SCOPE

Project number 327341
ACT – Accelerating CCS Technologies

European Commission

Accelerating CCS Technologies

Validation of a CESAR1 Solvent Model with a Focus on Water Wash Conditions

IEAGHG 7th Post Combustion Capture Conference
Pittsburgh, PA

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WP1 | Optimized Gas Treating, Inc.[1] , Hovyu B.V.[2]

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OGT

hovyu

Presentation Outline

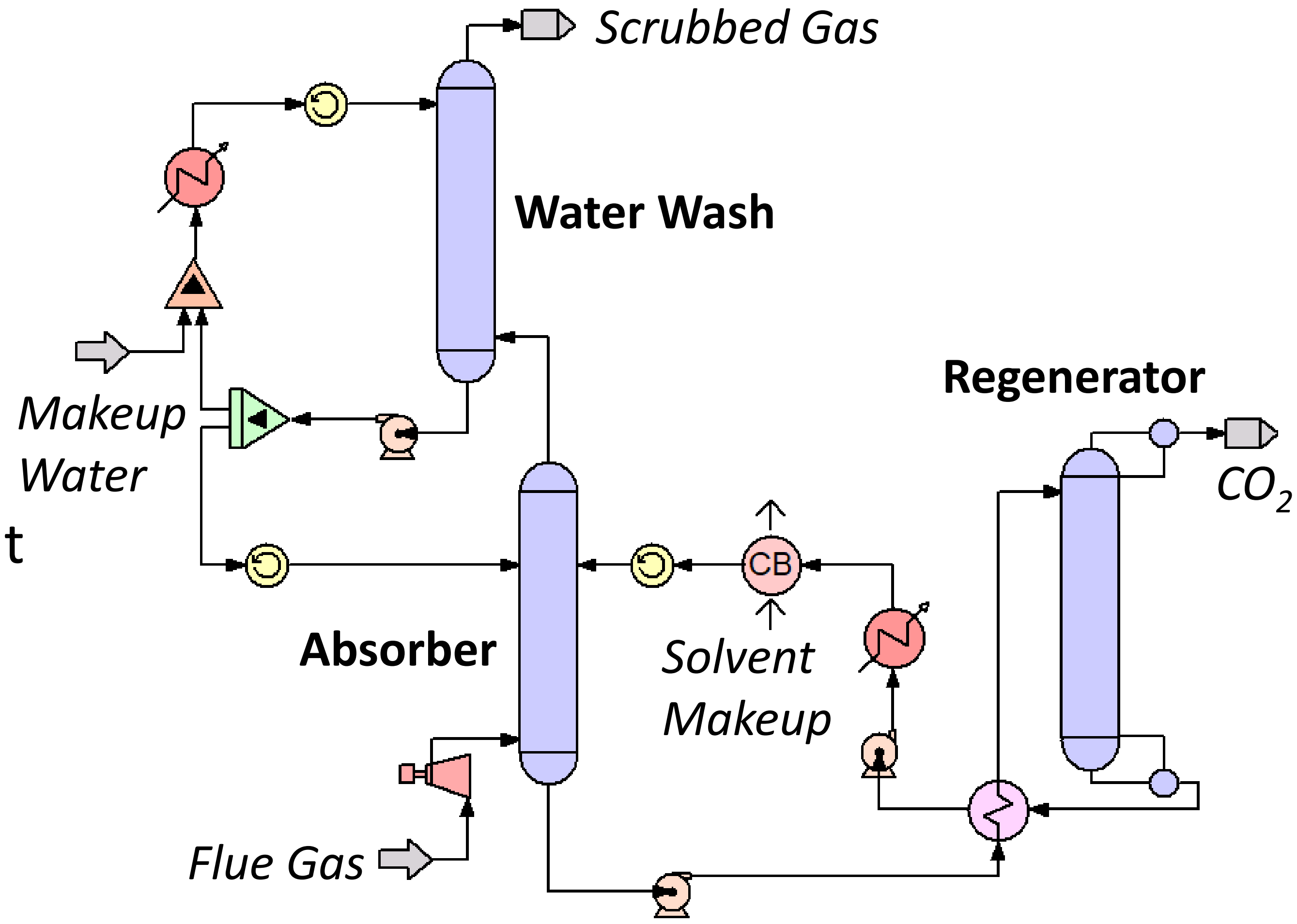
- Background
  - Absorber/regenerator loop with water-wash
  - CESAR1 solvent
  - SCOPE project
  - OGT’s role/objective

