Uncertainty Quantification of Properties Models: Application to a CO$_2$-Capture System

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Atlanta, GA
CCSI For Accelerating Technology Development

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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PRINCETON UNIVERSITY
West Virginia University
BOSTON UNIVERSITY

Industry

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FLUOR SOUTHERN COMPANY AEP AMERICAN ELECTRIC POWER
EXXONMOBIL EASTMAN ANSYS
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CCSI™ Carbon Capture Simulation Initiative
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
\[ \mathbf{\theta} = \mathbf{\theta}_j \ (j = 1, 2, \ldots, N) \]

Predictor Variables (M Observations)
\[ \mathbf{x} = \mathbf{x}_i \ (i = 1, 2, \ldots, M) \]

Mathematical Model (\( M \times N \) observations)
\[ \varphi_{ij} = F(\mathbf{x}_i, \mathbf{\theta}_j) \]
\( (i = 1, 2, \ldots, M; j = 1, 2, \ldots, N) \)

Response Surface Model
\[ \varphi \sim F^*(\mathbf{x}, \mathbf{\theta}) \]

Bayesian Inference
\[ \pi(\mathbf{\theta}|\mathbf{Z}) \propto P(\mathbf{\theta})L(\mathbf{Z}|\mathbf{\theta}) \]

Experimental Data with Uncertainty
\[ \mathbf{Z} = \{ Z_i(\mathbf{x}_i), i = 1, 2, \ldots, M \} \]

Posterior Parameter Distributions
\[ \mathbf{\theta}^* \]
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

Sample from Prior Parameter Distribution
\( \theta = \theta_j \) \((j = 1,2, ..., N)\)

Predictor Variables (M Observations)
\( x = x_i \) \((i = 1,2, ..., M)\)

Mathematical Model \((M \times N\) observations\)
\[ \varphi_{ij} = F(x_i, \theta_j) \]
\((i = 1,2, ..., M; j = 1,2, ..., N)\)

Response Surface Model
\[ \varphi \sim F^*(x, \theta) \]

Bayesian Inference
\[ \pi(\theta | Z) \propto P(\theta) L(Z | \theta) \]

Experimental Data with Uncertainty
\[ Z = \{Z_i(x_i), i = 1,2, ..., M\} \]

Posterior Parameter Distributions
\( \theta^* \)
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
Stochastic Modeling Methodology

Sample from Prior Parameter Distribution
\[ \theta = \theta_j \quad (j = 1,2, \ldots, N) \]

Predictor Variables (M Observations)
\[ x = x_i \quad (i = 1,2, \ldots, M) \]

Mathematical Model \((M \times N\) observations\)
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Response Surface Model
\[ \varphi \sim F^*(x, \theta) \]

Bayesian Inference
\[ \pi(\theta | Z) \propto P(\theta)L(Z | \theta) \]

Posterior Parameter Distributions
\[ \theta^* \]

Experimental Data with Uncertainty
\[ Z = \{Z_i(x_i), i = 1,2, \ldots, M\} \]
Down-selection by Parameter Screening

Response Surface Methodology

Sensitivity Matrix Methodology

\[ S_{ij} = \max \left| \frac{\partial}{\partial \hat{y}_i} \left( \frac{\partial \varphi}{\partial x_j} \right) \right| \]

\[ y_i = \bar{y}_i \hat{y}_i \]

\( \varphi \): 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: \( T^L \leq T \leq T^U \) \( X_{MEA}^L \leq X_{MEA} \leq X_{MEA}^U \) \( \alpha^L \leq \alpha \leq \alpha^U \) \( \hat{y}_i^L \leq \hat{y}_i \leq \hat{y}_i^U \)

Normalized version

\[ N_{ij} = \frac{S_{ij}}{\max_{i \in [1,n], j \in [1,m]} S_{ij}} \]
Viscosity Model

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

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<th>Parameter</th>
<th>Given Value(^1)</th>
<th>Calibrated Value</th>
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Viscosity Model/Data Comparison

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

\[ N_{fa} = 1 \]
\[ N_{ca} = 0.2176 \]
\[ N_{ea} = 0.0827 \]
Viscosity Model-Sample Posterior Distributions from Bayesian Inference

\[ N_{e\alpha} = 0.0827 \]

\[ N_{f\alpha} = 1 \]

\[ \mu_{sln} = \mu_{H_2O}(T) \exp \left( \frac{(aX_{MEA} + b)T + cX_{MEA} + d)(\alpha(eX_{MEA} + fT + g) + 1)X_{MEA}}{T^2} \right) \]
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
  
  - \( V_{CO_2} = a \)
  
  - \( V^* = b + cX_{MEA} \)
  
  - \( V^{**} = d + eX_{MEA} \)

<table>
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<th>Baseline Parameter Values</th>
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\(^1\) Weiland et al., Journal of Chemical & Engineering Data 1998, 43, 378-382
Density Model/Data Comparison

$r=0.3$

Data points from Jayaratna et al., Journal of Chemical & Engineering Data, 2013 58, 986-992
Surface Tension Model-Original Form\(^1\)

\[
\sigma_{\text{mix}} = \sigma_{\text{H}_2\text{O}} + \sum_{i=\text{CO}_2,\text{MEA}} \left(1 + \frac{b_i x_i}{(1-a_i)(1+\sum_{j=\text{CO}_2,\text{MEA}} a_j x_j)}\right) (x_i (\sigma_i - \sigma_{\text{H}_2\text{O}}))
\]

- 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
New Surface Tension Model

\[ \sigma_{\text{mix}} = \sigma_{\text{mix}}(T, \alpha, r) \]

\[ \sigma_{\text{mix}} = \sigma_{\text{H}_2\text{O}} + (\sigma_{\text{CO}_2} - \sigma_{\text{H}_2\text{O}})f(r, \alpha)X_{\text{CO}_2} + (\sigma_{\text{MEA}} - \sigma_{\text{H}_2\text{O}})g(r, \alpha)X_{\text{MEA}} \]

\[ f(r, \alpha) = a + b\alpha + c\alpha^2 + dr + erf^2 \]

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

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Surface Tension Model/Data Comparison

$r=0.2$

Data points from Jayarathna et al., Journal of Chemical & Engineering Data, 2013 58, 986-992
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 CO₂/mol MEA

• Effect of parametric uncertainty on percent CO₂ 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!

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