CCSI
Carbon Capture Simulation Initiative

# Uncertainty Quantification of Properties Models: Application to a $CO_2$-Capture System


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# CCSI For Accelerating Technology Development

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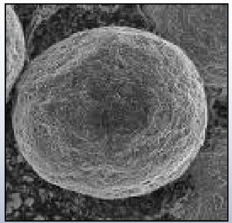
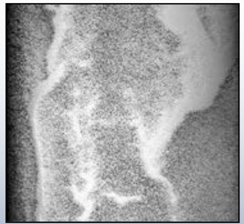
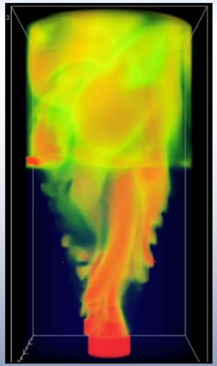


**Identify promising concepts** → **Reduce the time for design & troubleshooting** → **Quantify the technical risk, to enable reaching larger scales, earlier** → **Stabilize the cost during commercial deployment**

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# Outline

- Research Objectives and Motivation
- Overall Methodology
- Results
  - Viscosity model
  - Density model
  - Surface tension model
  - Application to absorber model
- Future Work

# Research Motivation

- Develop robust algorithm for uncertainty quantification of $CO_2$ based carbon capture system
- Starting point: "Gold Standard" MEA model
  - 30% aqueous MEA solution is industry standard
- Deterministic models of system have been considered
  - "Phoenix Model" (Rochelle Group at UT-Austin) used as baseline in this work

# Deterministic and Stochastic Modeling

**Deterministic Modeling**

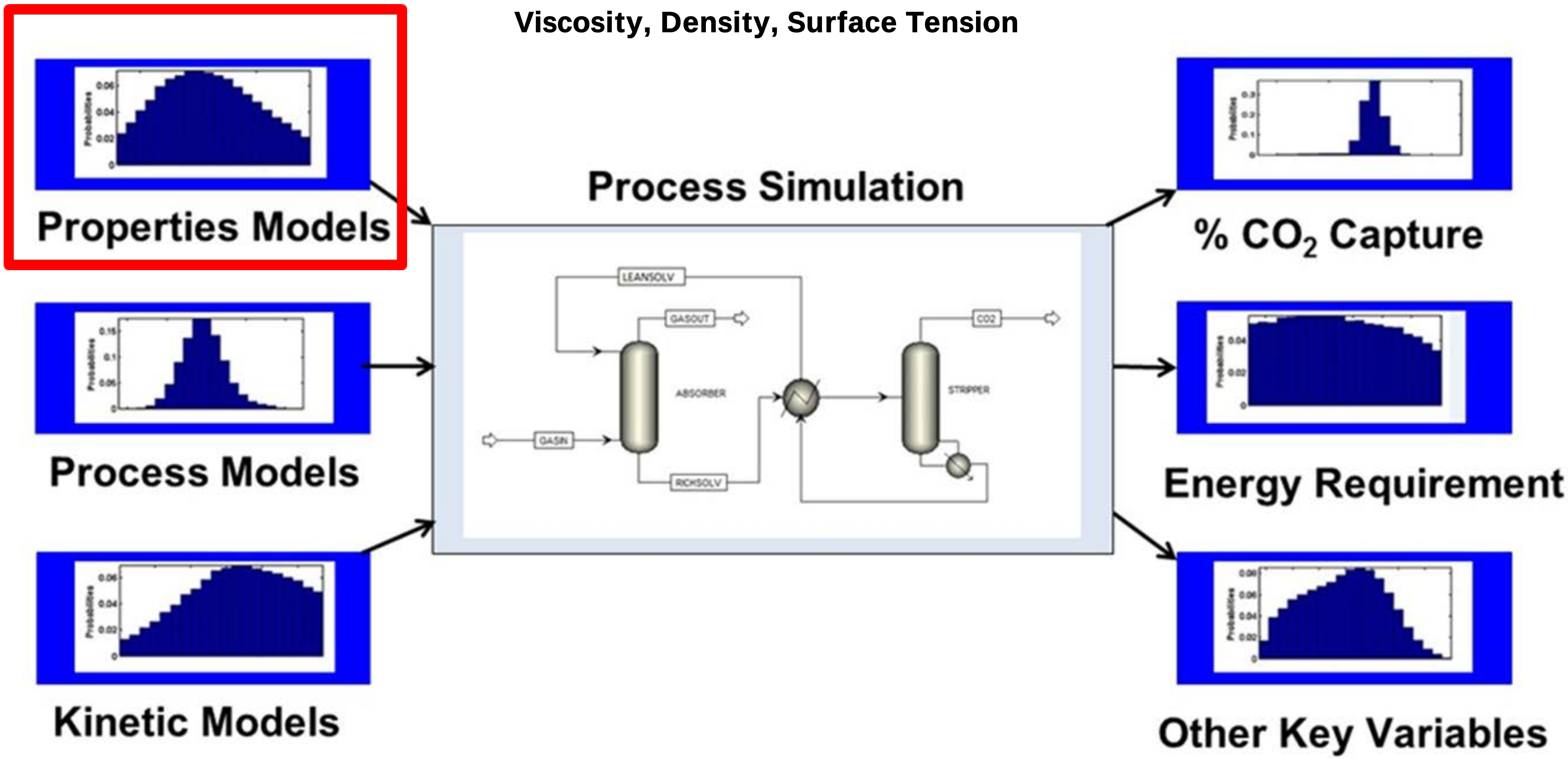
- Single value of
  - Predictor variables
  - Model parameters
  - Output variables
- Parameters calibrated from experiments
  - Best fit methods