- ProTreat® CESAR1 model development
  - OGT rate model
  - Physical properties
  - VLE

- Conclusion and upcoming work

CO_2 Capture Basics

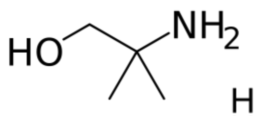
- Reaction with aq. amines in absorber/regenerator loop is most mature CO_2 capture technology
  - Water-wash design helps manage amine emissions
- 30 wt% MEA is the benchmark solvent
  - High absorption rate
  - High cyclic capacity
  - Large amount of literature
- Problem: high regeneration energy demand (~3.7 MJ/Kg_{CO2}[1])



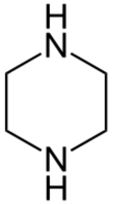
[1]Knudesen et al. (2011)

CESAR1 Solvent

- Developed by EU-funded CO_2 Enhanced Separation and Recovery (CESAR) project (2008 to 2011)
- Composition
  - 3.0 M AMP (~27 wt%)



  - 1.5 M Piperazine (~13 wt%)



- Regeneration energy of 2.6 to 2.8 MJ/Kg_{CO2}[1]
- Potential to replace MEA as benchmark solvent
  - Promising, but lacking literature
  - Questions over emissions control
  - Higher confidence needed in models

[1]Feron et al. (2020)

SCOPE Project

- Sustainable Operation of Post-combustion Capture Plants (SCOPE)
  - ACT-funded project (accelerating CCS technology)
  - Multinational consortium of 24 partners across 5 “work packages”

- SCOPE Objectives
  - Develop effective emissions control guidelines
  - Validate predictions against data from six different pilot plants (MEA and CESAR1)
  - Environmental risk assessment
  - Best policies and practices

- **OGT’s Role**
  - **WP 1: Emissions management tools**
  - **Develop and improve ProTreat® CESAR1 model**
  - **Use new VLE data generated through SCOPE, focus on water wash region**

OGT ProTreat® Rate Model

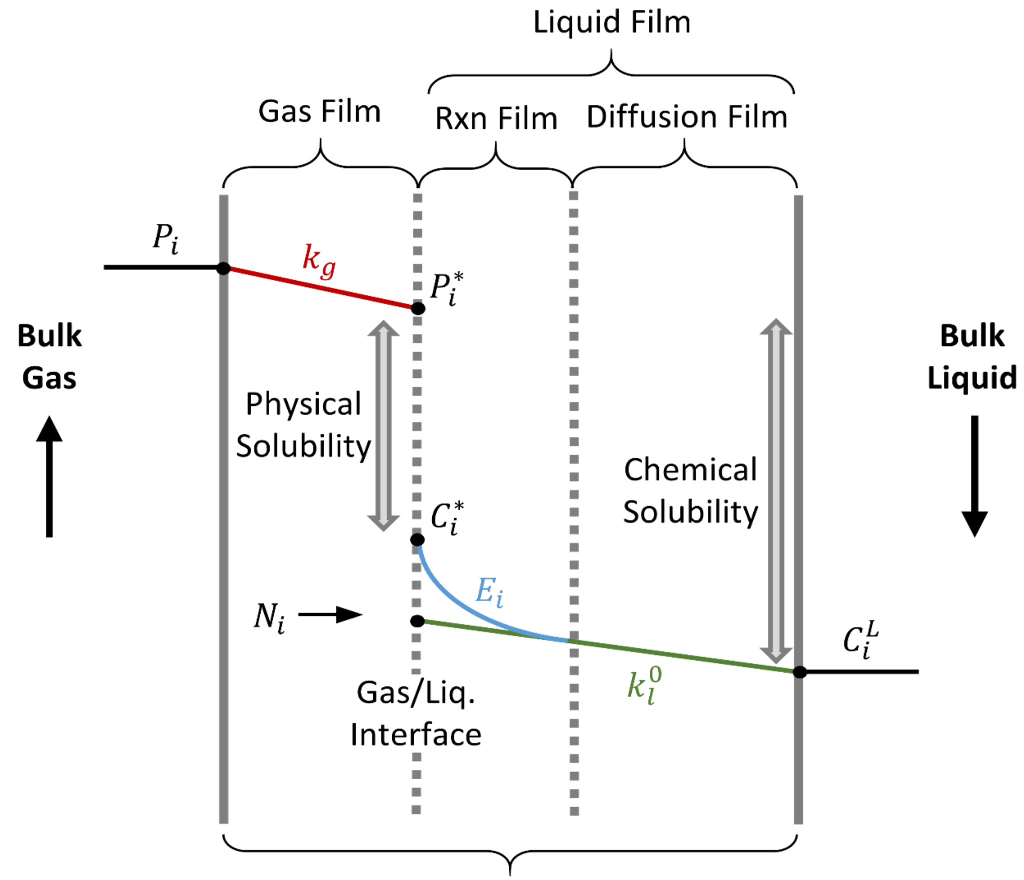
Absorber non-ideal behavior is better captured by rate-based models

