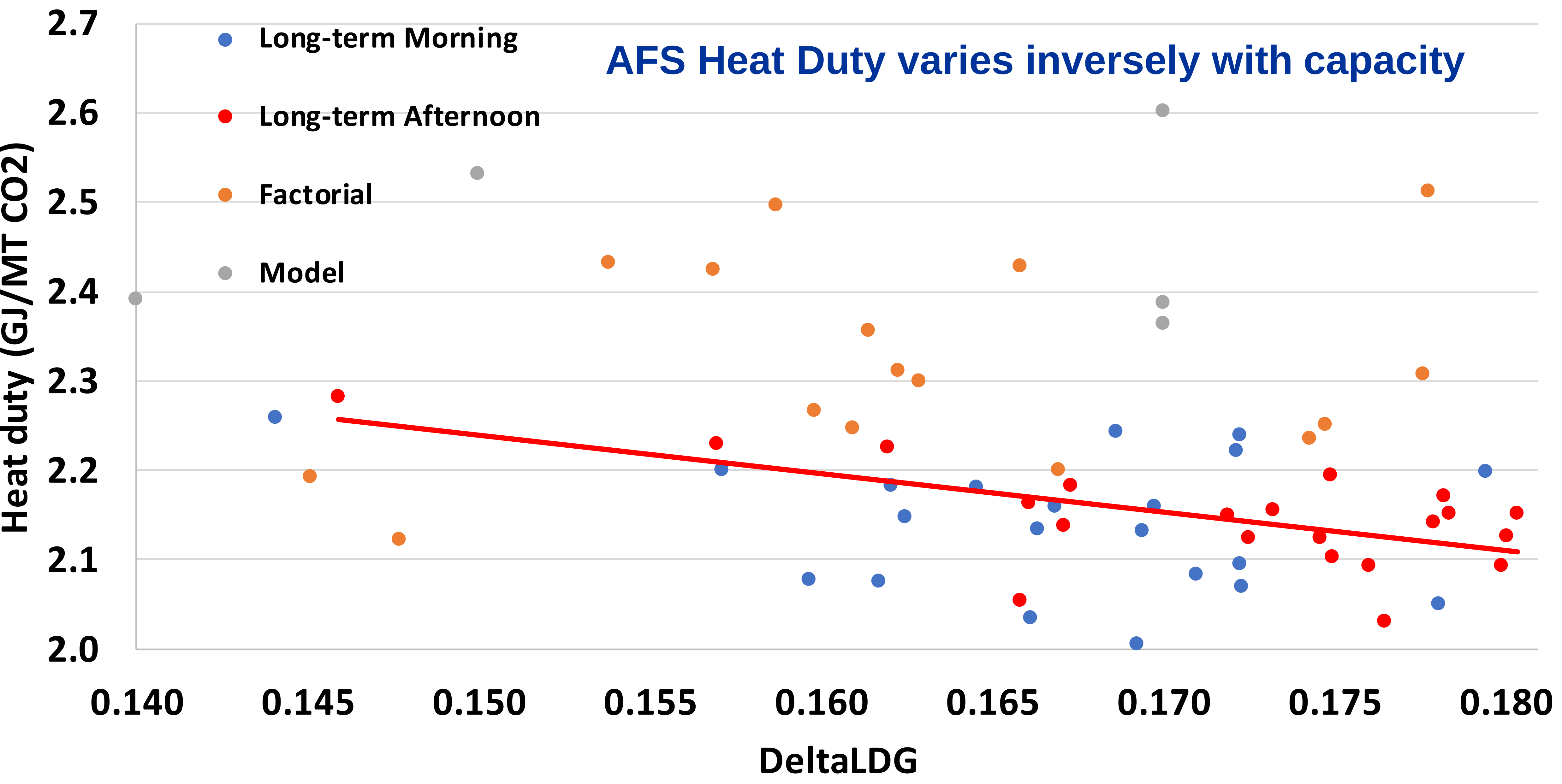




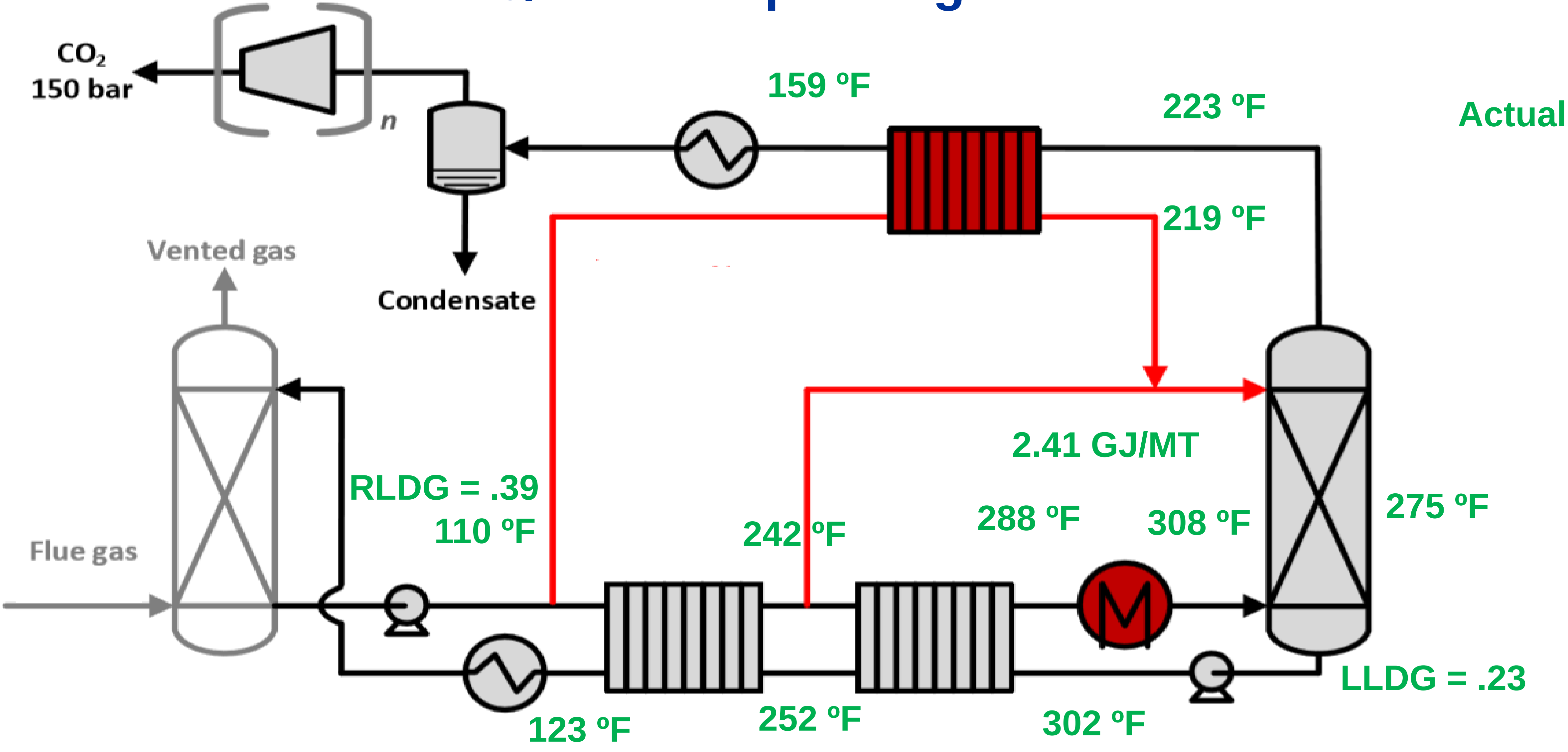
155
145
135
125
115
105
95
85
Temperature °F
L = 12931 lb/hr
G = 4132 lb/hr
0.229 lldg, 0.400 rldg
4.5 m PZ
T_{gas}
T_{liquid}
CO_2 flux
Y_{CO2}
IC inlet T
IC outlet T
0.15
0.1
0.05
0
CO_2 (mol frac), flux(kmol/hr)
0
0.2
0.4
0.6
0.8
1
Top
Z/Ztotal
Bottom