**Stochastic Modeling**

- Model inputs and outputs are probability distributions
- Rationale
  - Variability of measurements (input uncertainty)
  - Physical properties
    - Experimental data uncertainty
    - Model uncertainty

# Overall Approach

**Focus of this work:**
**Viscosity, Density, Surface Tension**



# Stochastic Modeling Methodology

Sample from Prior Parameter Distribution
$\boldsymbol{\theta} = \boldsymbol{\theta}_j \quad (j = 1,2, \dots N)$

Predictor Variables (M Observations)
$\boldsymbol{x} = \boldsymbol{x}_i \quad (i = 1,2, \dots, M)$

Mathematical Model ($M \times N$ observations)
$\varphi_{ij} = F(\boldsymbol{x}_i, \boldsymbol{\theta}_j)$
$(i = 1,2, \dots, M; j = 1,2, \dots, N)$

Response Surface Model
$\varphi \sim F^*(\boldsymbol{x}, \boldsymbol{\theta})$

Bayesian Inference
$\pi(\boldsymbol{\theta}|\mathbf{Z}) \propto \mathrm{P}(\boldsymbol{\theta}) L(\boldsymbol{Z}|\boldsymbol{\theta})$

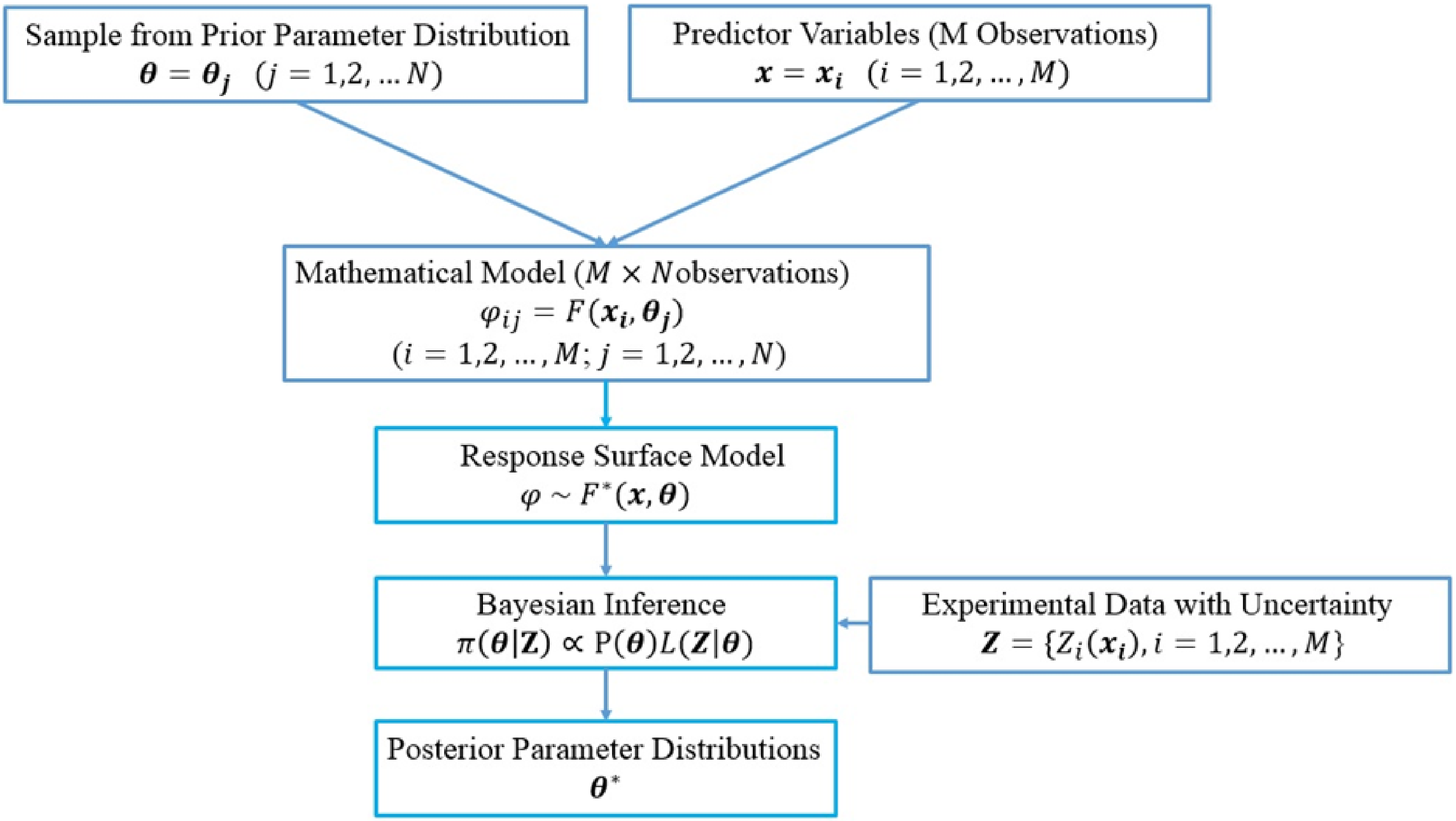
Experimental Data with Uncertainty
$\boldsymbol{Z} = \{Z_i(\boldsymbol{x}_i), i = 1,2, \dots, M\}$