Four Step Mass Transfer w/ Reaction

1. Gas diffusion (driving force)
2. Gas solubility in liquid (equilibrium)
3. Chemical Reaction (liquid phase)
4. Liquid diffusion (driving force)

Separation and Transfer Rates depend on:

- Area for mass/heat transfer
- Vapor & liquid loads
- System Kinetics
- Composition, physical and transport properties (c_p, μ, σ, ρ, Ɗ)
- Driving force - phases are not in equilibrium



$$N_i = k_g(P_i - P_i^*) = E_i k_l^0 (C_i^* - C_i^L)$$

$$Rate_i = K_G \times A \times (P_i - P_i^*)$$

Property Modeling

Need to model relevant compositions of AMP/PZ/Water/CO_2 system

Constant Properties

- Critical Pressure
- Critical Temperature
- Critical Volume
- Critical Compressibility Factor
- Acentric Factor
- Dipole Moment
- Boiling Point

Pure and Aqueous Properties

- Vapor Pressure
- Density
- Viscosity
- Thermal Conductivity
- Surface Tension
- Heat Capacity
- Heat of Absorption

Reaction Properties

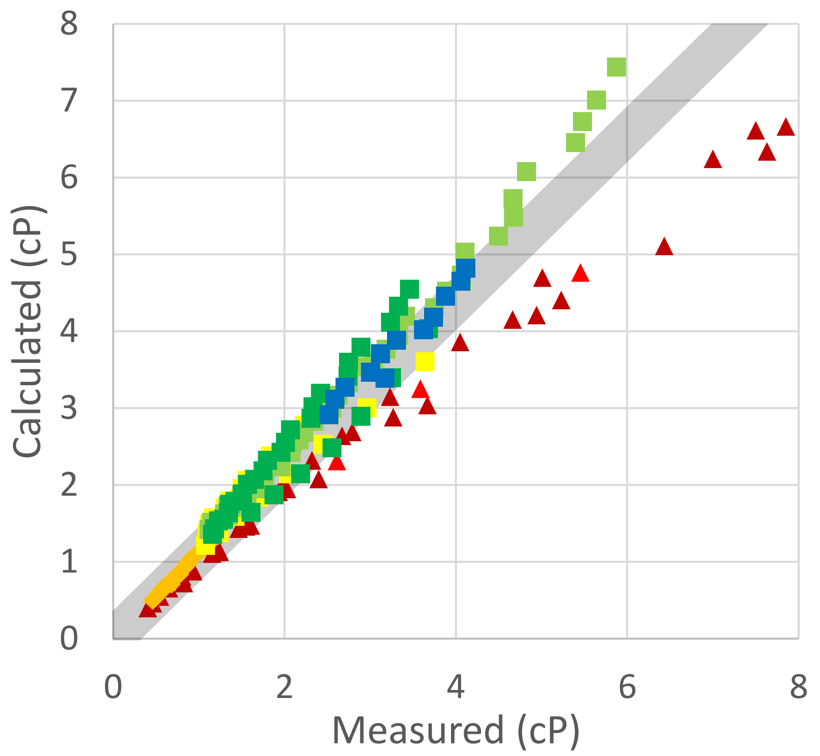
- CO_2 Kinetics
- pKa of Protonation

Checked each against literature, updated in ProTreat® model as necessary

AMP/Water Viscosity

$$*Relative\ Error\ \% = 100 * \left|\frac{Calc - Meas}{Meas}\right|$$

ProTreat® Legacy Model



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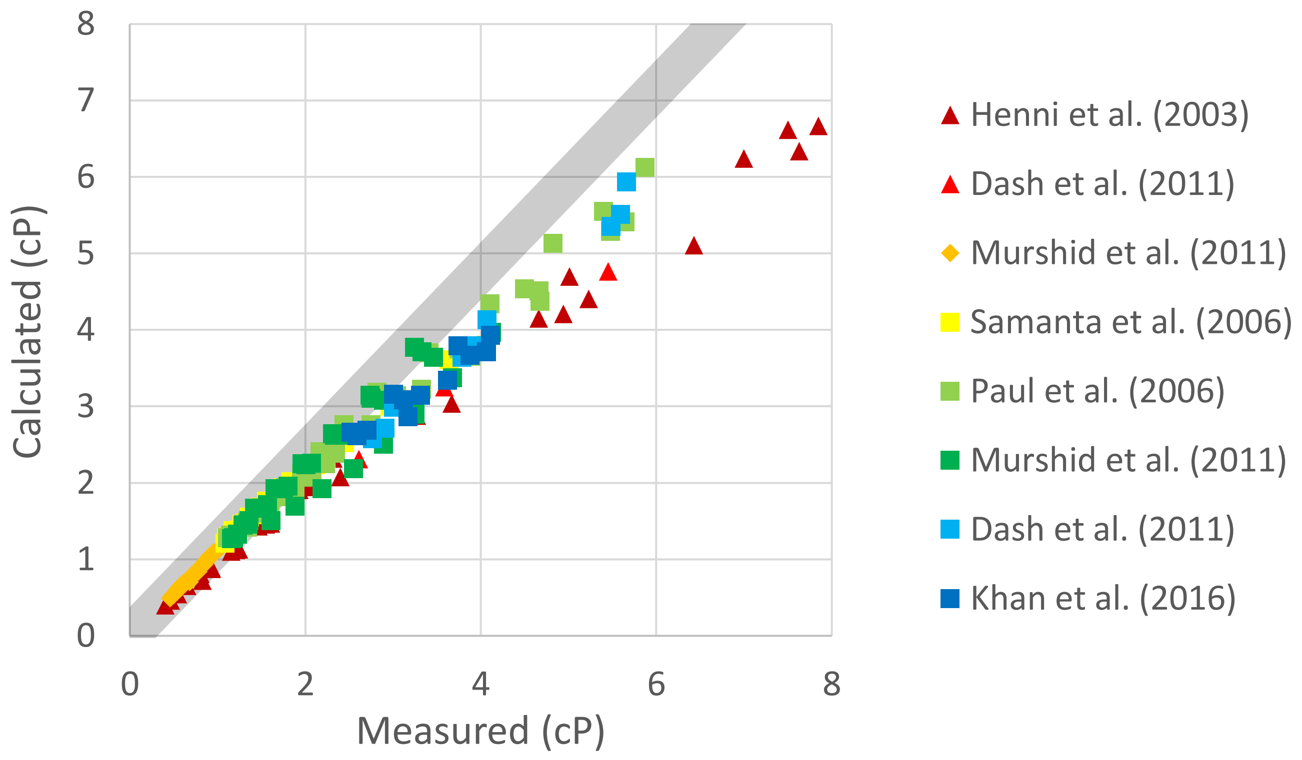
ProTreat® Updated Model



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VLE Model

- “OGT Gas Treating” Thermo Method
  - ProTreat® proprietary methods
  - Deshmukh-Mather Activity coefficient model[1]
    - Used with Peng-Robinson EOS
    - Poynting correction included
    - Ion-ion, molecule-ion, molecule-molecule interactions parameters regressed, both with and without CO_2 and H_2S