NCCC Stripper Modeling

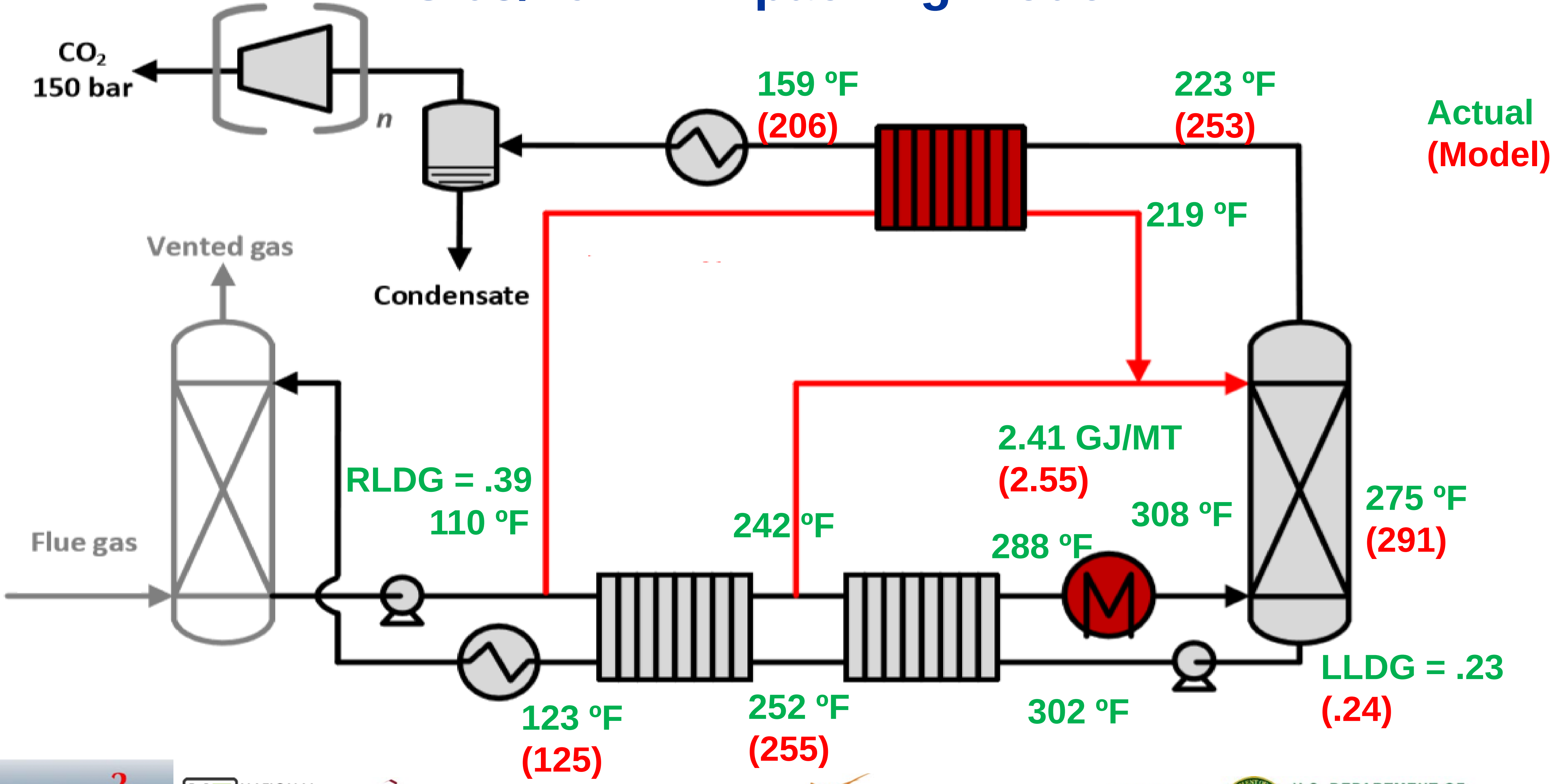
- Empirical representation of heat duty
- Performance underpredicted by Independence


AFS Heat Duty varies inversely with capacity
Long-term Morning
Long-term Afternoon
Factorial
Model
Heat duty (GJ/MT CO2)
2.7
2.6
2.5
2.4
2.3
2.2
2.1
2.0
0.140
0.145
0.150
0.155
0.160
0.165
0.170
0.175
0.180
DeltaLDG

