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Carbon Capture Simulation Initiative

Uncertainty Quantification of Properties Models for an MEA System

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WestVirginiaUniversity

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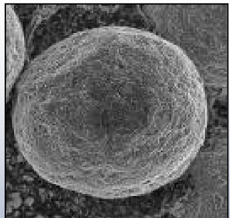
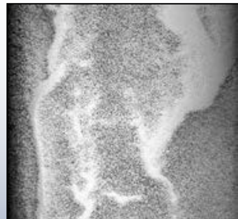
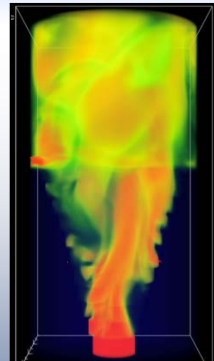





Identify promising concepts → **Reduce the time for design & troubleshooting** → **Quantify the technical risk, to enable reaching larger scales, earlier** → **Stabilize the cost during commercial deployment**

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
- Institute for Clean and Secure Energy, The University of Utah

Industry

- ADA Environmental Solutions
- ALSTOM
- B&W the babcock&wilcox company
- GE
- EPRI Electric Power Research Institute
- Fluor
- Southern Company
- Phillips 66
- AEP American Electric Power
- Southern California Edison, An Edison International Company, San Onofre Nuclear Generating Station
- Chevron
- ExxonMobil
- URS
- Air Products
- Eastman
- ANSYS
- aspentech
- invensys
- PSE

Presentation Outline

- Research Objectives and Motivation
- Physical Property Model Development
  - Model choice
  - Deterministic modeling
  - Parameter screening
  - Stochastic modeling
- Results
  - Viscosity Model
  - Density Model
  - Surface Tension Model

Research Objectives

- Development of an algorithm for determining physical property models for solvent-based carbon capture with uncertainty quantification (UQ) capability
  – Consider monoethanolamine (MEA) as baseline solvent
  – Use Phoenix Model (University of Texas-Austin) as a starting point
- Validation of models with plant scale data

Model Development Overview

- Identify models that give physical properties as functions of solution conditions (e.g. temperature and composition)
- Deterministic modeling: Calibrate model parameters to fit available experimental data (best fit optimization)
- Parameter screening: Surface response analysis and sensitivity analysis
- Stochastic modeling: Use Bayesian inference to represent model parameters as probability distribution functions

Model Identification

- Use Phoenix model developed by Dr. Rochelle's group at UT Austin as starting point for model choice
- Started with simple/independent properties (viscosity, density, surface tension)
  - Necessary for design and evaluation of separation equipment (e.g. flooding and mass transfer correlations)
- Solution physical properties given as functions of temperature and composition only
  - Composition represented by two independent variables (generally CO_2 loading and MEA weight fraction/percent)

Solution Chemistry

- Represented as ternary MEA-H_2O-CO_2 system in available models and process data
- Simplified electrolytic speciation:

$$2MEA + CO_2 \leftrightarrow MEA^{+} + MEACOO^{-}$$

$$MEA + CO_2 + H_2O \leftrightarrow MEA^{+} + HCO_3{}^{-}$$

  – Does not consider presence of other ions (H^+,OH^-,CO_3^{2-}) found to be in negligible concentration
- Electrolyte presence generates complexity in properties modeling (highly non-ideal solution)

Deterministic Modeling

- Function inputs (variables/parameters) and outputs are represented as single values
- General procedure
  - Gather as much relevant data as possible
  - Optimize model parameters to minimize sum of square error (SSE) between data values and model predictions

Parameter Screening

- Determine parameters to which the model is most sensitive
  - UQ necessary for parameters of high sensitivity
  - Parameters of low sensitivity may be eliminated from UQ analysis not only to avoid unnecessary computation, but also for computational tractability
- Response surface method: qualitative parameter screening
- Sensitivity calculation method: quantitative parameter screening

Response Surfaces

- Multivariate Adaptive Regression Splines (MARS) regression technique
  - Reduces mathematical model into non-parametric form that maintains capability of describing relationships between input and output variables
- Computationally inexpensive
- Generated using PSUADE software developed by LLNL
  - Input: Uniform distribution of model variables and parameter and associated output
  - Output: Response surface
- Parameter sensitivity determined by response surface shape

Sensitivity matrix calculation

- For generic physical property:

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

$$y_i = \bar{y}_i \hat{y}_i$$

φ: 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

$$\hat{y}_i{}^L \leq \hat{y}_i \leq \hat{y}_i{}^U \qquad T^L \leq T \leq T^U \quad \alpha^{\mathrm{L}} \leq \alpha \leq \alpha^{\mathrm{U}} \quad X_{MEA}{}^{\mathrm{L}} \leq X_{MEA} \leq X_{MEA}{}^{\mathrm{U}}$$