Binary

AMP-Water (ProTreat® Proprietary)

PZ-Water (ProTreat® Proprietary)

Ternary

AMP-Water-CO2 (Deshmukh-Mather)

PZ-Water-CO2 (Deshmukh-Mather)

Quaternary

AMP-PZ-Water-CO2 (Deshmukh-Mather)

[1]Deshmukh, R. D. & A. E. Mather, *Chem. Eng. Sci.*, **1981**, 36, 355-362

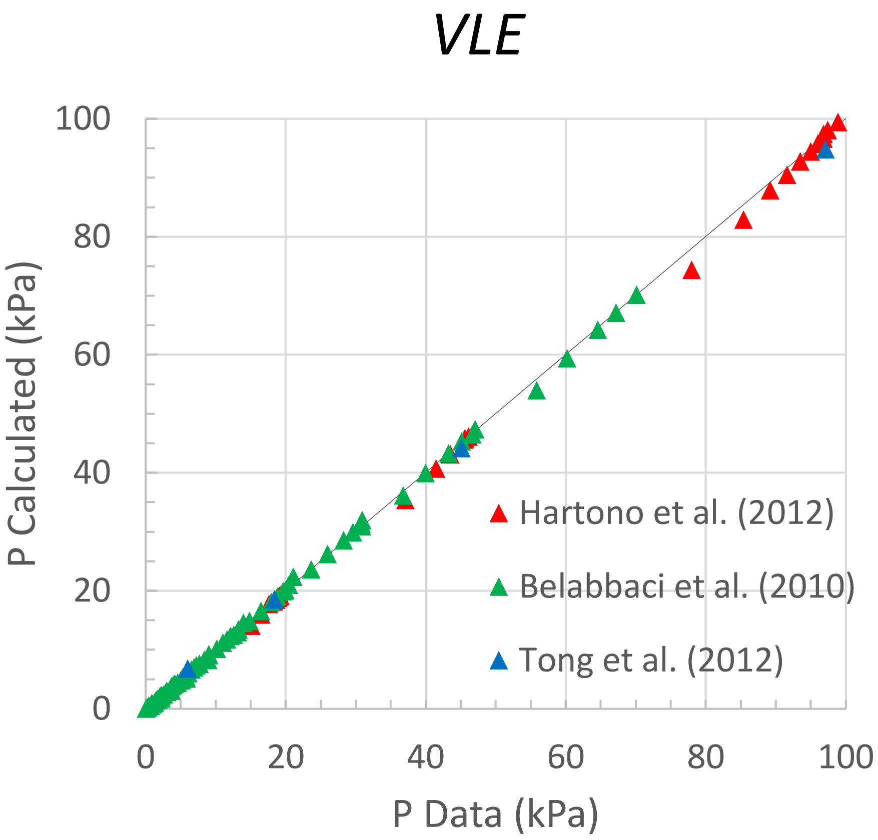
Activity Coefficient Fitting AMP/Water

VLE
- 120 data points
- 3 sources
- 293 to 497 K
- Large conc. range

Freezing Point Depression
- 29 data points
- 2 sources

Excess Enthalpy
- 16 data points
- 1 source

Excess Heat Capacity
- 210 data points
