CCSI

Carbon Capture Simulation Initiative

Validation and Uncertainty Quantification of a High-Fidelity Model of a MEA-Based CO_2 Capture System

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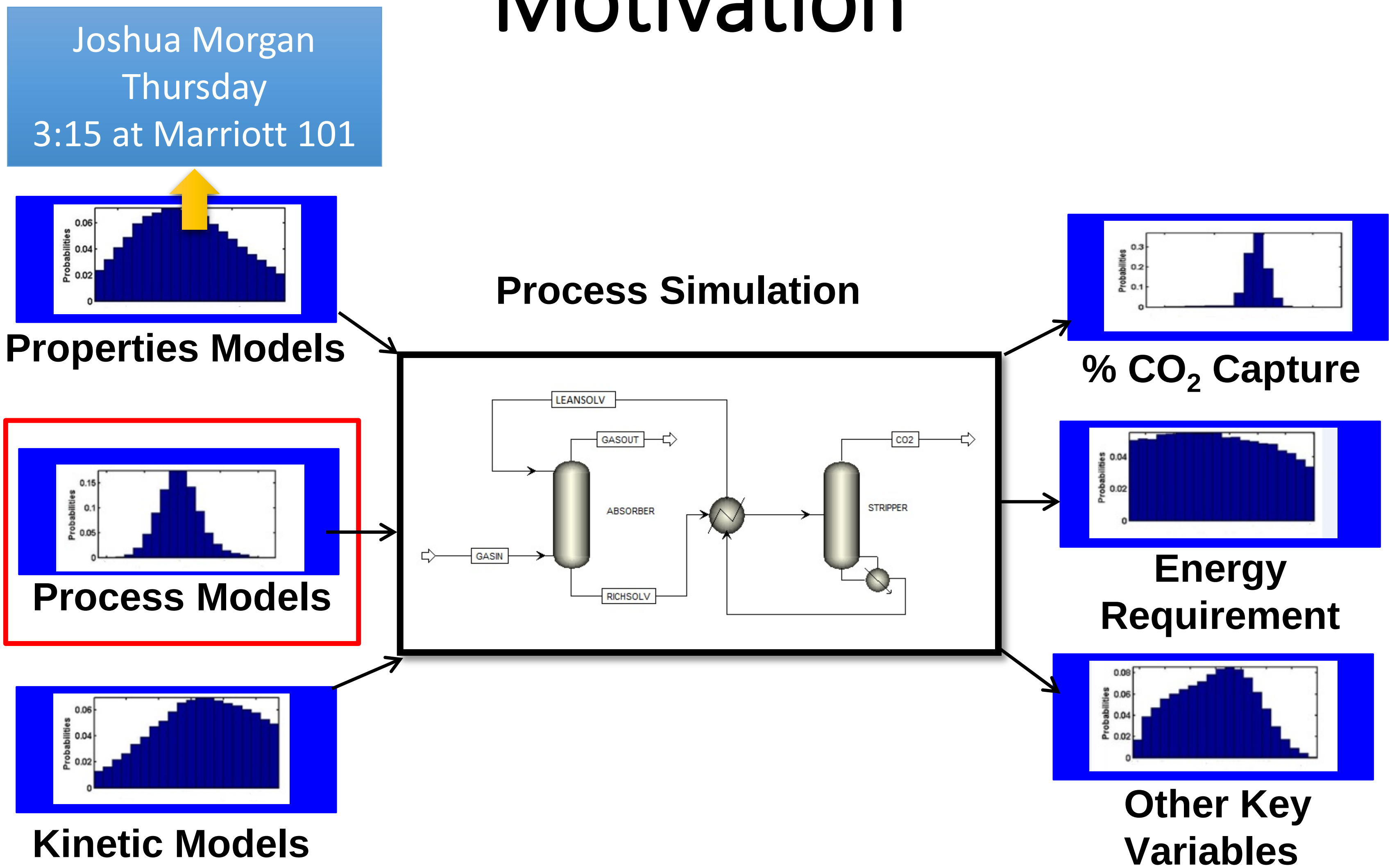
AICHE Annual Meeting 2014
Atlanta, GA

Outline

- Motivation
- Approach
  - Deterministic model
  - Uncertainty Quantification
- Results
  - Holdup
  - Pressure Drop
  - Interfacial Area
  - Mass Transfer Coefficients
  - Uncertainty Propagation
- Conclusion

Motivation


Joshua Morgan
Thursday
3:15 at Marriott 101
Properties Models
Process Models
Kinetic Models
Process Simulation
LEANSOLV
GASOUT
CO2
ABSORBER
STRIPPER
GASIN
RICHSOLV
% CO_2 Capture
Energy Requirement
Other Key Variables
Probabilities

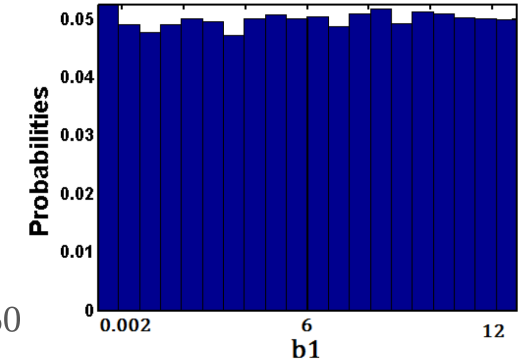
Process Model

- **Hydraulic Model**
  - Holdup
  - Pressure Drop
- **Mass Transfer Model**
  - Interfacial Area
  - Mass Transfer Coefficients
- **Heat Transfer Model**
  - Heat Transfer Coefficients