- Normalized version

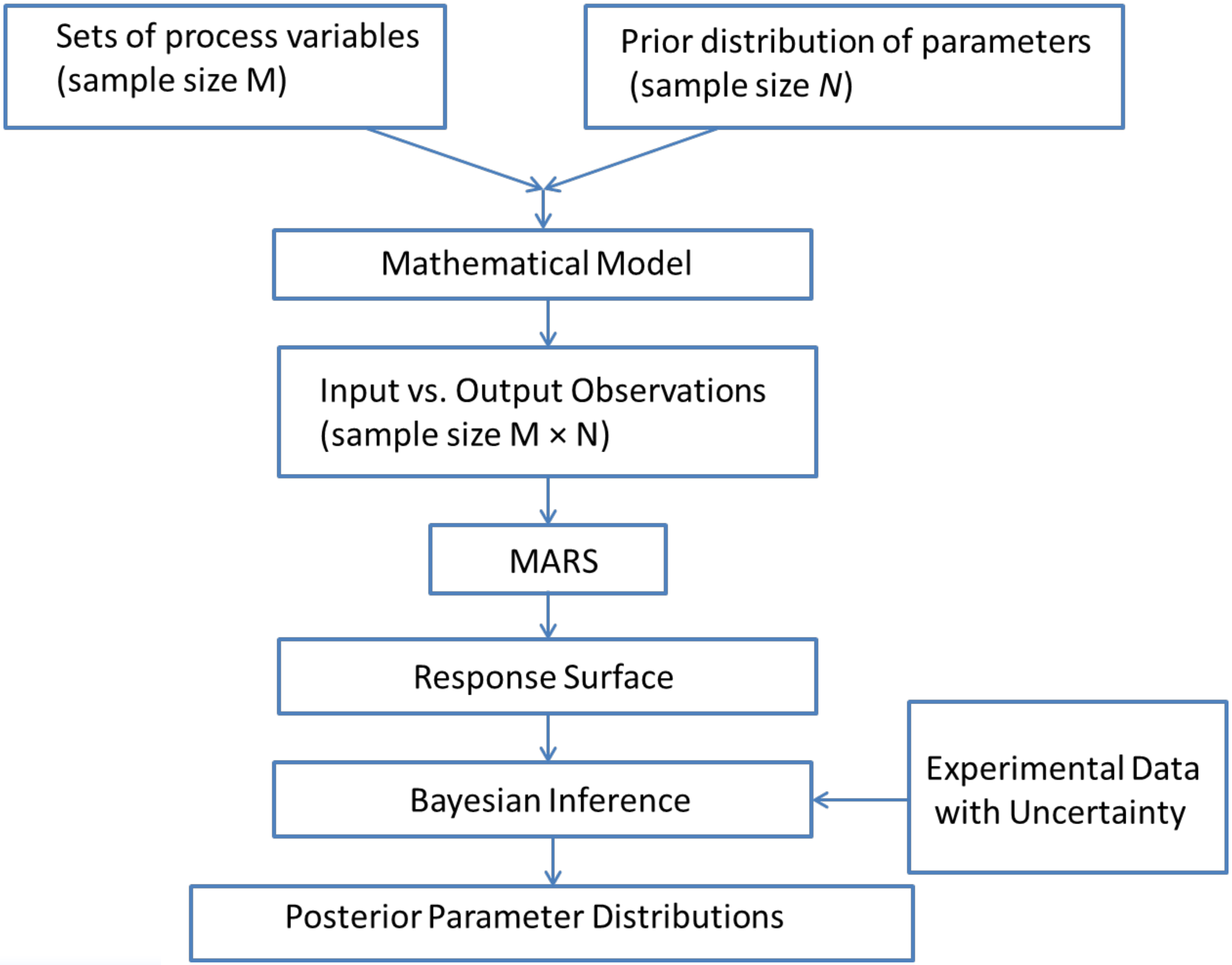
$$N_{ij} = \frac{S_{ij}}{\max_{i\epsilon[1,n],j\epsilon[1,m]} S_{ij}}$$

- Parameter sensitivity determined by value of N_{ij}
- Method may be more convenient than visualizing surface responses

Stochastic Modeling

- Function inputs and outputs are represented as PDFs
- Sources of uncertainty
  - Process variable measurements (input uncertainty)
  - Physical property measurements (output uncertainty)
  - Functional form of physical property models (model uncertainty)
- Bayesian inference may be used to quantify parametric uncertainty
  - Prior distributions of parameters are updated as additional information is acquired (sampling of experimental data)
  - Markov Chain Monte Carlo (MCMC) method using Gibbs sampling

Bayesian Inference



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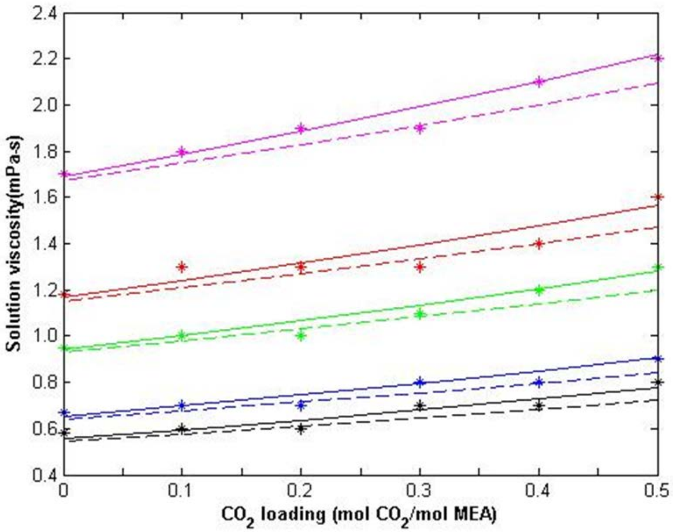
Viscosity Model