Posterior Parameter Distributions
$\boldsymbol{\theta}^*$

# Response Surface Analysis

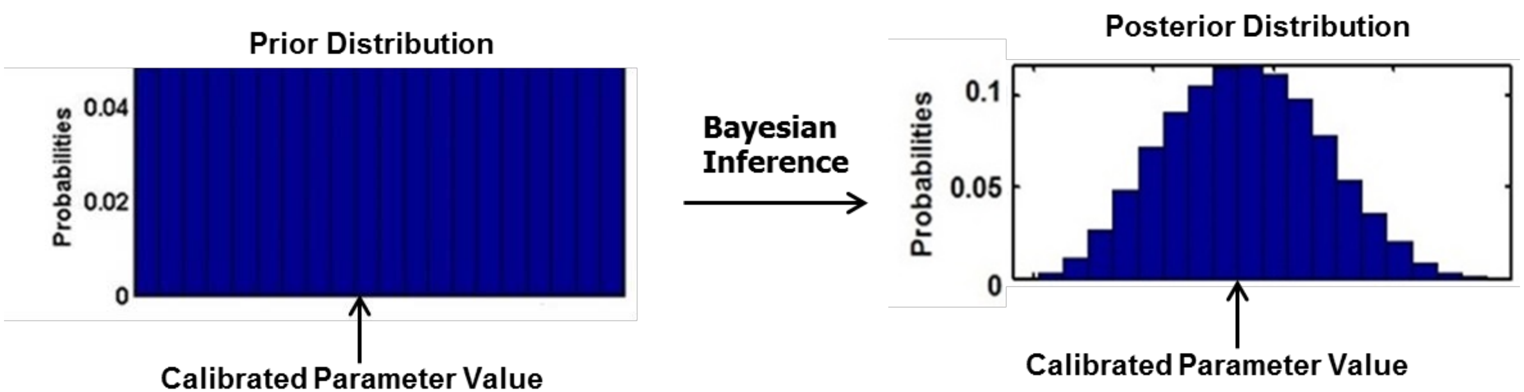
- Computationally inexpensive surrogate models
- Method
  – Multivariate Adaptive Regression Splines (MARS)
- Procedure
  – Generate input sample
  – Collect output from model simulation
  – Select a response surface scheme and perform fitting
  – Validate the response surface

# Stochastic Modeling Methodology



# Bayesian Inference

- Bayesian inference seeks to update prior beliefs of parameter uncertainties in view of data
  - Idea: scan intelligently the prior parameter uncertainty space to identify values that match well with available data
  - Algorithm: Markov Chain Monte Carlo (MCMC) method using Gibbs sampling



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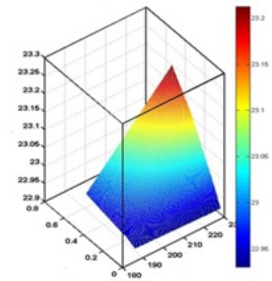
$\pi(\boldsymbol{\theta}|\mathbf{Z}) \propto \mathrm{P}(\boldsymbol{\theta})L(\boldsymbol{Z}|\boldsymbol{\theta})$

**Experimental Data with Uncertainty**
$\boldsymbol{Z} = \{Z_i(\boldsymbol{x}_i), i = 1,2, \ldots, M\}$

**Posterior Parameter Distributions**
$\boldsymbol{\theta}^*$

# Down-selection by Parameter Screening

Response Surface Methodology



Sensitivity Matrix Methodology

$$S_{ij} = max\left|\frac{\partial}{\partial \hat{y}_i}\left(\frac{\partial \varphi}{\partial x_j}\right)\right| \qquad y_i = \bar{y}_i \hat{y}_i$$