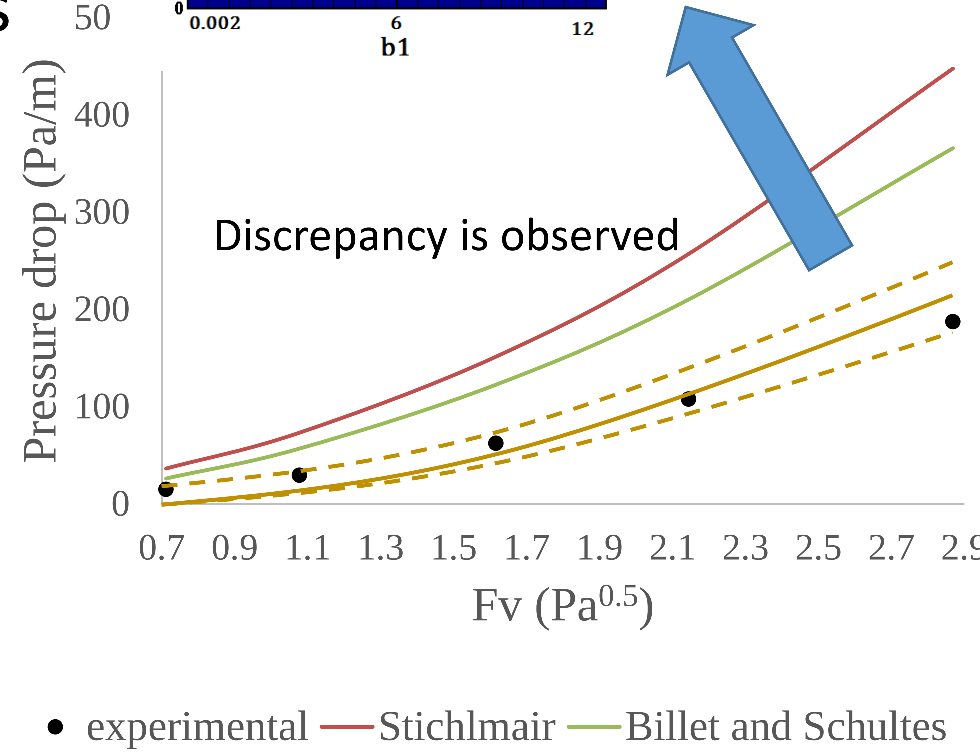
A Close Look on Uncertainty in Modeling: Pressure Drop Model