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

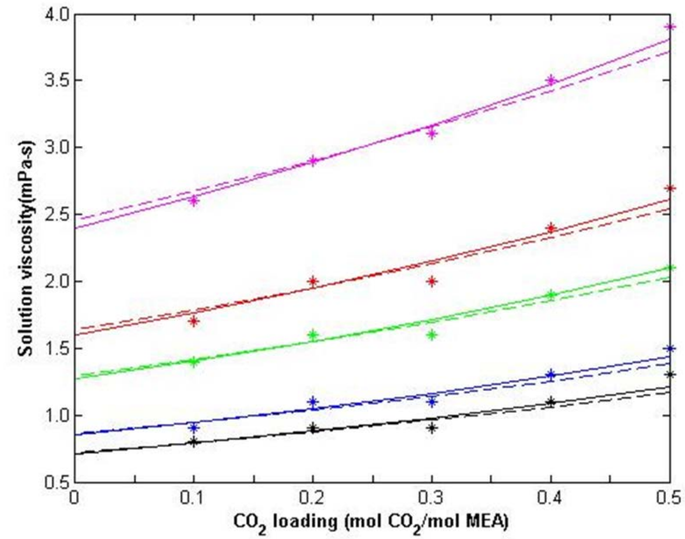
Parameter	Given Value	Calibrated Value
a	0	-0.0838
b	0	2.8817
c	21.186	33.651
d	2373	1817
e	0.01015	0.00847
f	0.0093	0.0103
g	-2.2589	-2.3890