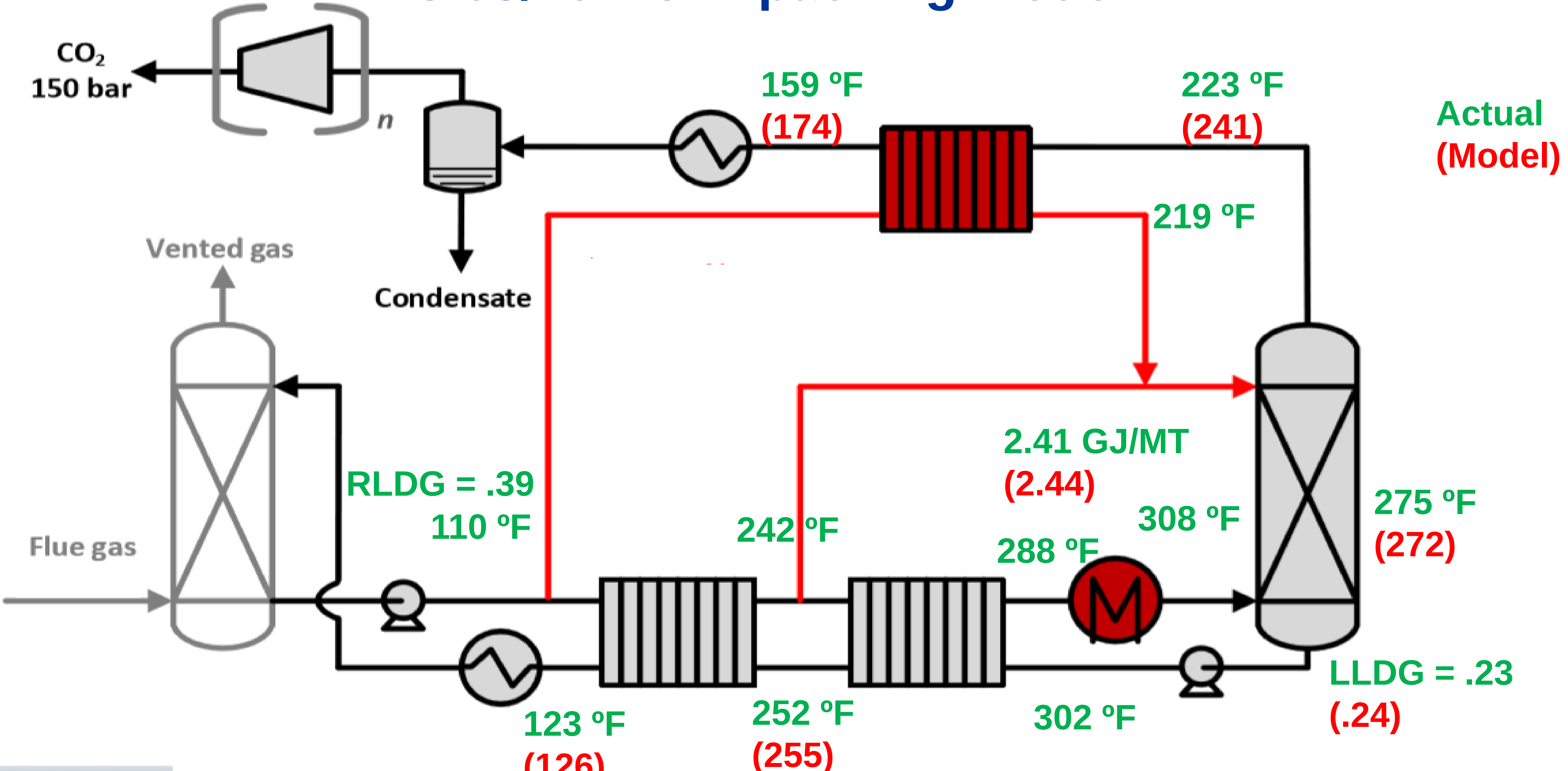
AFS 03/26 – 4 m packing model



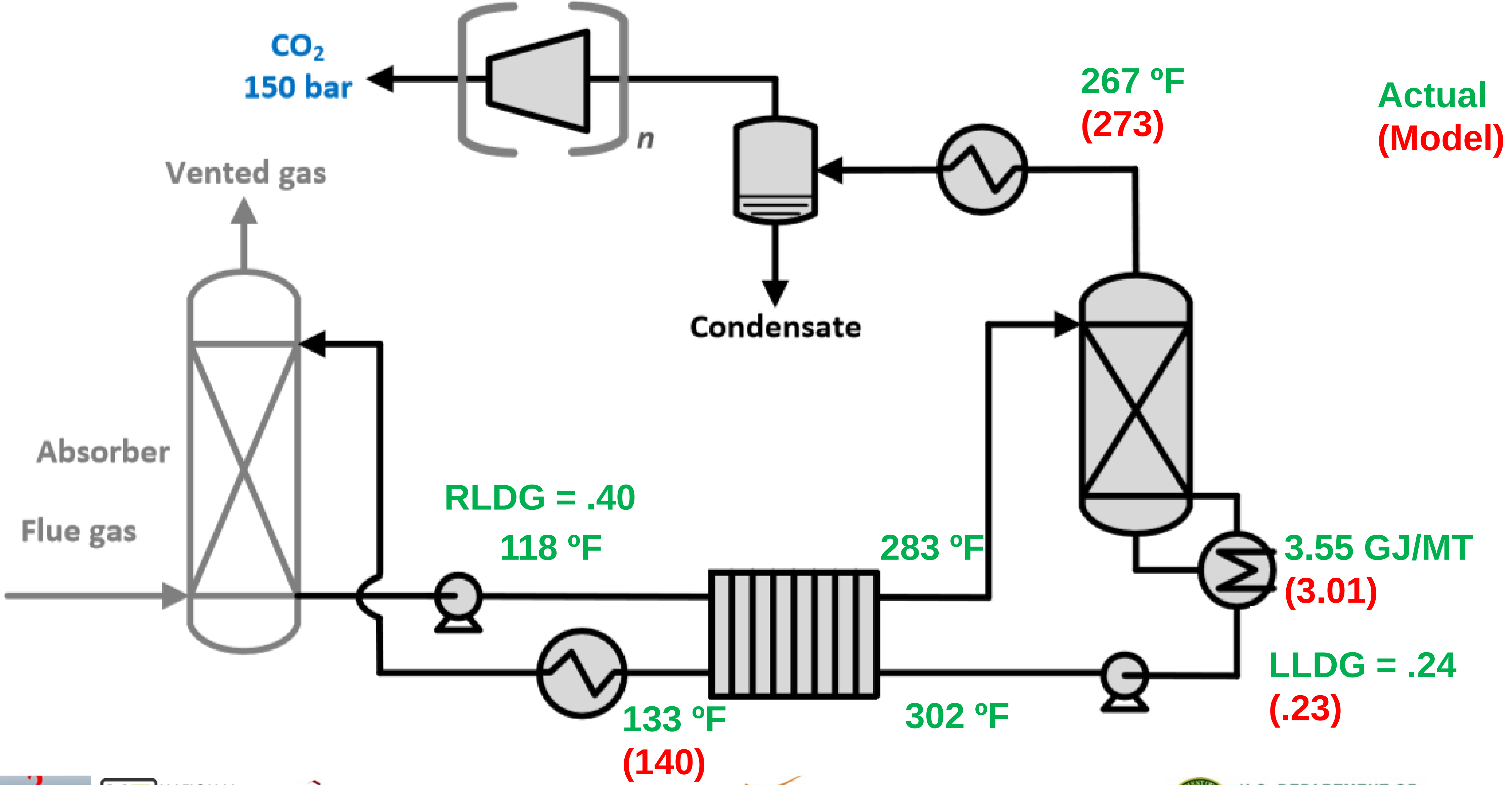
AFS 03/26 – 4 m packing model



AFS 03/26 – 8 m packing model

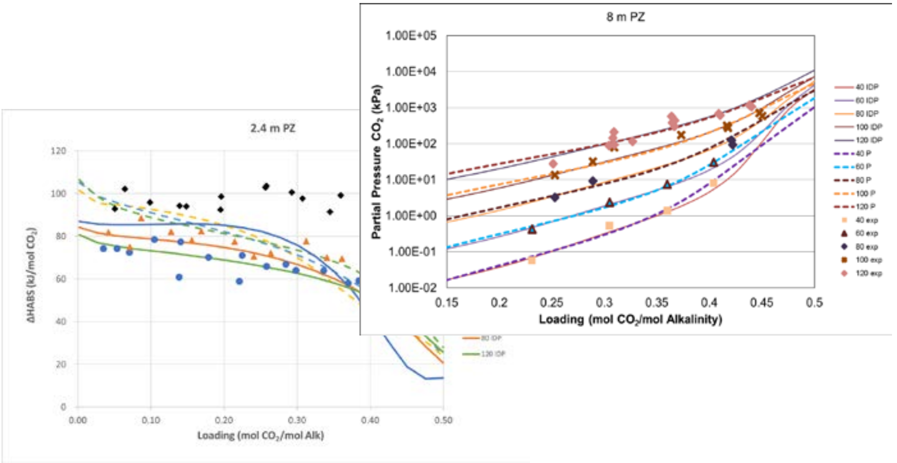


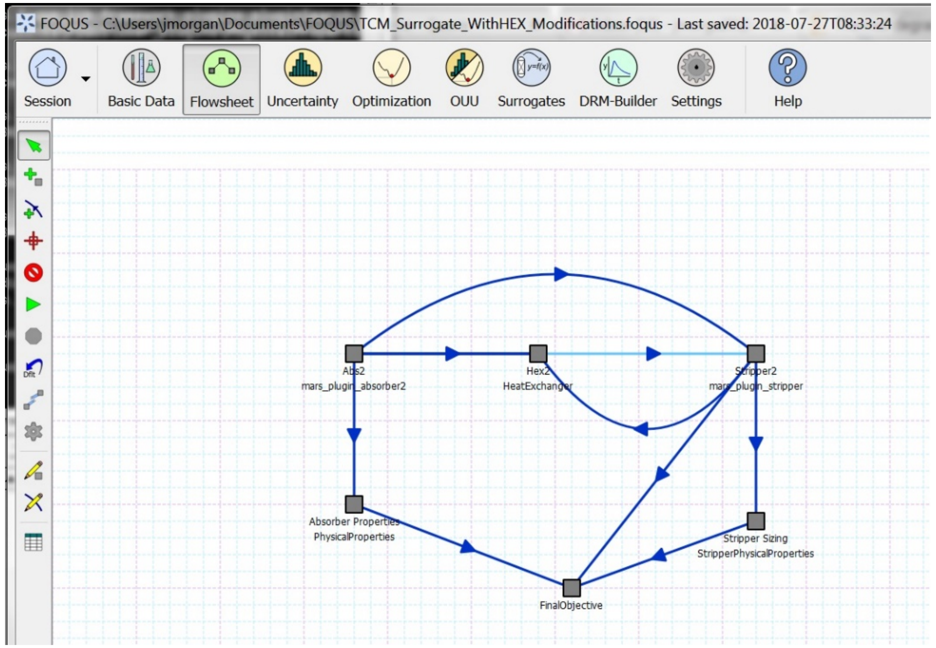
Simple Stripper 05/24



Improvements to Independence Model

- Rigorous optimization of AFS requires highly predictive model
  - Use of opensource CCSI Toolset
  - MEA solvent
- Accuracy of thermodynamic model has significant effect on
  - Column design
  - Regeneration energy cost
  - Energy balance calculations
- Issues
  - energy balance not closing and estimation of heat loss
- A robust and validated, thermodynamically consistent VLE model helps to reduce scale-up uncertainty and reduce impact of data gaps