- Evaluation of literature models
  - Billet and Schultes
  - Stichlmair

Packing Type
Liquid/gas system
Operating Conditions

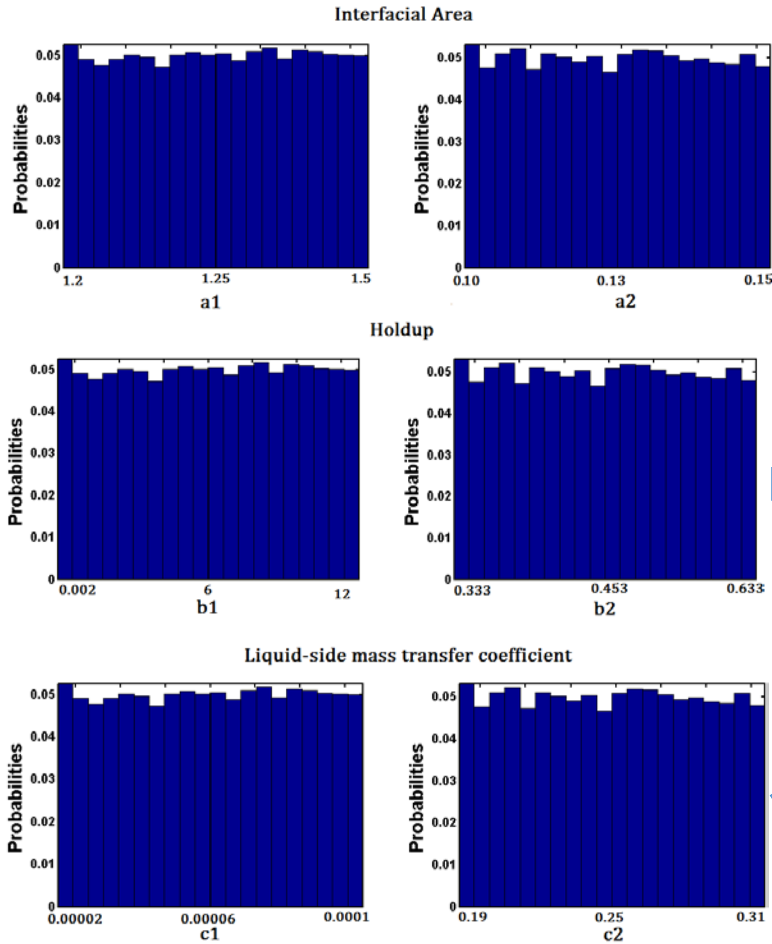


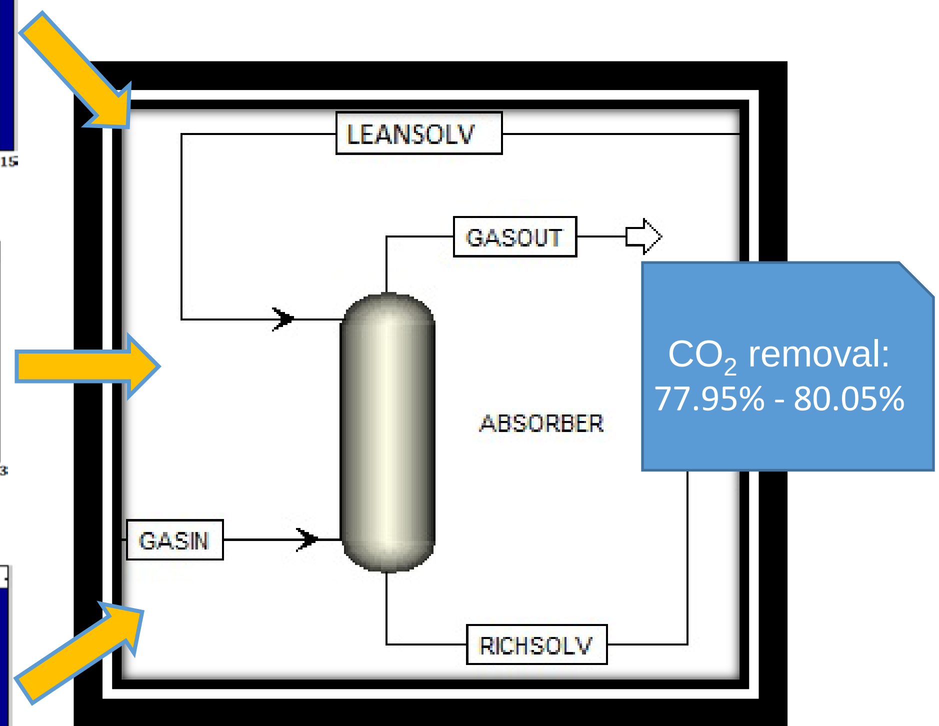
Parameter range and probabilities



Parametric Uncertainty Propagation

Models from Plaza (2012)[1]: Phoenix Model



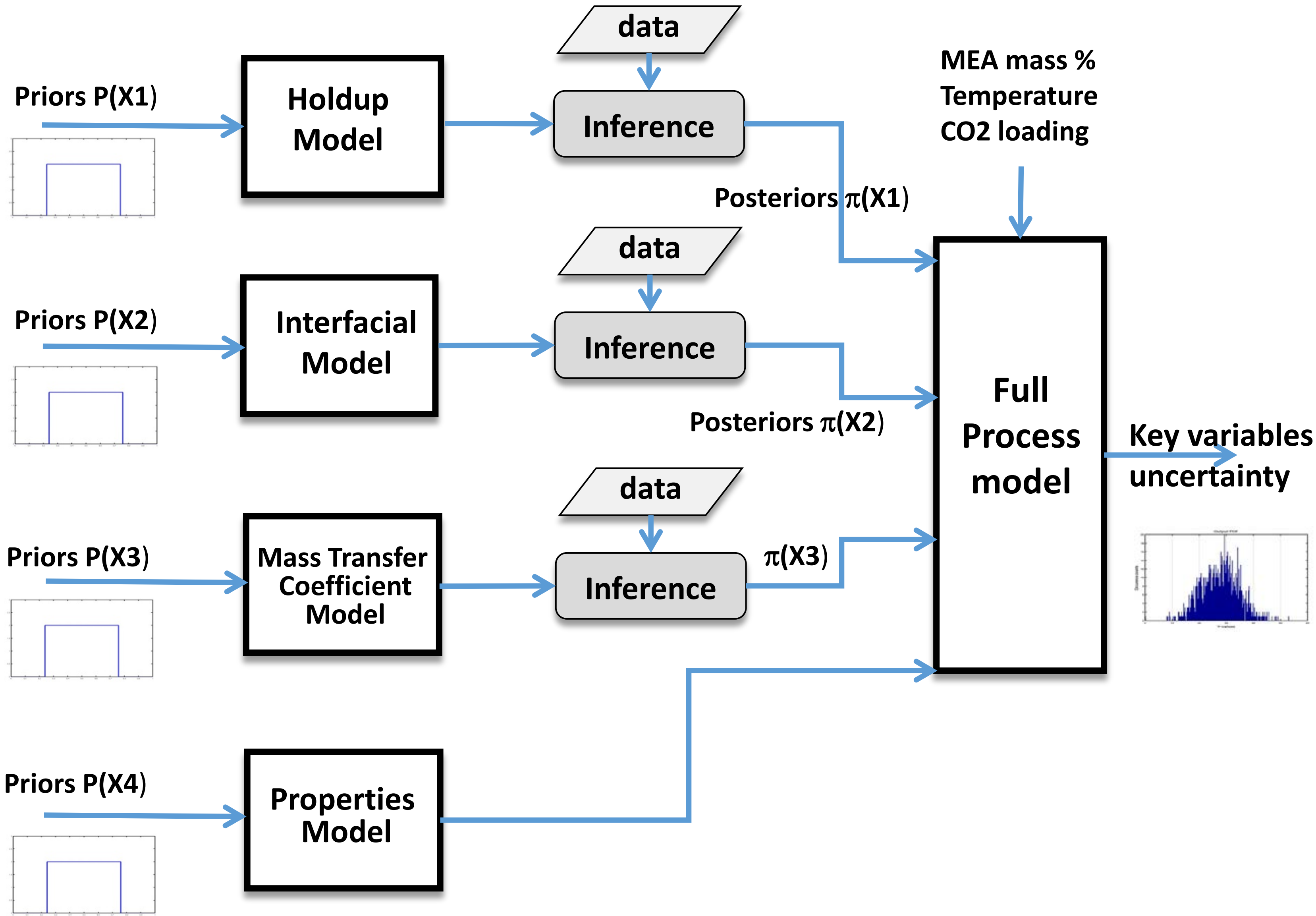