$\varphi$: physical property of interest
$x_j$: variable
$y_i$: actual parameter
$\bar{y}_i$: baseline parameter value
$\hat{y}_i$: parameter deviation term

Subject to: $T^L \le T \le T^U$ $\quad {X_{MEA}}^{\mathrm{L}} \le X_{MEA} \le {X_{MEA}}^{\mathrm{U}}$ $\quad \alpha^{\mathrm{L}} \le \alpha \le \alpha^{\mathrm{U}}$ $\quad {\hat{y}_i}^{L} \le \hat{y}_i \le {\hat{y}_i}^{U}$

Normalized version $\quad N_{ij} = \dfrac{S_{ij}}{\max\limits_{i\epsilon[1,n],j\epsilon[1,m]} S_{ij}}$

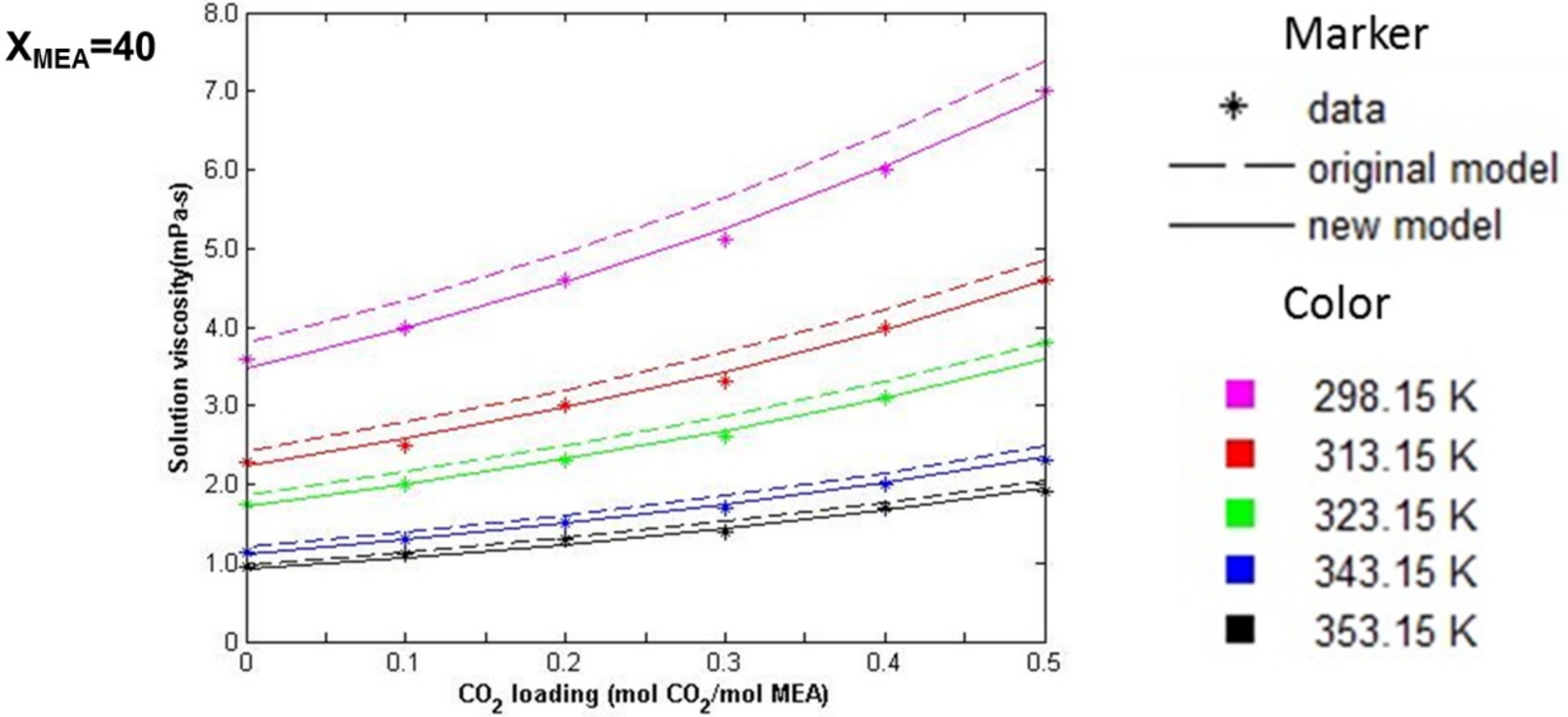
# Viscosity Model

$$\mu_{sln} = \mu_{H_2O}(T)\, exp\left(\frac{((aX_{MEA} + b)T + cX_{MEA} + d)(\alpha(eX_{MEA} + fT + g) + 1)X_{MEA}}{T^2}\right)$$

| Parameter | Given Value[1] | Calibrated Value |
|---|---|---|
| a | 0 | -0.0838 |
| b | 0 | 2.8817 |
| c | 21.186 | 33.651 |
| d | 2373 | 1817 |
| e | 0.01015 | 0.00847 |
| f | 0.0093 | 0.0103 |
| g | -2.2589 | -2.3890 |