Viscosity Model/Data Comparison

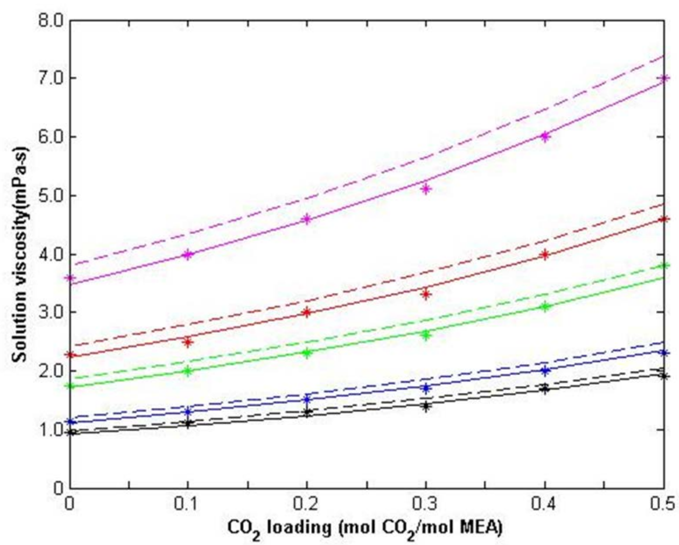
X_{MEA}=20

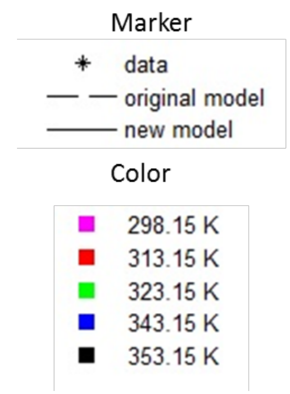


X_{MEA}=30



X_{MEA}=40

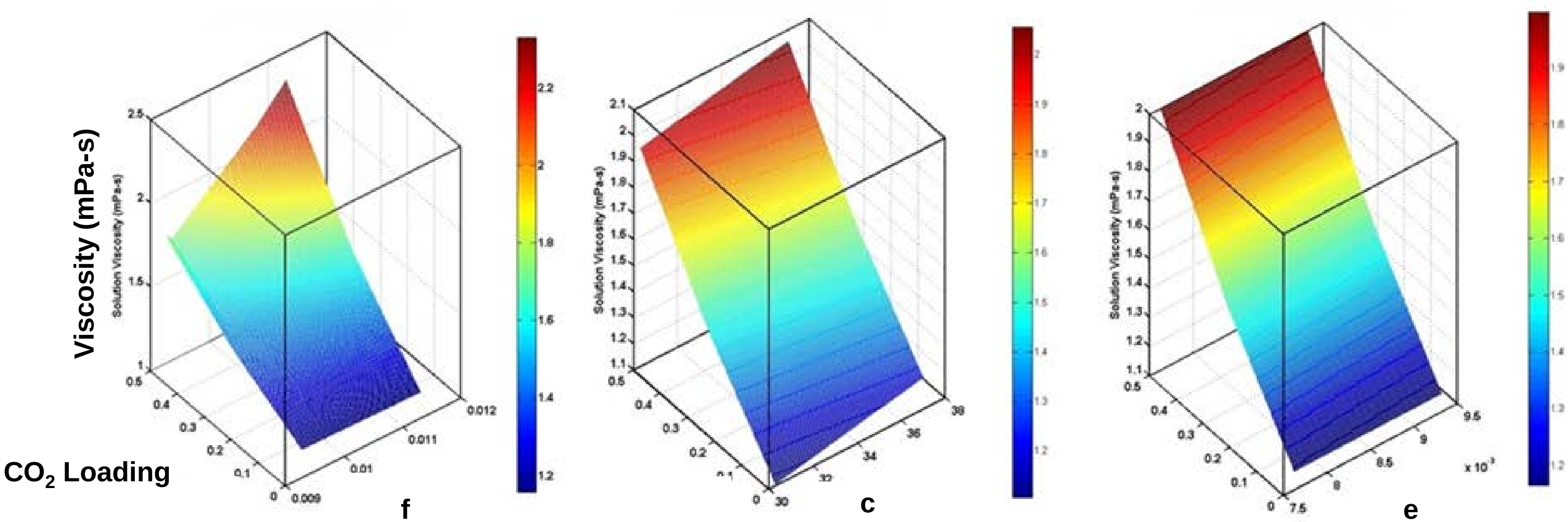




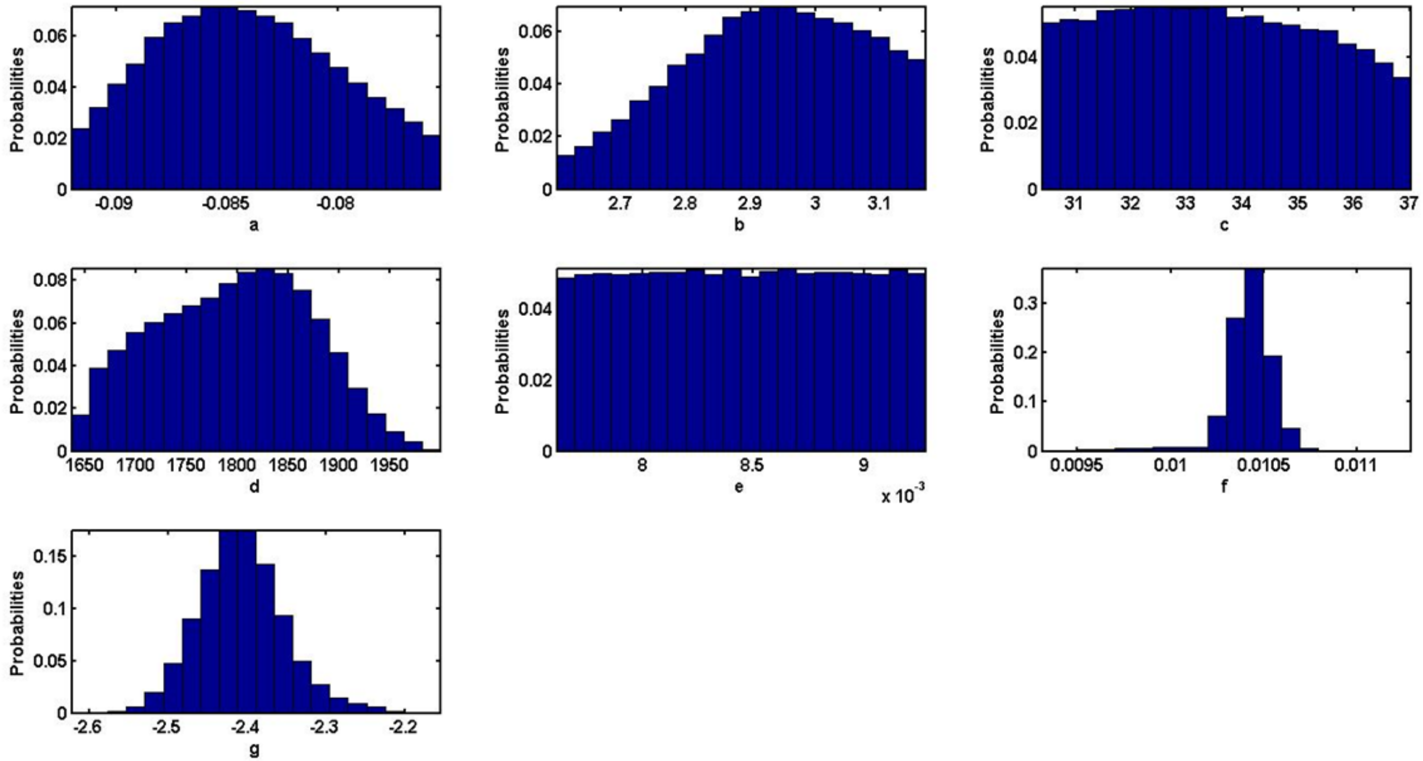
Viscosity Model-Sensitivity Analysis

- $$N = max\begin{bmatrix} \left|\frac{\partial}{\partial \hat{a}}\left(\frac{\partial \mu}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{a}}\left(\frac{\partial \mu}{\partial X_{MEA}}\right)\right| & \left|\frac{\partial}{\partial \hat{a}}\left(\frac{\partial \mu}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{b}}\left(\frac{\partial \mu}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{b}}\left(\frac{\partial \mu}{\partial X_{MEA}}\right)\right| & \left|\frac{\partial}{\partial \hat{b}}\left(\frac{\partial \mu}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{c}}\left(\frac{\partial \mu}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{c}}\left(\frac{\partial \mu}{\partial X_{MEA}}\right)\right| & \left|\frac{\partial}{\partial \hat{c}}\left(\frac{\partial \mu}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{d}}\left(\frac{\partial \mu}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{d}}\left(\frac{\partial \mu}{\partial X_{MEA}}\right)\right| & \left|\frac{\partial}{\partial \hat{d}}\left(\frac{\partial \mu}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{e}}\left(\frac{\partial \mu}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{e}}\left(\frac{\partial \mu}{\partial X_{MEA}}\right)\right| & \left|\frac{\partial}{\partial \hat{e}}\left(\frac{\partial \mu}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{f}}\left(\frac{\partial \mu}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{f}}\left(\frac{\partial \mu}{\partial X_{MEA}}\right)\right| & \left|\frac{\partial}{\partial \hat{f}}\left(\frac{\partial \mu}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{g}}\left(\frac{\partial \mu}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{g}}\left(\frac{\partial \mu}{\partial X_{MEA}}\right)\right| & \left|\frac{\partial}{\partial \hat{g}}\left(\frac{\partial \mu}{\partial \alpha}\right)\right| \end{bmatrix} = \begin{bmatrix} 0.0022 & 0.0089 & 0.1566 \\ 0.0019 & 0.0058 & 0.1329 \\ 0.0034 & 0.0123 & 0.2176 \\ 0.0048 & 0.0134 & 0.3063 \\ 0.0009 & 0.0028 & 0.0827 \\ 0.0090 & 0.0254 & 1.0000 \\ 0.0074 & 0.0186 & 0.7246 \end{bmatrix}$$

Viscosity Model-Surface Response Analysis



Viscosity Model-Posterior Distributions from Bayesian Inference



Density Model

- Three sources of data available for parameter calibration

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

- Solution molecular weight calculation takes electrolyte speciation into account in new model
- 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**

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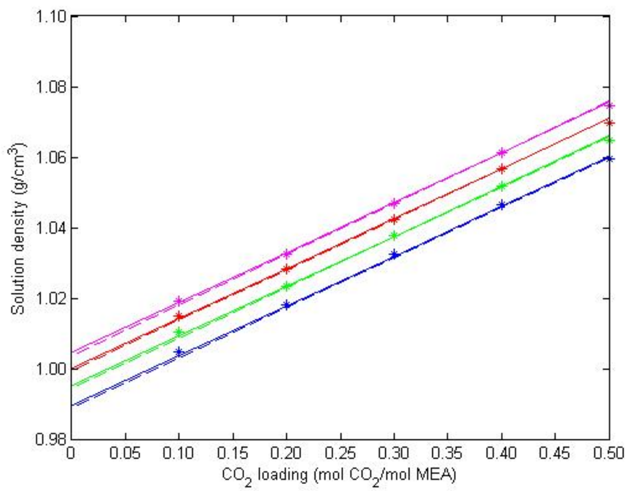
U.S. Department of Energy