1. Jorge Mario Plaza, Ph.D. Dissertation, UT Austin, May 2012

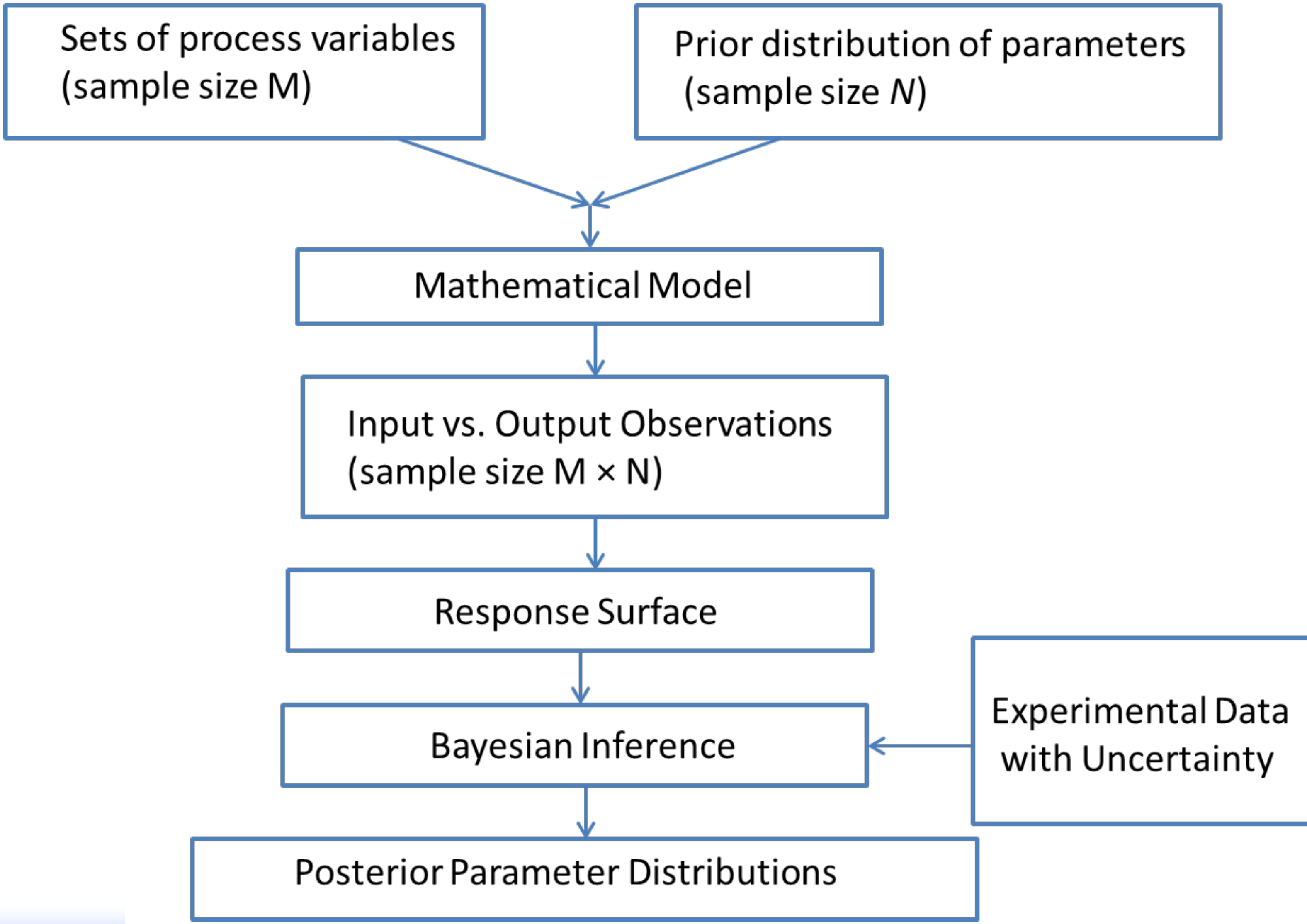
Overall Approach to UQ

- **Deterministic Model Identification**
  - Identification of Model and Data
  - Parameter Calibration (with model form correction)
  - Implementation in Aspen Plus® (Fortran User Models)
- **Parametric Uncertainty Quantification**
- **Uncertainty Propagation Through Process Model**