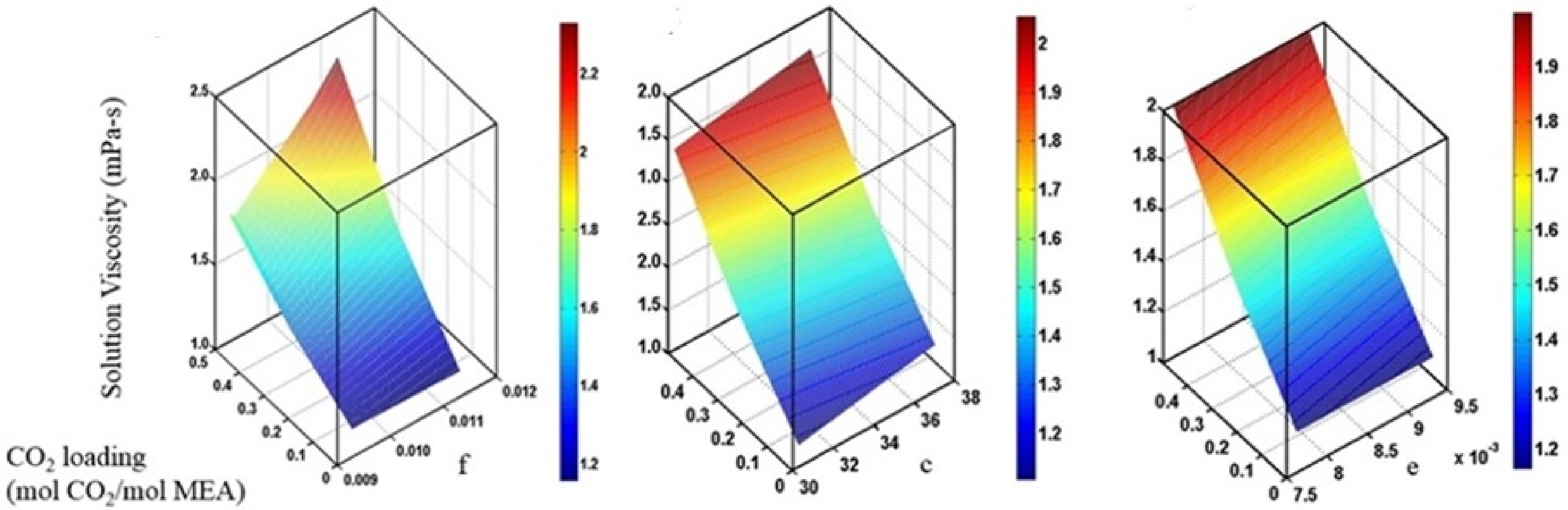
1. Weiland et al., Journal of Chemical & Engineering Data 1998, 43, 378-382.

# Viscosity Model/Data Comparison




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

# Viscosity Model-Sensitivity Analysis




$$N_{f\alpha} = 1 \qquad N_{c\alpha} = 0.2176 \qquad N_{e\alpha} = 0.0827$$

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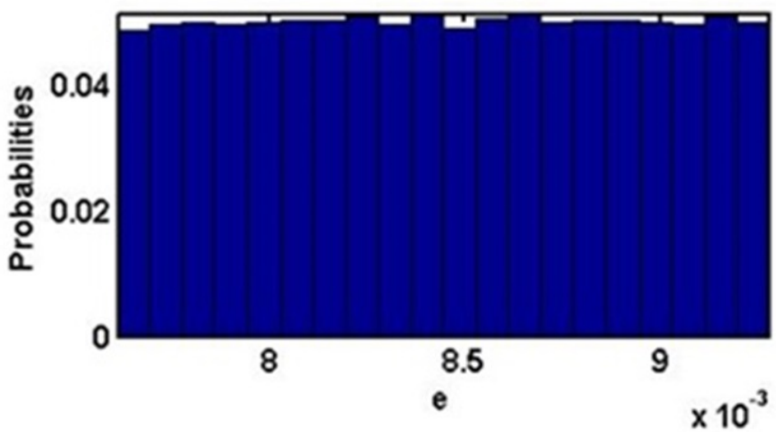
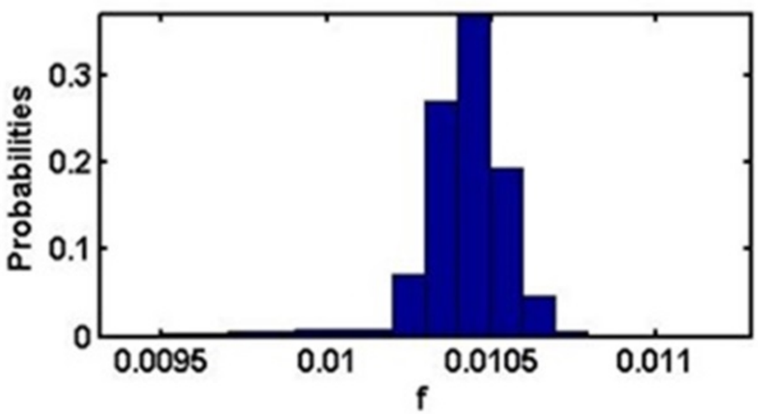
# Viscosity Model-Sample Posterior Distributions from Bayesian Inference