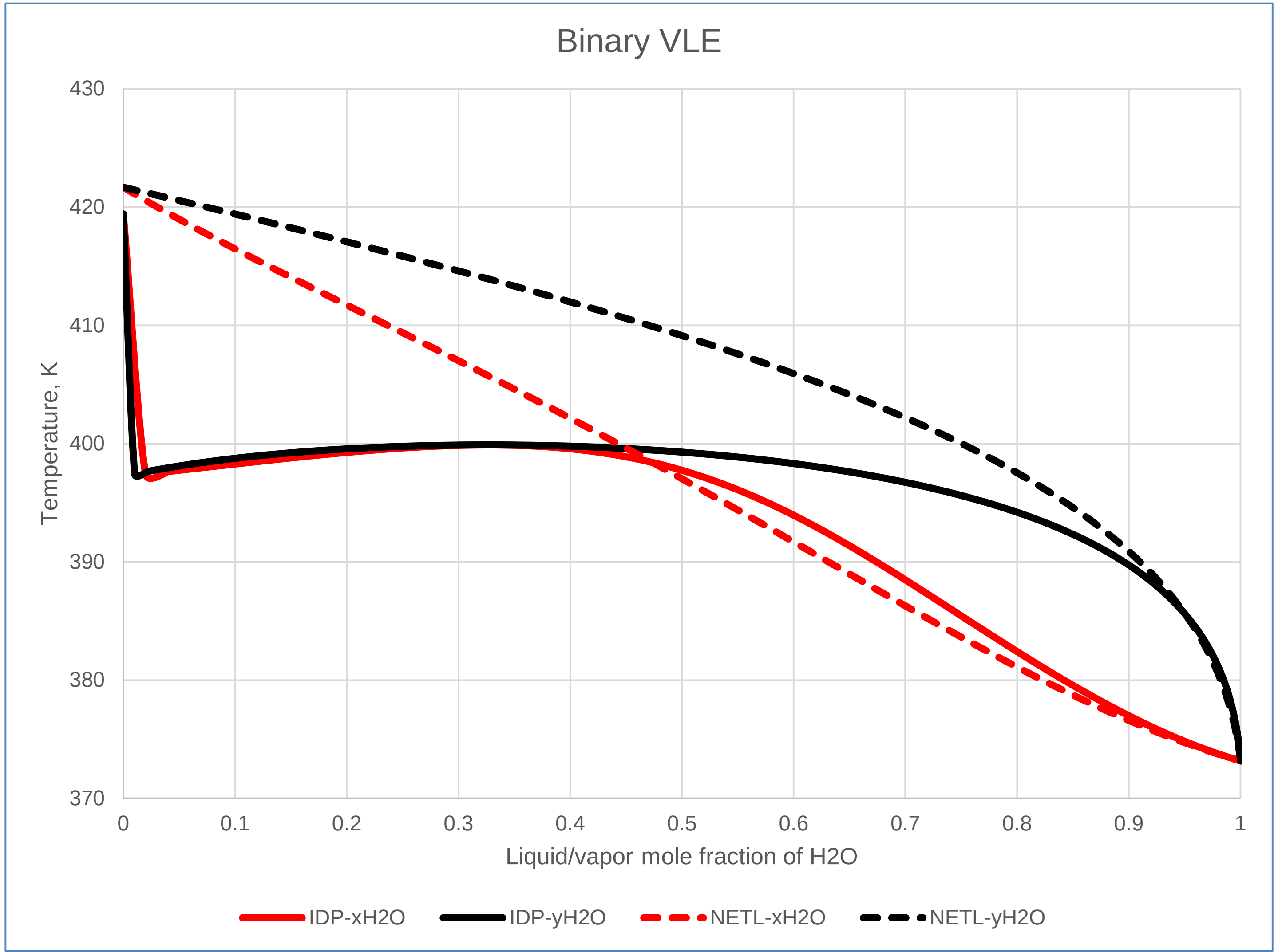
Thermodynamic Model Development

- **Sequential regression methodology was used**
  - Binary (PZ/H_2O) → Ternary (PZ/H_2O/CO_2)

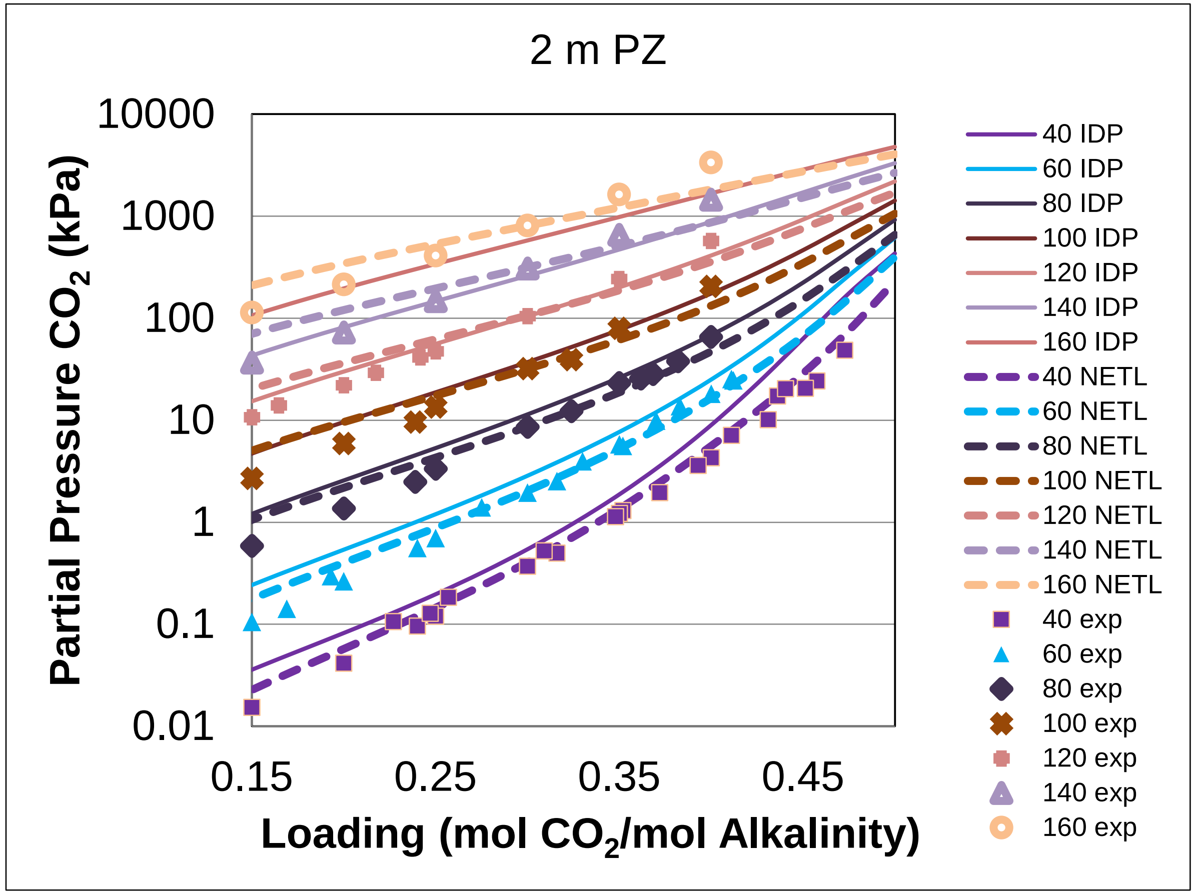
- **Binary VLE**:
  - PZ/H_2O VLE data
  - PZ volatility data
  - Freezing point depression data
    - to get water activity
  - Unloaded C_p data