Physical Properties, Hydraulic, and Mass Transfer Models



Stochastic Modelling Approach



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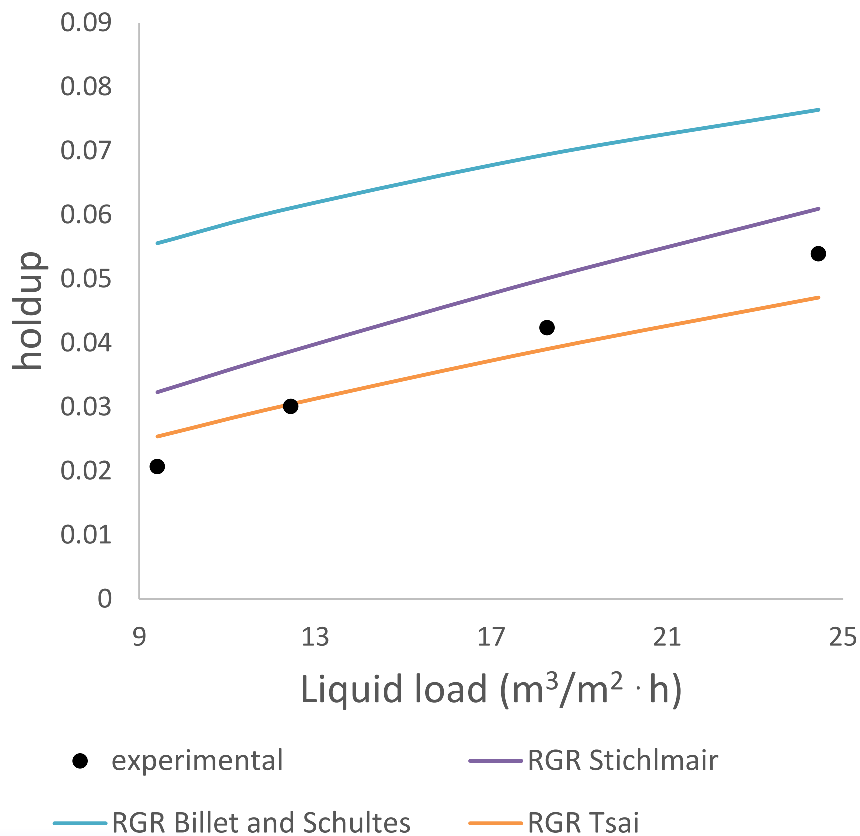
U.S. Department of Energy

Holdup Sub-model Uncertainty Quantification

Step 1 – Model Parameter Calibration: Holdup

- 2 Parameters Calibrated



Tsai (2010)[2] Holdup Correlation:

$$h_L = \mathrm{A1}\left[\frac{1}{S^2 g^{2/3}}\left(\frac{\mu_L}{\rho_L}\right)^{1/3}\frac{Q}{L_P}\right]^{\mathrm{A2}}$$

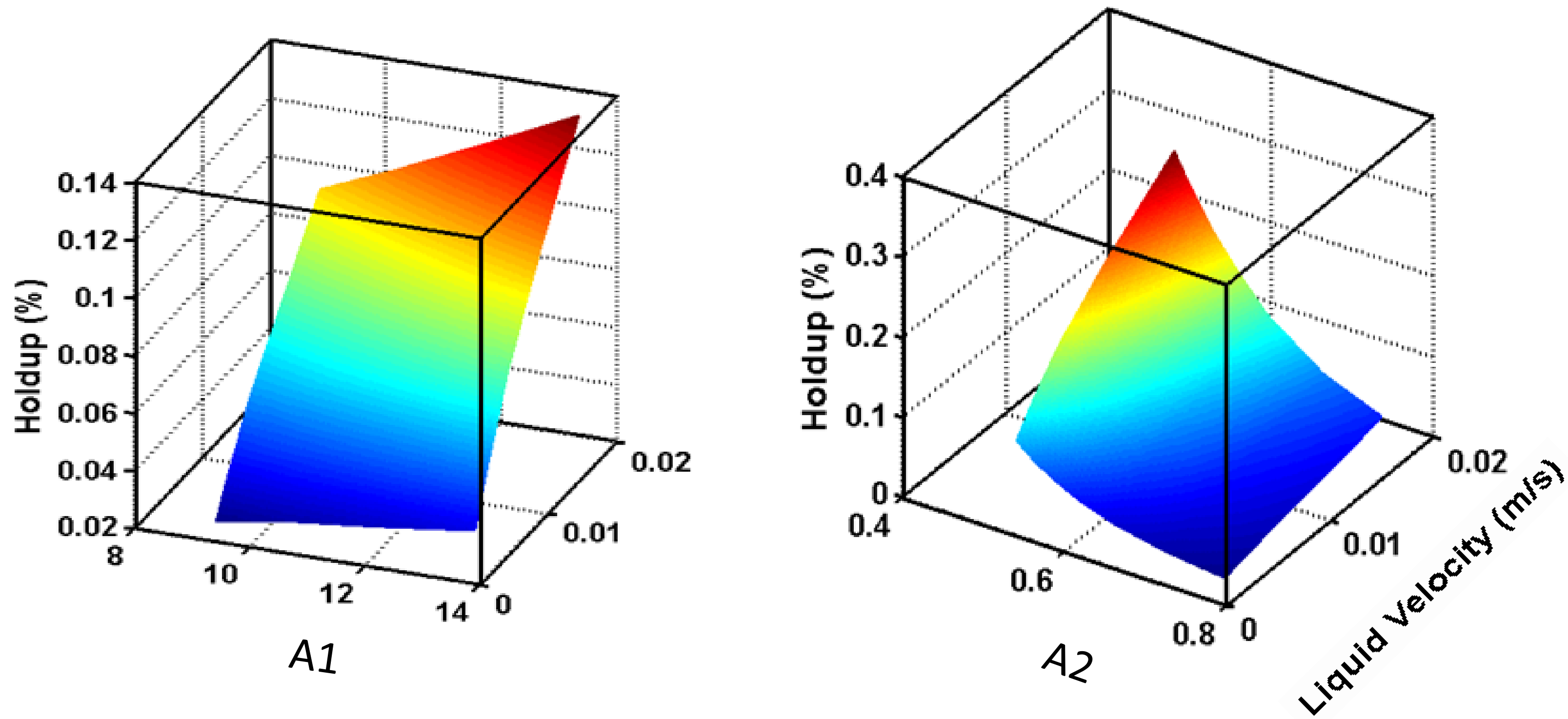
Parameter	Initial	Calibrated
A1	6.94	11.450
A2	0.573	0.647