$N_{e\alpha} = 0.0827$




$N_{f\alpha} = 1$

$$\mu_{sln} = \mu_{H_2O}(T)\, exp\left(\frac{((aX_{MEA} + b)T + cX_{MEA} + d)(\alpha(eX_{MEA} + fT + g) + 1)X_{MEA}}{T^2}\right)$$

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# Density Model[1]

- Three sources of data available for parameter calibration

$$\rho_{sln} = \frac{MW_{sln}}{X_{MEA}V_{MEA} + X_{H_2O}V_{H_2O} + X_{CO_2}V_{CO_2} + X_{MEA}X_{H_2O}V^{*} + X_{MEA}X_{CO_2}V^{**}}$$

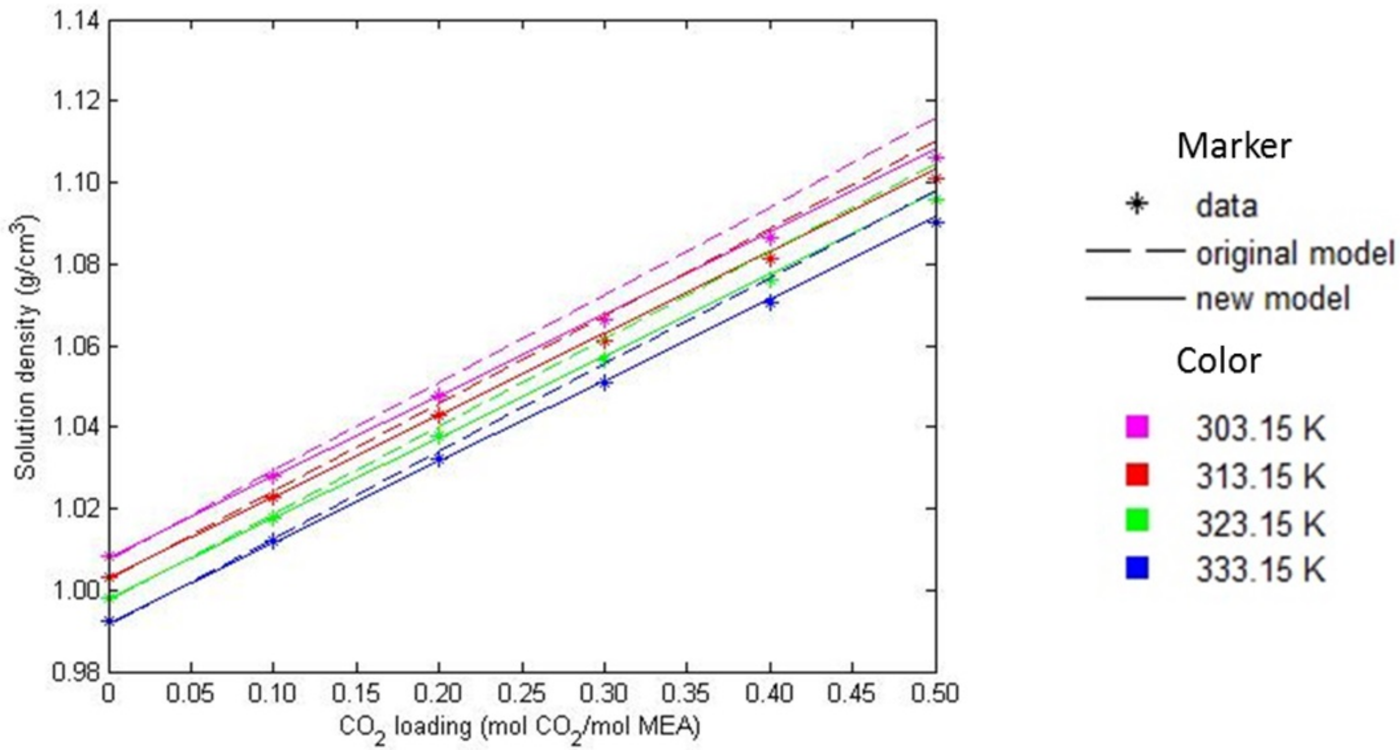
- Modified molecular weight calculation
- Five uncertain parameters
  - $V_{CO_2} = a$
  - $V^{*} = b + cX_{MEA}$
  - $V^{**} = d + eX_{MEA}$

| Baseline Parameter Values | |
|---|---|
| a | 10.2074 |
| b | -2.2642 |
| c | 3.0059 |
| d | 207 |
| e | -563.3701 |