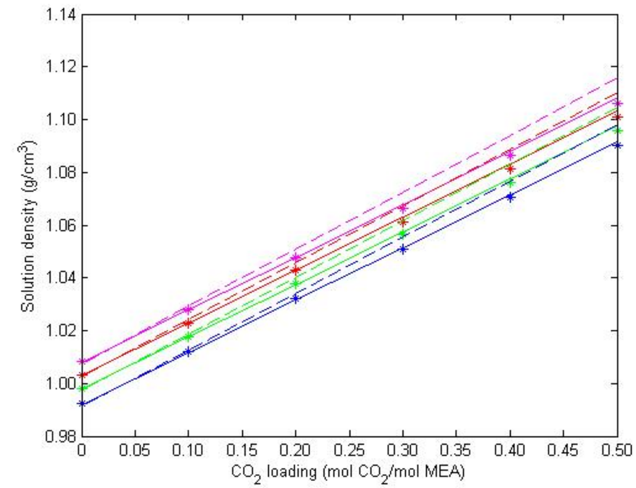
Density Model/Data Comparison

- Results shown for one data source only

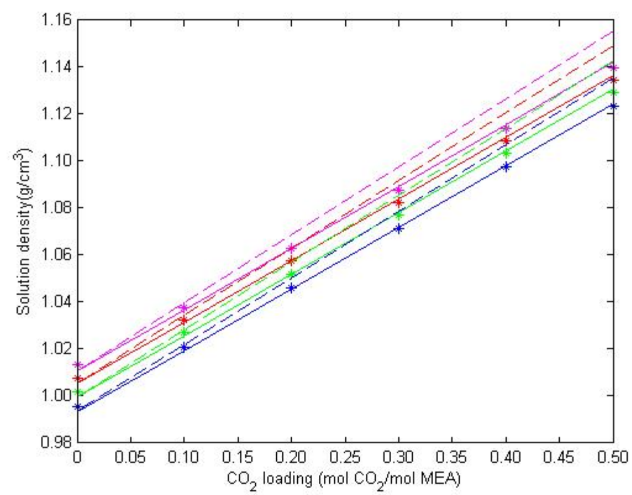
r=0.2

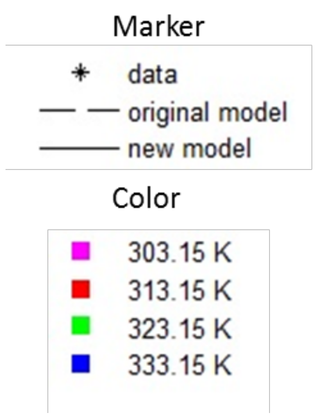


r=0.3



r=0.4

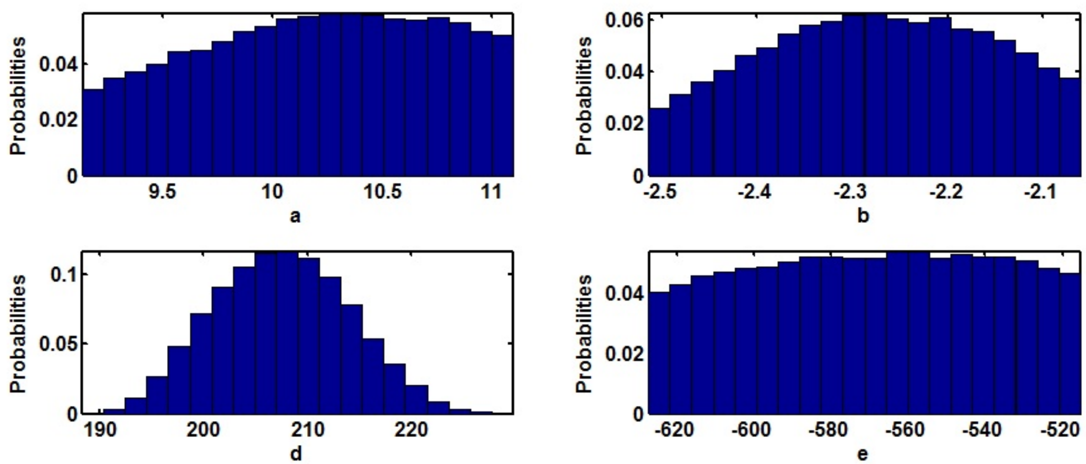




Density Model-Sensitivity Analysis

- $$N = \begin{bmatrix} \left|\frac{\partial}{\partial \hat{a}}\left(\frac{\partial V}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{a}}\left(\frac{\partial V}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{a}}\left(\frac{\partial V}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{b}}\left(\frac{\partial V}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{b}}\left(\frac{\partial V}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{b}}\left(\frac{\partial V}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{c}}\left(\frac{\partial V}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{c}}\left(\frac{\partial V}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{c}}\left(\frac{\partial V}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{d}}\left(\frac{\partial V}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{d}}\left(\frac{\partial V}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{d}}\left(\frac{\partial V}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{e}}\left(\frac{\partial V}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{e}}\left(\frac{\partial V}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{e}}\left(\frac{\partial V}{\partial \alpha}\right)\right| \end{bmatrix} = \begin{bmatrix} 0 & 0.1624 & 0.1092 \\ 0 & 0.0566 & 0.0067 \\ 0 & 0.0277 & 0.0022 \\ 0 & 1.000 & 0.3639 \\ 0 & 0.6199 & 0.1628 \end{bmatrix}$$

Density Model-Posterior Distributions from Bayesian Inference



Surface Tension Model-Original Form

- $\sigma_{mix} = \sigma_{H_2O} + \sum_{i=CO_2,MEA}\left(1 + \frac{b_i x_i}{(1-a_i)(1+\sum_{j=CO_2,MEA}\frac{a_j}{(1-a_j)}x_j)}\right)(x_i(\sigma_i - \sigma_{H_2O}))$

- Parameters a_i and b_i regressed individually for data sets with given value of MEA weight fraction
- Cannot be used to represent solvents over a range of temperature and composition

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New Surface Tension Model

- Continuous function of temperature, CO_2 loading(α), and MEA weight fraction (r) on CO_2-free basis

$$\sigma_{mix} = \sigma_{H_2O} + \left(\sigma_{CO_2} - \sigma_{H_2O}\right) f(r,\alpha) x_{CO_2} + (\sigma_{MEA} - \sigma_{H_2O}) g(r,\alpha) x_{MEA}$$
$$f(r,\alpha) = a + b\alpha + c\alpha^2 + dr + er^2$$
$$g(r,\alpha) = f + g\alpha + h\alpha^2 + ir + jr^2$$