2. Robert Edison Tsai, Ph.D. Dissertation, UT Austin, 2010

Step 2 - Response Surface Model:Holdup

- 69 Sets of Process Variables
- Uniform Prior Distribution (Monte Carlo Simulation)
  - Sample size = 100
  - ± 20% range assumption from calibrated values
- Results obtained from the deterministic model (6900 points)
- Multivariate Adaptive Regression Splines (MARS) method to fit a response surface

Step 2 - Response Surface Model: Holdup

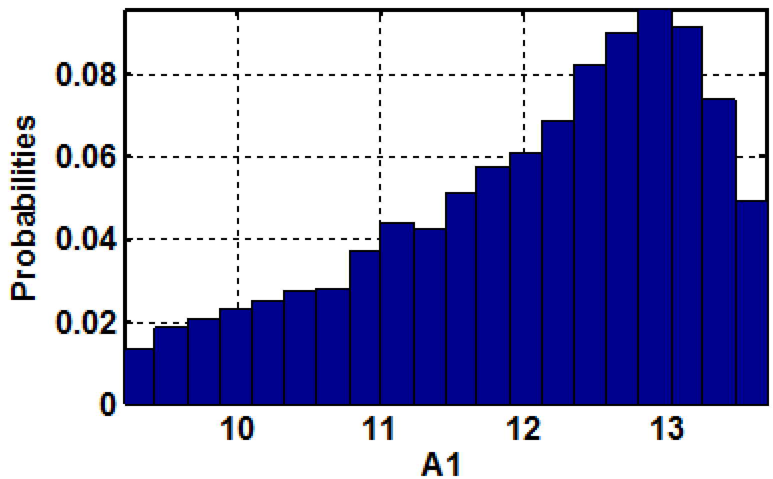


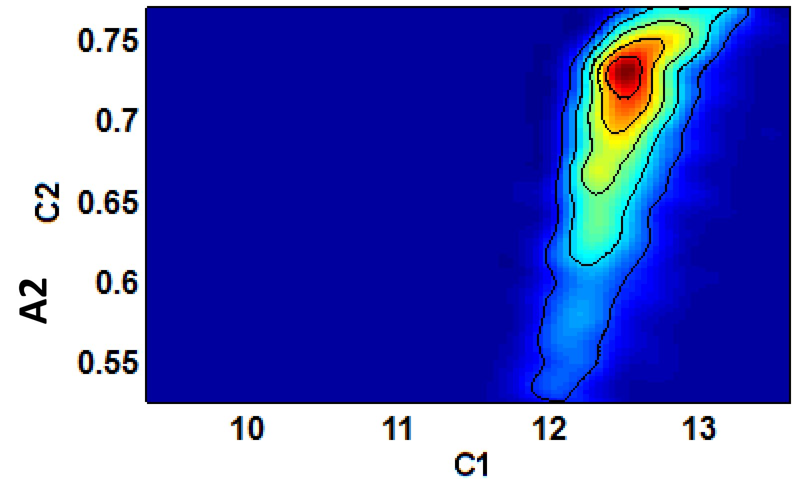
Step 3 – Bayesian Inference

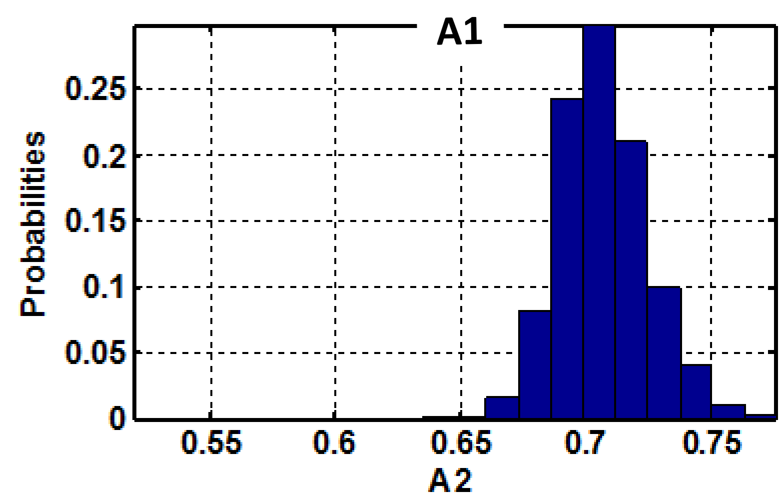
- Posterior distribution of the parameters are generated by maximizing expectation of finding the experimental data given the uncertainty in observation and initial guess of parametric uncertainty