1 Weiland et al., Journal of Chemical & Engineering Data 1998, 43, 378-382

# Density Model/Data Comparison

**r=0.3**




**Data points from Jayarathna et al., Journal of Chemical & Engineering Data, 2013 58, 986-992**

# Surface Tension Model-Original Form[1]

- $\sigma_{mix} = \sigma_{H_2O} + \sum_{i=CO_2,MEA}\left(1 + \frac{b_i x_i}{(1-a_i)(1+\sum_{j=CO_2,MEA}\frac{a_j}{(1-a_j)}x_j)}\right)(x_i(\sigma_i - \sigma_{H_2O}))$
- Function of temperature and composition
- Parameters $a_i$ and $b_i$ regressed individually for data sets with a given value of MEA weight fraction
- Cannot be used to represent solvents over a range of temperature and composition

1. Jayarathna et al., Journal of Chemical & Engineering Data, 2013 58, 986-992

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# New Surface Tension Model

$$\sigma_{mix} = \sigma_{mix}(T, \alpha, r)$$

$$\sigma_{mix} = \sigma_{H_2O} + \left(\sigma_{CO_2} - \sigma_{H_2O}\right) f(r, \alpha) X_{CO_2} + \left(\sigma_{MEA} - \sigma_{H_2O}\right) g(r, \alpha)\ X_{MEA}$$

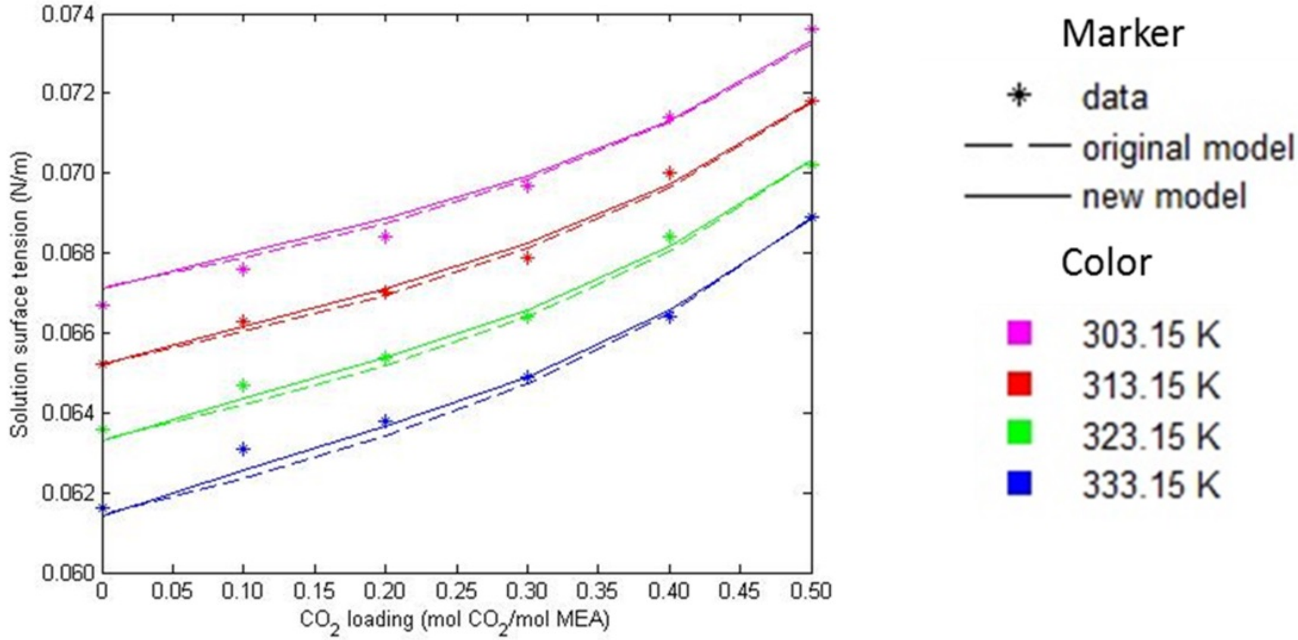
$$f(r, \alpha) = a + b\alpha + c\alpha^2 + dr + er^2$$

$$g(r, \alpha) = f + g\alpha + h\alpha^2 + ir + jr^2$$

| Parameter | Value | Parameter | Value |
|---|---|---|---|
| a | 2.4558 | f | 2.3122 |
| b | -1.5311 | g | 4.5608 |
| c | 3.4994 | h | -2.3924 |
| d | -5.6398 | i | 5.3324 |
| e | 10.2109 | j | -12.0494 |