- 4 sources



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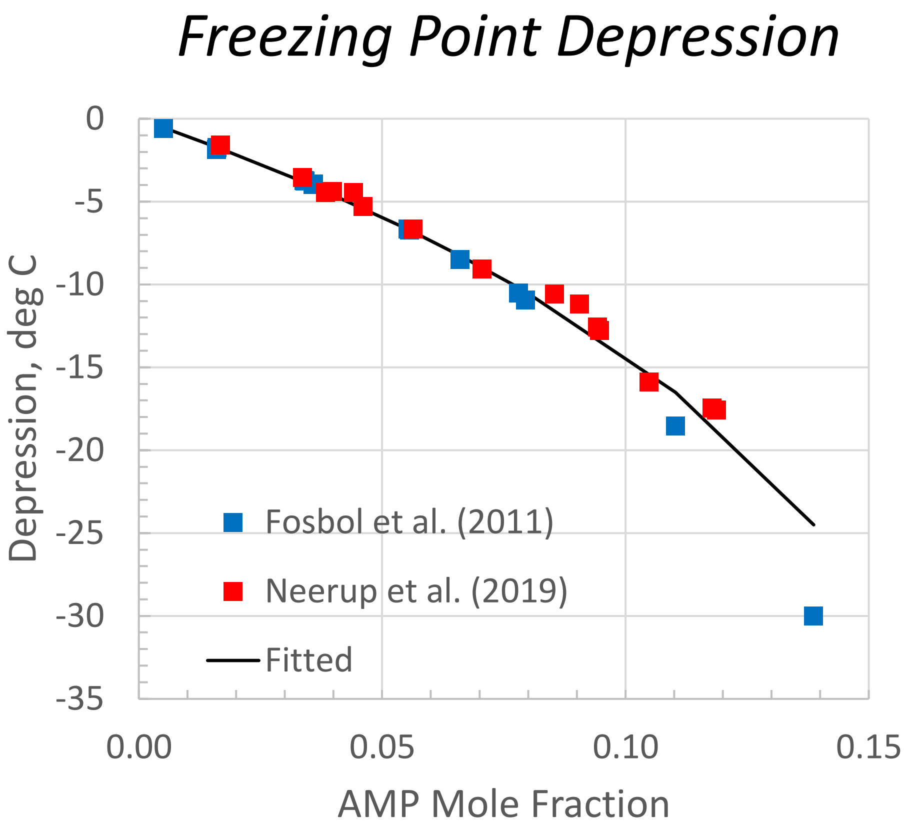

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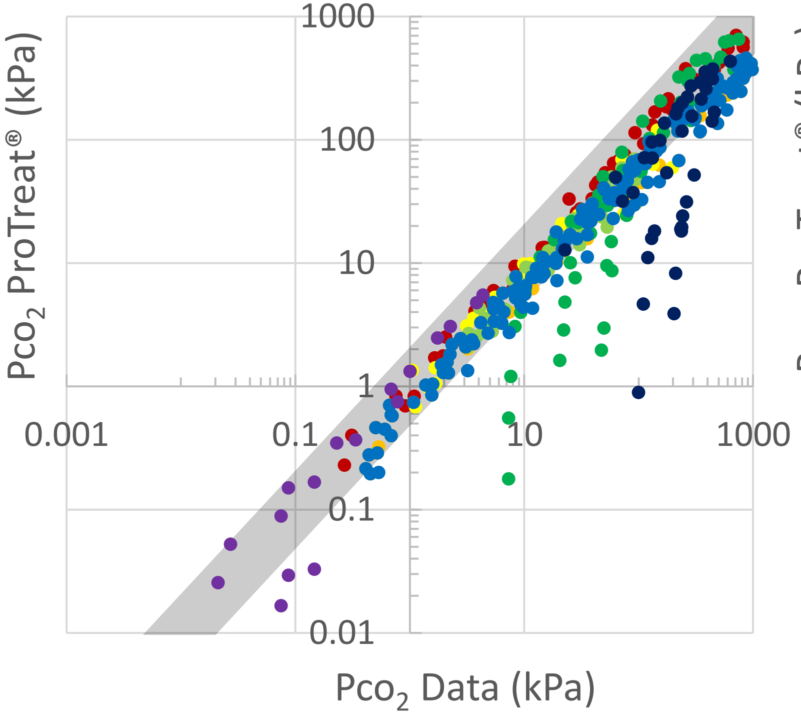
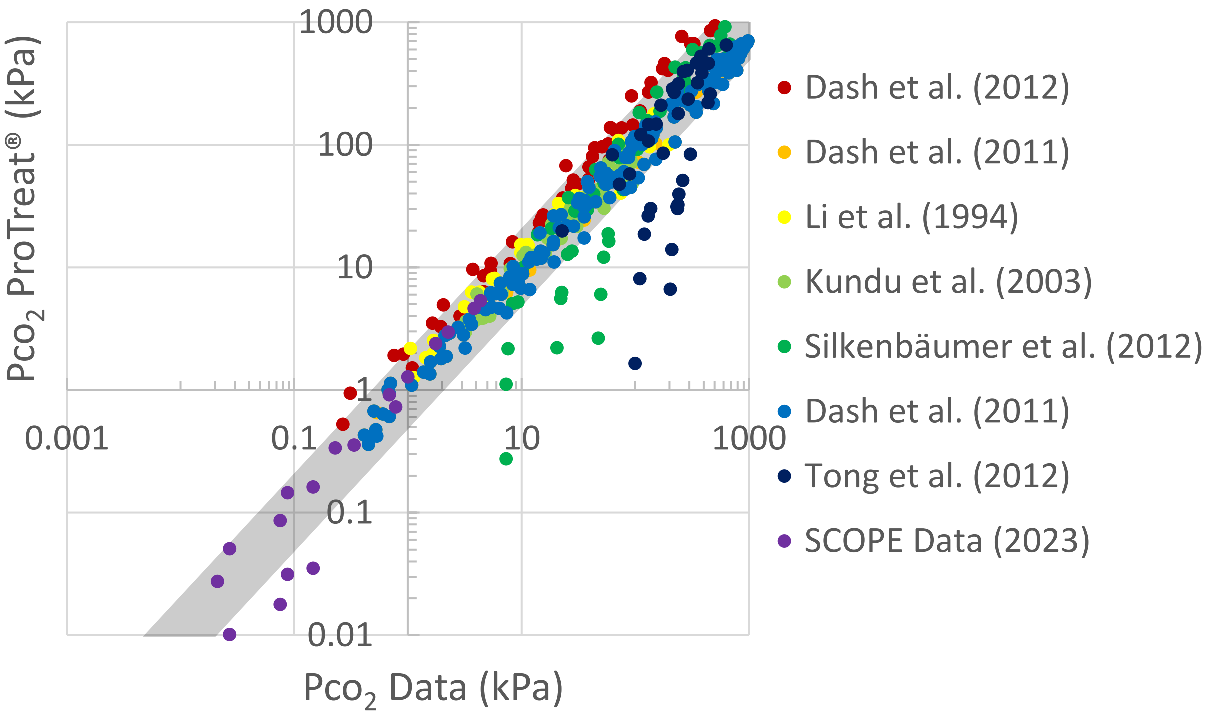
Deshmukh-Mather Fitting: AMP/Water/CO_2