- Method: Markov Chain Monte Carlo
- Software: PSUADE

Step 3 – Bayesian Inference

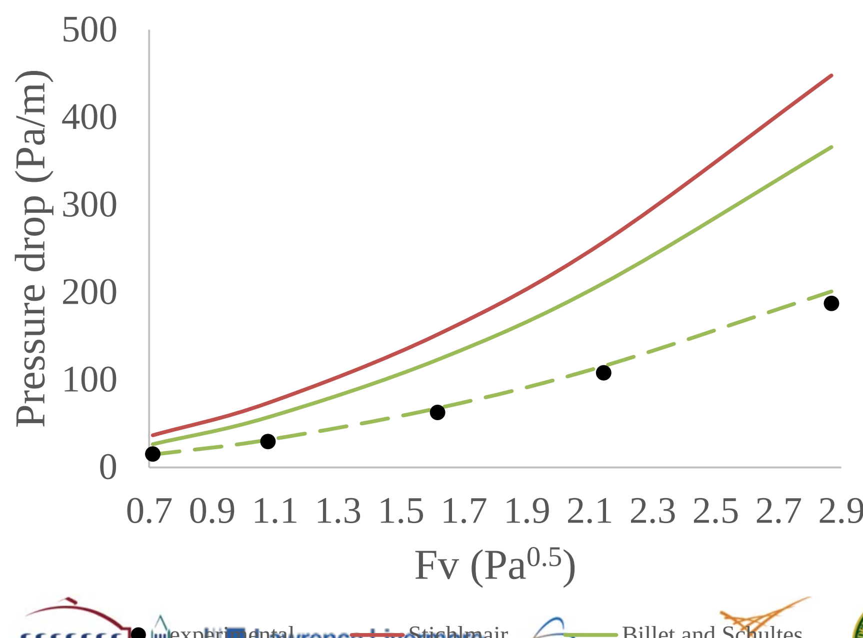






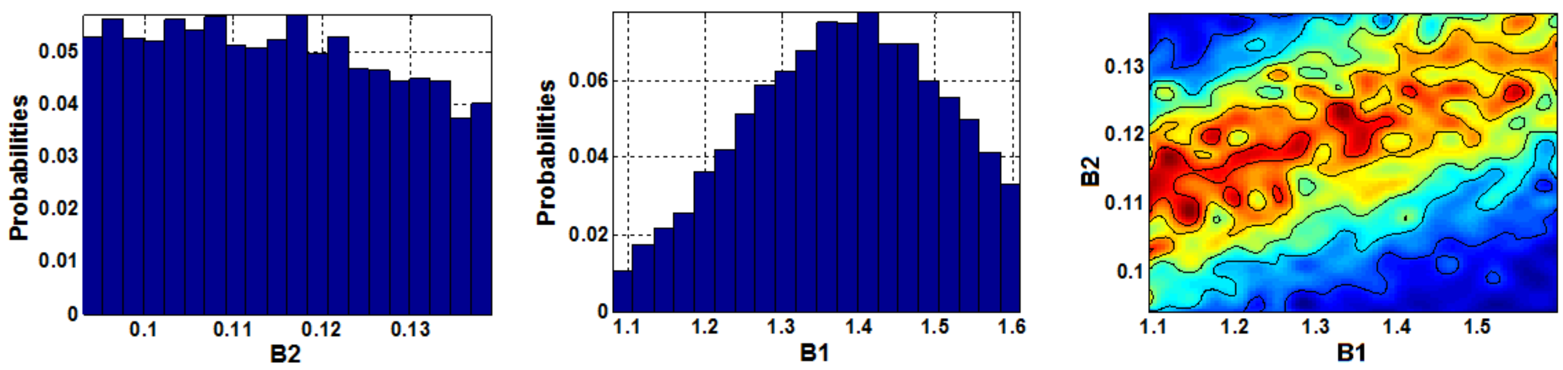
Pressure Drop

- Billet and Schultes' correlation was evaluated
- Calibration of 1 Parameter
- For holdup, modified Tsai (2010) model was considered



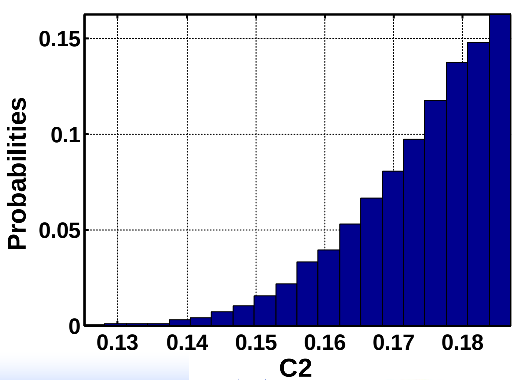
Interfacial Area

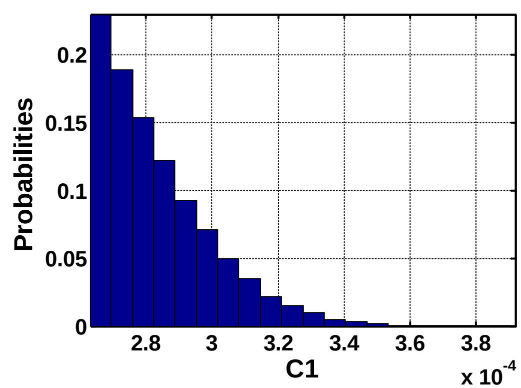
- Tsai (2010) correlation was selected
- No calibration was performed
- Uncertainty considered in 2 Parameters