# Surface Tension Model/Data Comparison

**r=0.2**




**Data points from Jayarathna et al., Journal of Chemical & Engineering Data, 2013 58, 986-992**

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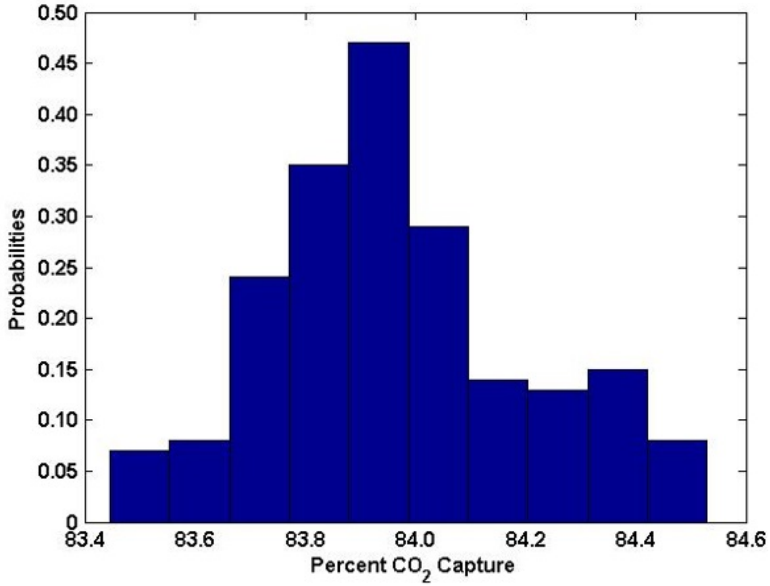
# Case Study: Application of Parametric Uncertainty to Absorber Model

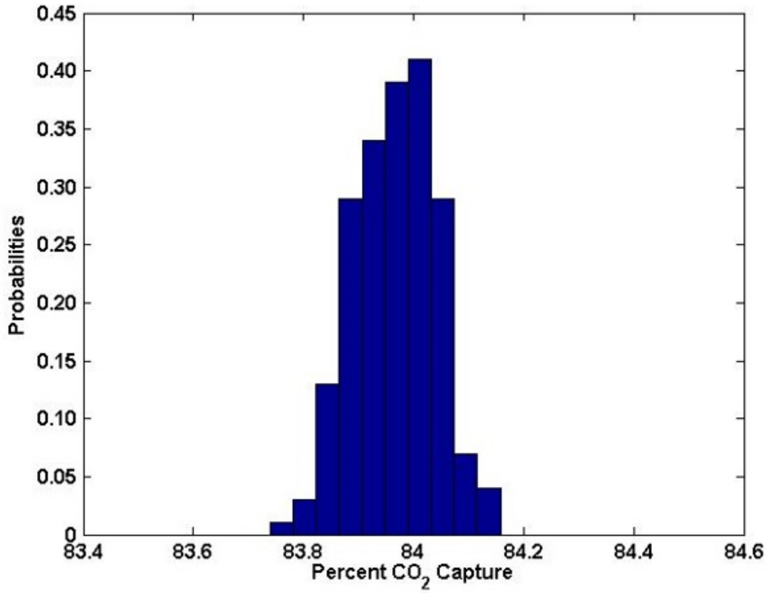
- Considered stochastic absorber model (Phoenix model) for two cases
  - Prior distributions (±10% of deterministic value) for all parameters not eliminated by sensitivity matrix methodology
  - Posterior distributions of all parameters not eliminated by sensitivity matrix methodology or Bayesian inference output
- Key input variables for absorber simulation
  - Inlet lean solvent mass flowrate: 3000 kg/hr
  - L/G mass ratio: 4.42
  - Lean solvent concentration: 35.4 wt% MEA; 0.35 mol $CO_2$/mol MEA
- Effect of parametric uncertainty on percent $CO_2$ capture observed

# Case Study Results

Prior Distribution Case




Posterior Distribution Case




Sample size is 200 simulations

# Future Work

- Complete physical property models uncertainty quantification
  - e-NRTL thermodynamic framework: VLE, heat capacity, heat of absorption
  - Diffusivity
- Propagate all stochastic models (e.g. physical properties, kinetics, mass transfer and hydraulics) through process simulation
- Validation of overall stochastic model with process data
  - Steady state data from UT Austin pilot plant
  - Steady state and dynamic data from NCCC

# Thank you!

## Acknowledgements

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