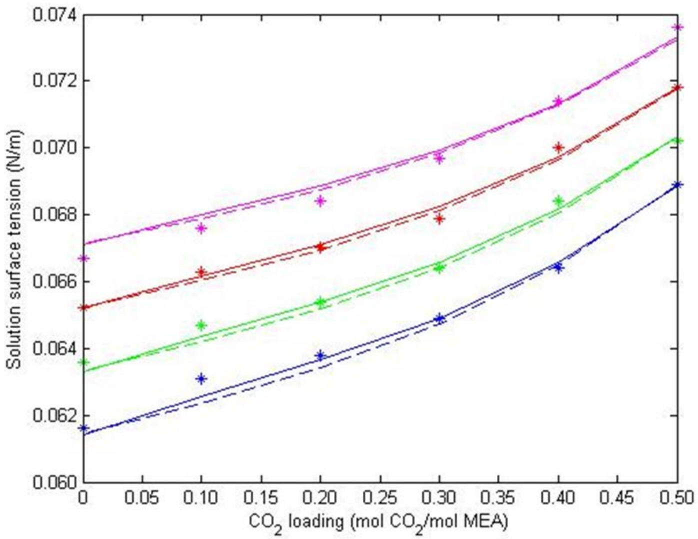
- Functionally similar to original model
- Preserves quality of fit between model and experimental data

Surface Tension Model-Calibrated Parameter Values

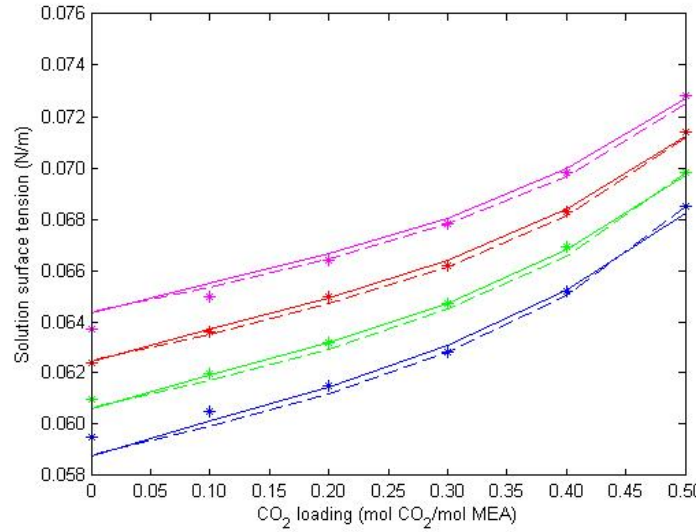
Parameter	Value	Parameter	Value
a	2.4558	f	2.3122
b	-1.5311	g	4.5608
c	3.4994	h	-2.3924
d	-5.6398	i	5.3324
e	10.2109	j	-12.0494