- ~700 data points
- 9 sources
- 293 to 393 K
- 0.9 wt% to 50wt% AMP unloaded
- .0001 to 1.94 CO_2 loading
- Partial and total pressure
- 3 SCOPE data sets

ProTreat® Legacy Model



ProTreat® Updated Model

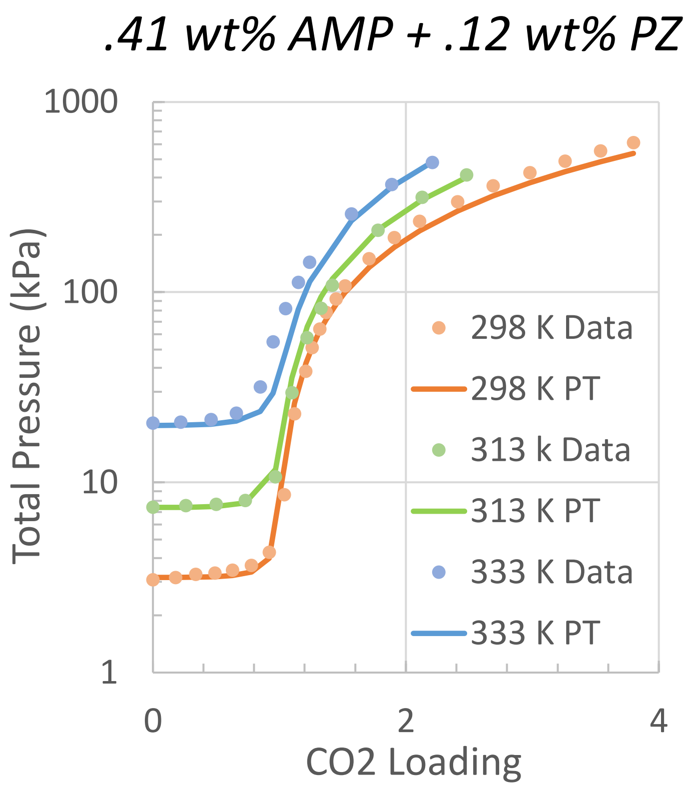


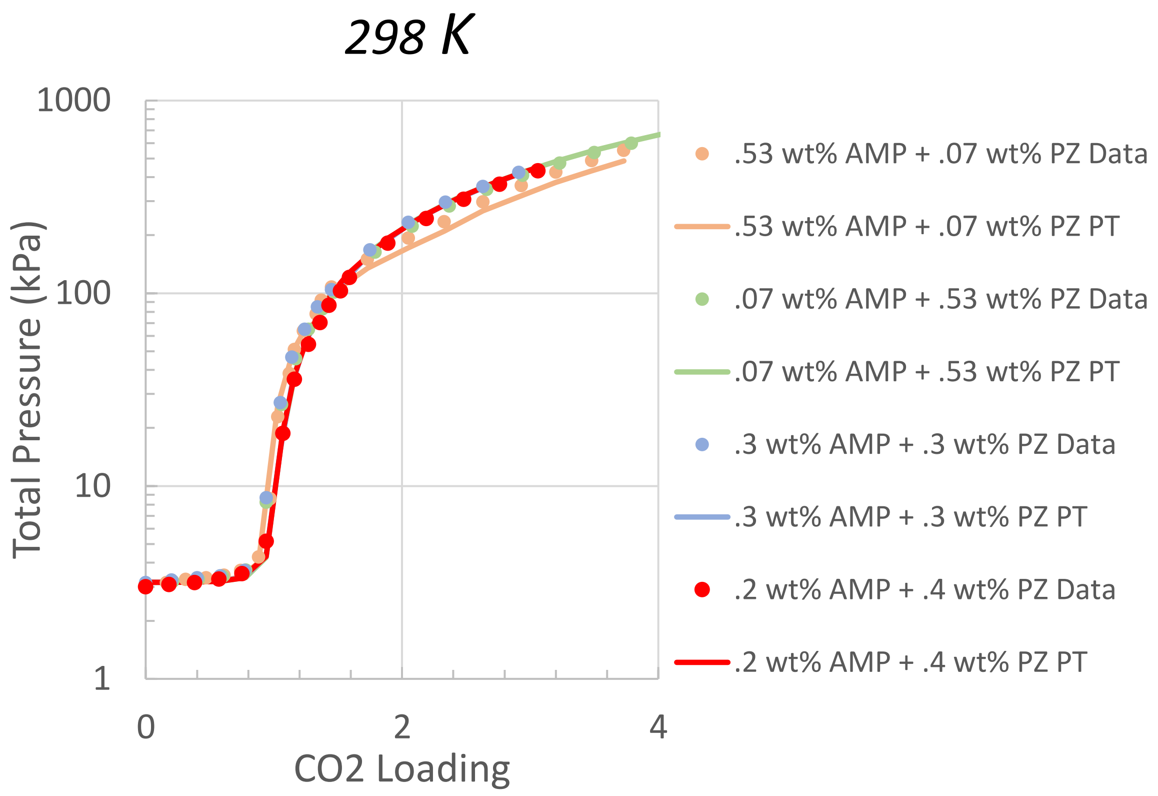
Deshmukh-Mather Fitting: AMP/PZ/Water/CO_2

Fitting

- ~530 data points
- 5 sources
- 293 to 393 K
- Large conc. range
- .035 to 3.79 CO_2 loading
- 2 SCOPE data sets

SCOPE Data (2023)





Relative Error: 10.7%

Conclusions

- Large amount of data processed to create high accuracy ProTreat® CESAR1 model
- Why?
  - High accuracy models needed for CESAR1 evaluation, design, etc.
  - Rate-based models have predictive capabilities
  - Model is currently being used by other SCOPE partners for plant validation, uncertainty quantification
  - Model eventually accessible to public through ProTreat® commercial software
- Upcoming work: Internal plant validation and tuning of model

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