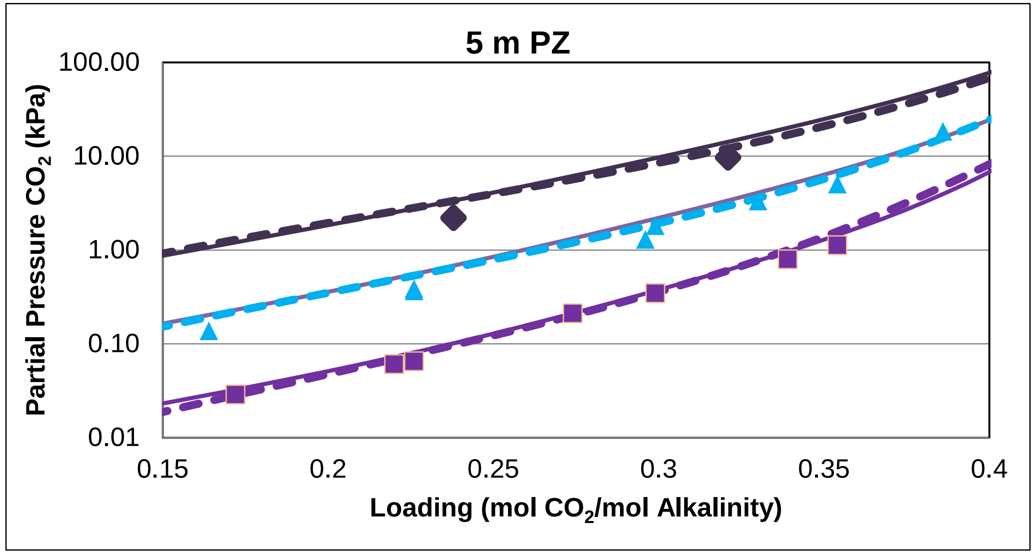
- **Ternary VLE** :(PZ+H_2O+CO_2)
  - PZ+H_2O+CO_2 VLE data
    - P_{CO2} data
    - Total pressure data
    - PZ volatility data
    - NMR speciation data
  - Heat of absorption data
  - pKa and pH
  - N_2O solubility
    - to regress activity of CO_2 in the solution via N_2O analogy: Crucial for kinetics
  - Loaded Cp data

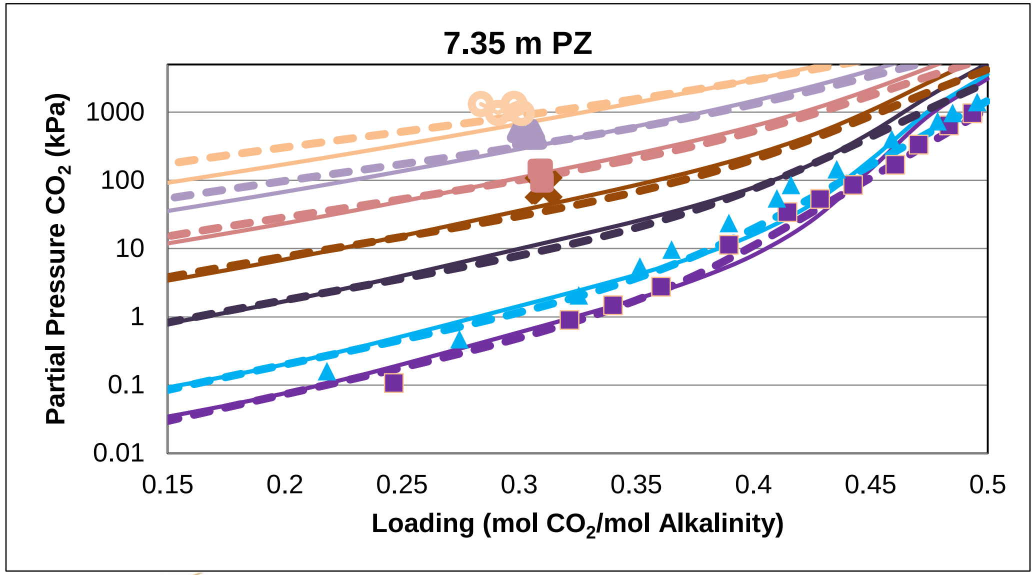
Binary VLE


Binary VLE
430
420
410
400
390
380
370
Temperature, K
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Liquid/vapor mole fraction of H2O
IDP-xH2O
IDP-yH2O
NETL-xH2O
NETL-yH2O