Surface Tension Model/Data Comparison

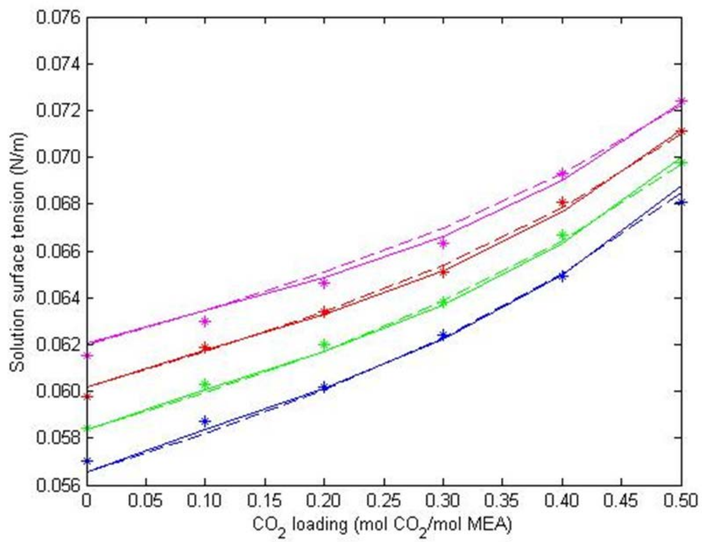
r=0.2

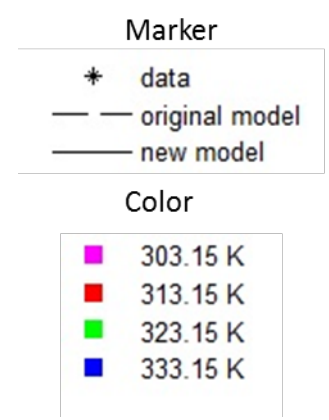


r=0.3



r=0.4

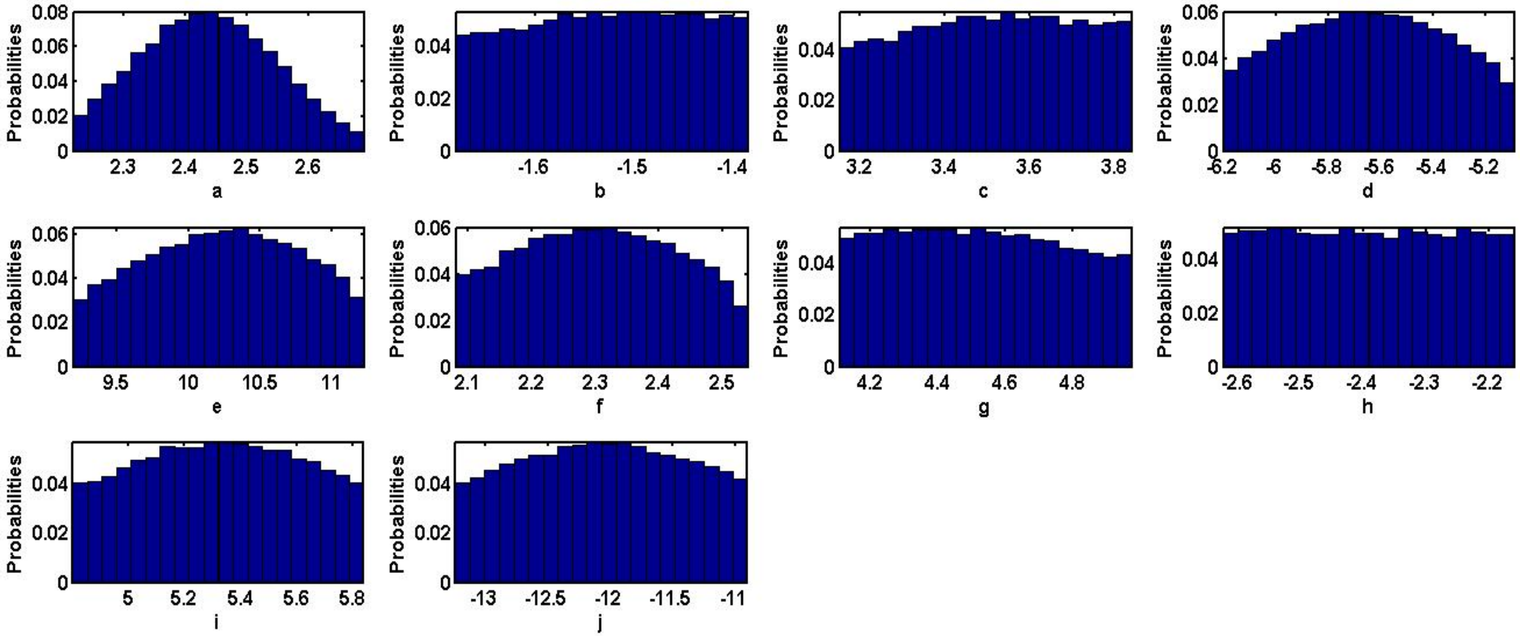




Surface Tension Model-Sensitivity Analysis

- $$N = \begin{bmatrix} \left|\frac{\partial}{\partial \hat{a}}\left(\frac{\partial\sigma}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{a}}\left(\frac{\partial\sigma}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{a}}\left(\frac{\partial\sigma}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{b}}\left(\frac{\partial\sigma}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{b}}\left(\frac{\partial\sigma}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{b}}\left(\frac{\partial\sigma}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{c}}\left(\frac{\partial\sigma}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{c}}\left(\frac{\partial\sigma}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{c}}\left(\frac{\partial\sigma}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{d}}\left(\frac{\partial\sigma}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{d}}\left(\frac{\partial\sigma}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{d}}\left(\frac{\partial\sigma}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{e}}\left(\frac{\partial\sigma}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{e}}\left(\frac{\partial\sigma}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{e}}\left(\frac{\partial\sigma}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{f}}\left(\frac{\partial\sigma}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{f}}\left(\frac{\partial\sigma}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{f}}\left(\frac{\partial\sigma}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{g}}\left(\frac{\partial\sigma}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{g}}\left(\frac{\partial\sigma}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{g}}\left(\frac{\partial\sigma}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{h}}\left(\frac{\partial\sigma}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{h}}\left(\frac{\partial\sigma}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{h}}\left(\frac{\partial\sigma}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{\imath}}\left(\frac{\partial\sigma}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{\imath}}\left(\frac{\partial\sigma}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{\imath}}\left(\frac{\partial\sigma}{\partial \alpha}\right)\right| \\ \left|\frac{\partial}{\partial \hat{\jmath}}\left(\frac{\partial\sigma}{\partial T}\right)\right| & \left|\frac{\partial}{\partial \hat{\jmath}}\left(\frac{\partial\sigma}{\partial r}\right)\right| & \left|\frac{\partial}{\partial \hat{\jmath}}\left(\frac{\partial\sigma}{\partial \alpha}\right)\right| \end{bmatrix} = \begin{bmatrix} 0.0008 & 0.6143 & 0.5005 \\ 0.0002 & 0.1918 & 0.2771 \\ 0.0003 & 0.2192 & 0.4816 \\ 0.0007 & 0.8493 & 0.4594 \\ 0.0005 & 1.0000 & 0.3330 \\ 0.0001 & 0.3298 & 0.0158 \\ 0.0001 & 0.2782 & 0.1865 \\ 0.0000 & 0.0727 & 0.0875 \\ 0.0001 & 0.5227 & 0.0148 \\ 0.0001 & 0.6702 & 0.0126 \end{bmatrix}$$

Surface Tension Model-Posterior Distributions from Bayesian Inference



Future Work

- Complete physical properties models/UQ for MEA
  - Vapor-liquid equilibrium
  - Heat capacity
  - Thermal conductivity
  - Diffusion coefficient
- Implement models in Aspen Plus® to allow for quantification of uncertainty in process variables (e.g. capture efficiency)
- Validate models with process data
  - UT-Austin Pilot Plant
  - National Carbon Capture Center (NCCC)
- Shift focus to high viscosity solvents

Thank you!

Disclaimer