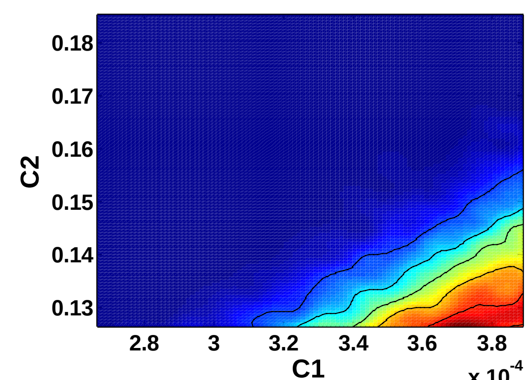


Liquid Side Mass Transfer Coefficient

- None of the existing correlations that were evaluated gave satisfactory result in comparison to the experimental data
- Wang (2013)[3] was selected for being a complementary study to Tsai (2010)
- Calibration of 2 Parameters
- Uncertainty considered in 2 Parameters







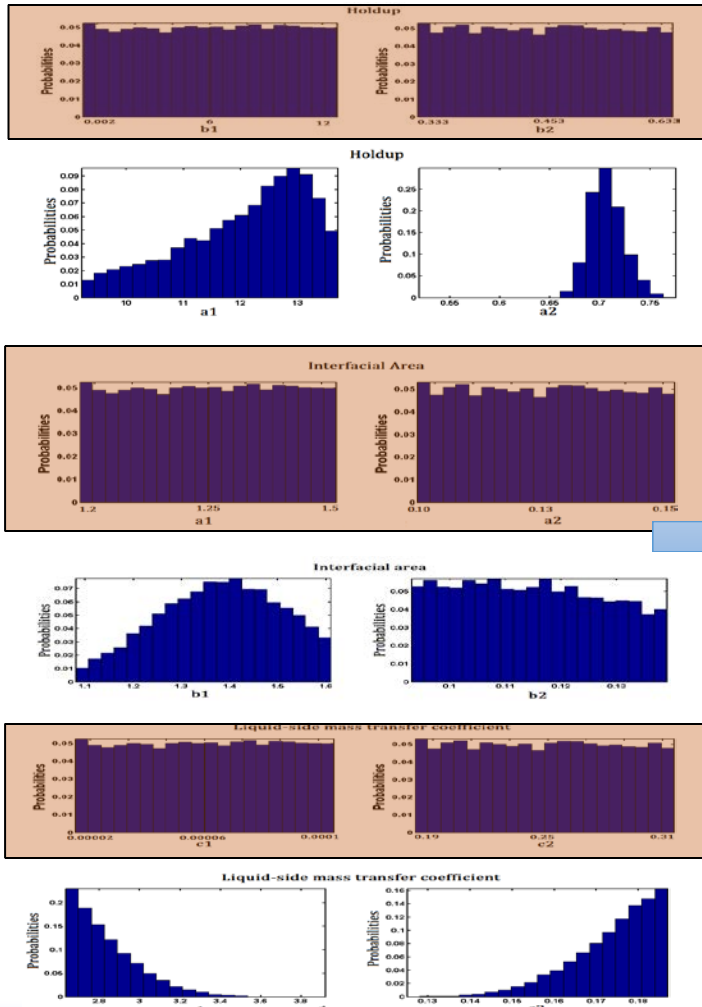
3. Wang, C.B., Perry, M., Rochelle, G.T., Seibert, A. F., 2013. Characterization of Novel Structured Packings for CO2 Capture. Energy Procedia 37, 2145-2153.

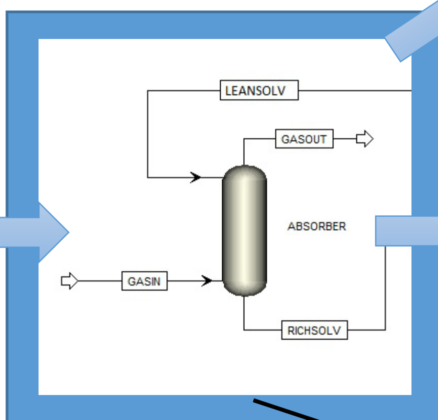
Parametric Uncertainty Propagation

- Posterior distributions from Bayesian Inference are considered
- User models developed in FORTRAN, compiled and used in Aspen Plus environment
- For each set of parameters and process variables, Aspen Workbook was used to run the Aspen simulations

Initial vs Final Results

(Hold up, interfacial area, and liquid-side mass transfer coefficient only)





Initial

CO_2 removal:
77.95% - 80.05%

Final

CO_2 removal:
84.01% - 84.77%

Validation: Data from Recently Conducted Test Runs at NCCC

Lean solvent :	**Flue gas :**
Flowrate = 6000 kg/h	Flowrate = 2260 kg/h
T = 44 °C	T = 43.4 °C
P = 101.3 kPa	P = 111.7 kPa
29.65% MEA	16% CO_2

Conclusion

- A methodology for quantification of parametric uncertainty of process models is developed.
- Starting from an initial guess, the methodology generates a more precise estimate of parametric uncertainty if the observation data and their uncertainty are known
- The methodology improves the overall estimate, both deterministic and stochastic, of the key variables.

Acknowledgment

As part of the National Energy Technology Laboratory's Regional University Alliance (NETLRUA), a collaborative initiative of the NETL, this technical effort was performed under the RES contract DE-FE0004000.

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