VLE model



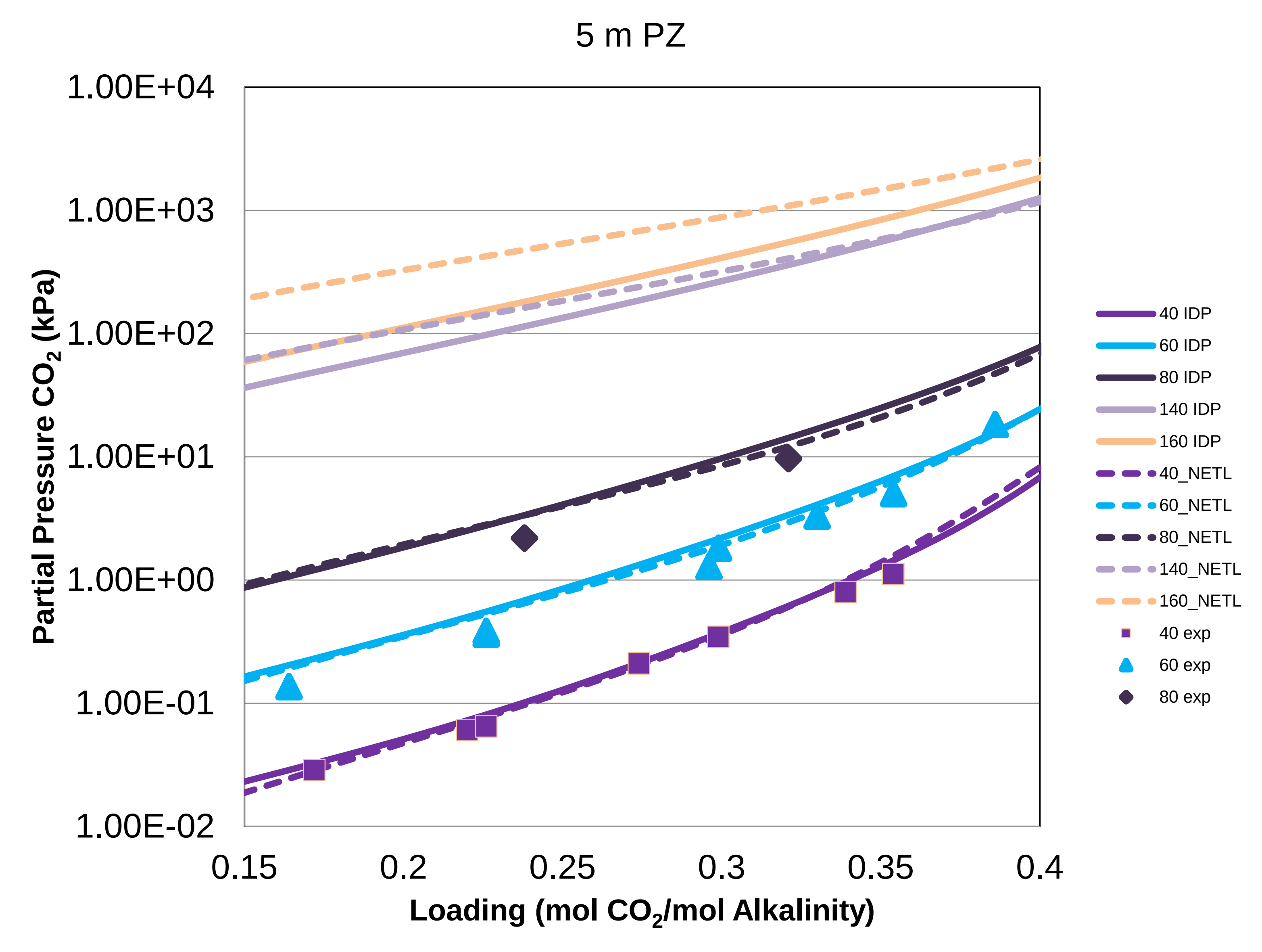




R. E. Dugas, Carbon Dioxide Absorption, Desorption, and Diffusion in Aqueous Piperazine and Monoethanolamine, PhD Thesis, University of Texas Austin, 2009.
S. K. Dash, A. Samanta, A. N. Samanta, and S. S. Bandyopadhyay, Fluid Phase Equilibria **300**, 145 (2011).
M. D. Hilliard, A Predictive Thermodynamic Model for an Aqueous Blend of Potassium Carbonate, Piperazine, and Monoethanolamine for Carbon Dioxide Capture from Flue Gas, 2008

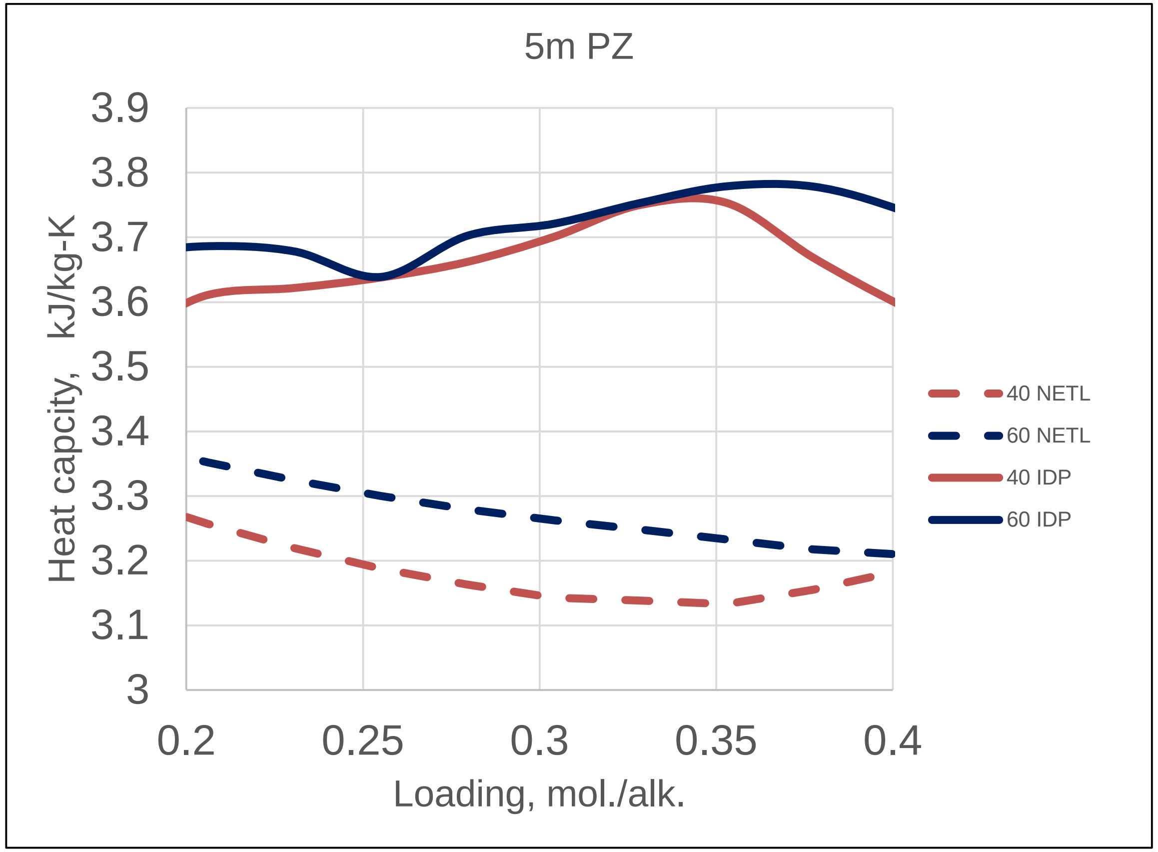
VLE model results

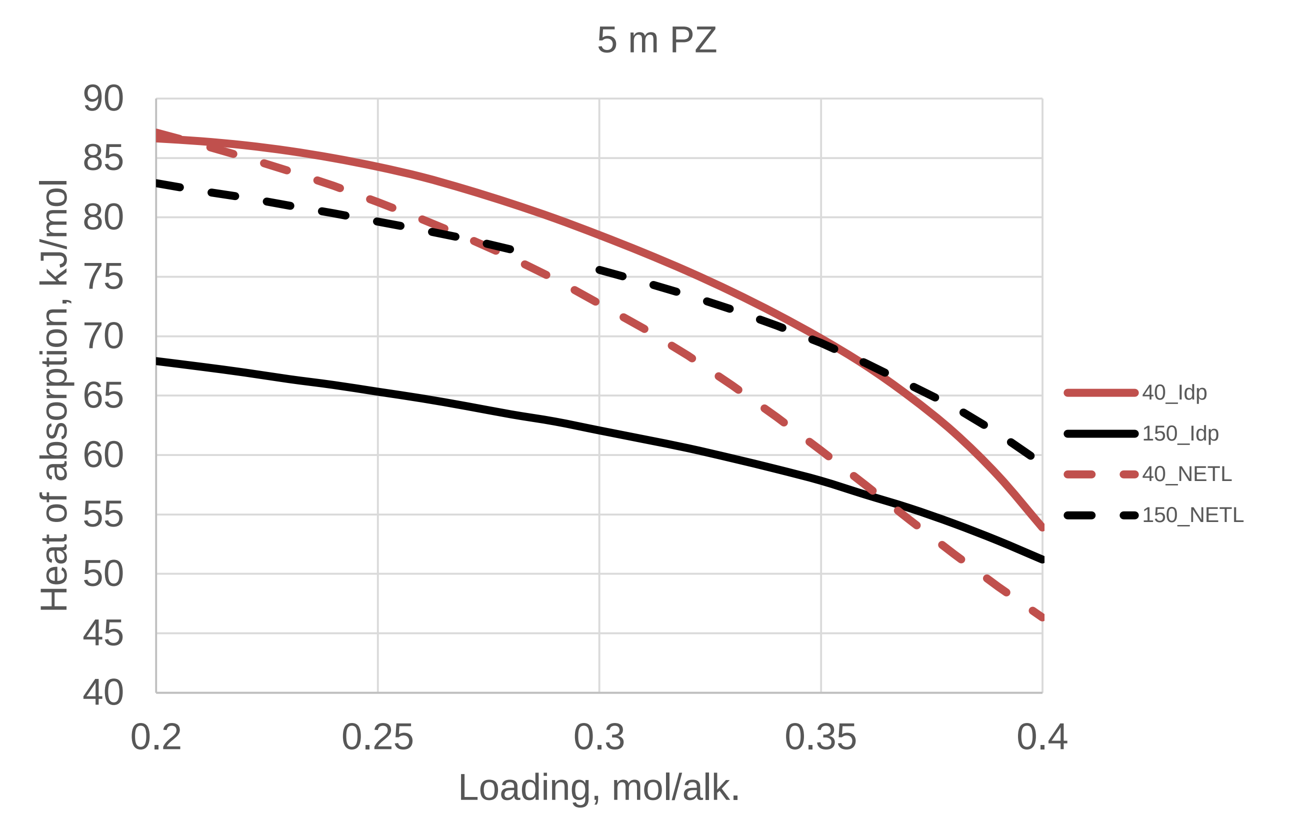
- **Ternary VLE** :($PZ+H_2O+CO_2$)
  - **Only P_{CO2} data available**
  - Missing data
    - Total pressure data
    - PZ volatility data
    - NMR speciation data
    - Heat of absorption data
    - N_2O solubility
    - Loaded Cp data



Dugas (2009)

Heat Capacity and Heat of Absorption



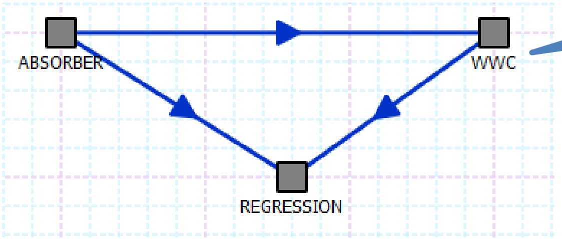


Energy balance (1,000 Btu/hr)

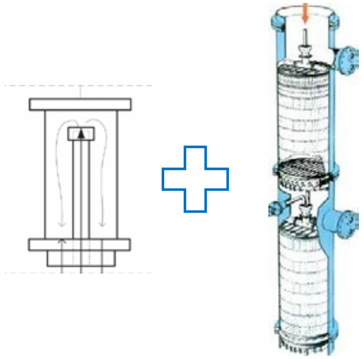
	Independence model		NETL model	
	Simple stripper	Long term AFS	Simple stripper	Long term AFS
Steam heat duty	883	536	883	536
Sensible heat, Lean – Rich	-113	-138	-104	-129
CO_2 ΔH desorption	-384	-398	-435	-441
Condenser	-192	-27	-192	-27
Total (heat loss)	194	10	145	-18

Development of Integrated Mass Transfer Model

- Properties (diffusivity, viscosity, surface tension), interfacial area, mass transfer coefficients, and reaction kinetics all affect mass transfer calculation
- 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
- Turbine facilitates faster computation



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



- Diffusivity
- Mass Transfer coefficients
- Reaction kinetics
- Interfacial area

Conclusions

- Viscosity and Density can be reliable indicators of solvent composition.
- 90-98% removal was achieved with 40 ft packing.
- Heat duty with PZ/AFS at NCCC is 2.1 GJ/tonne CO_2.
  - 10% uncertainty from energy balance and heat loss
- Independence underpredicts absorber and stripper performance.
- New NETL model represents basic data well.
  - Modeling important for experimental validation, estimation of heat loss.
- Reliable model essential for scale-up and optimization
  - CCSI Toolset being used for development of integrated mass transfer model.

For more information
https://www.acceleratecarboncapture.org/

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