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Reliable Predictive Computational Fluid Dynamics Models for Coal Gasifier Simulations with Uncertainty Quantification

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Presentation Outline

- Motivation and Objective
- Overview of Uncertainty Quantification Frameworks
- Results from Two Non-intrusive UQ Analysis Methods
  - NETL's B22 riser simulations
- Summary & Conclusions
- Future Work

Motivation and Objectives

- Computational science and simulation based engineering (SBE) have become an indispensible tool for resolving complex engineering problems through simulation.
- Reactive multiphase flow models and simulation tools (e.g., MFIX) play important role in development of new technologies for fossil fuel based clean energy.
- Increasingly strong need for assessment of credibility of the predictions from simulations for wider acceptance of SBE.
- Uncertainty quantification (UQ) methods provide a yardstick.

Objective:

- Determine the best set of UQ methods and tools applicable for reactive multiphase flow simulation.

Quick Overview of
Uncertainty Quantification (UQ) Methods

Intrusive UQ

Uncertain inputs → **Model** → **Uncertainty information**

Stochastic simulation
(UQ embedded in the model)

Several Available Methods:

- Polynomial Chaos Expansions (PCE)
- Stochastic Expansion

Pro:

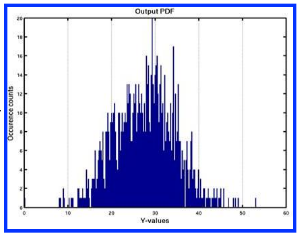
- Quick prediction

Con:

- Surgery in the code and long development time

Non-Intrusive UQ

Uncertain inputs → **UQ Toolbox** (**Model**) →



UQ achieved by sampling
many deterministic simulations

Several Available Methods:

- Surrogate Model + Monte Carlo
- Polynomial Chaos Expansions
- Bayesian Techniques

Pro:

- Short development time

Con:

- Sampling error

Source: An Introduction to Uncertainty Quantification Methodologies and Methods, C. Tong (2012) & Comparing Uncertainty Quantification Methods Under Practical Industry Requirements, Wang (2012)

Several Questions To Be Addressed By Using Non-intrusive Uncertainty Quantification and Propagation In Our Simulations?

Questions Addressed with Uncertainty Quantification:

- **What is the effect of variability in system input on the quantities of interest (QoI)?**

  E.g. How is the gasifier yield affected from operating condition variability or batch to batch coal feed variations?

  ➔ Forward Propagation of Input Uncertainties

- **Which input contributes most to variability of QoI?**

  E.g. If the variability in yield of gasifier output exceeds the allowable process limits, which system input factor needs to be managed or investigated to reduce uncertainty.

  ➔ Sensitivity Analysis

- **How to use observed data to calibrate system parameters?**

  ➔ Bayesian Calibration

- **What is the uncertainty in CFD simulation based predictions for scale-up studies?**

  ➔ Total Prediction Uncertainty Quantification

Non-Intrusive UQ Methodology Demonstration Results

Demonstration of applicability of UQ methods in answering questions through representative problems:

- Case A: 3D Transient Fluidized Bed Riser Simulation
  - Non-reacting multiphase flow simulation with MFiX
  - B-22 riser at NETL with experimental data from 2010 NETL/ PSRI Fluidization Challenge Problem.
- Case B: 2D Transient Gasifier Simulation
  - Reacting multiphase flow simulation with MFiX
- Case C: 3D Transient Fluidized Bed Gasifier
  - Reacting multiphase flow simulation with Fluent
  - UQ compatible experimental data from Canadian collaborators

Case A: 3D Transient Fluidized Bed Riser Simulation (in collaboration with T. Li, B. Gopalan, M. Syamlal)

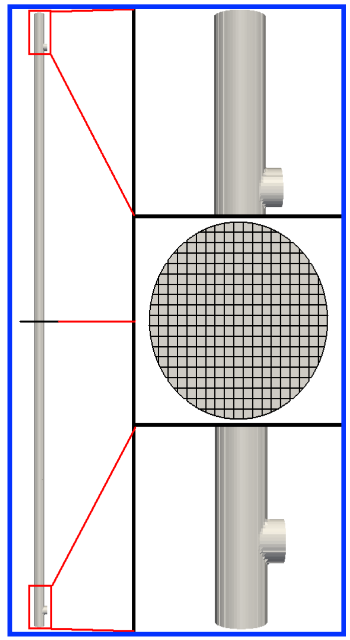
Uncertainty Quantification Study Properties:

Input parameters with Uncertainty [min-max range]:
(1) Superficial gas velocity (m/s):
[7.2 – 8.12]
(2) Gas flow through distributor (kg/s)
[12.6 – 15.98]

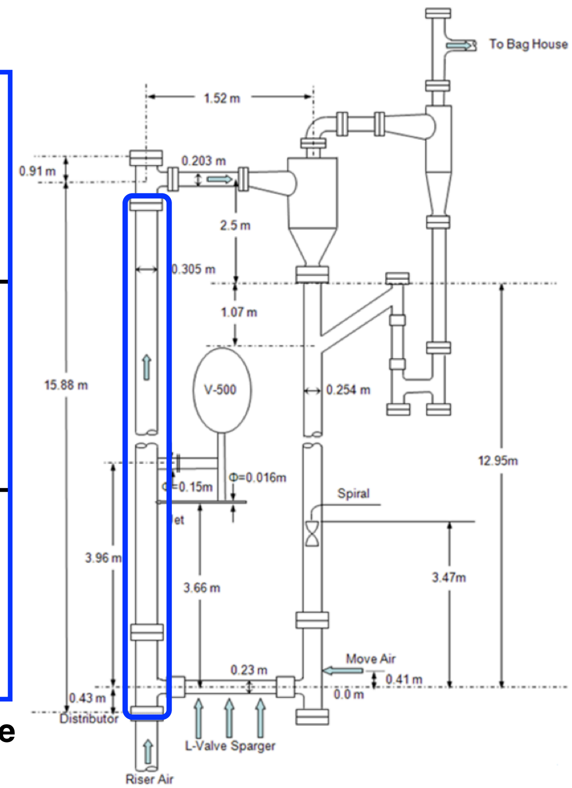
Quantity of Interest: Pressure Drop (kPa)

Sampling Method: Central Composite
Sample Size = 13

Computational time/sample: ~22 days on 80 cores



Enlarged view of the simulated section



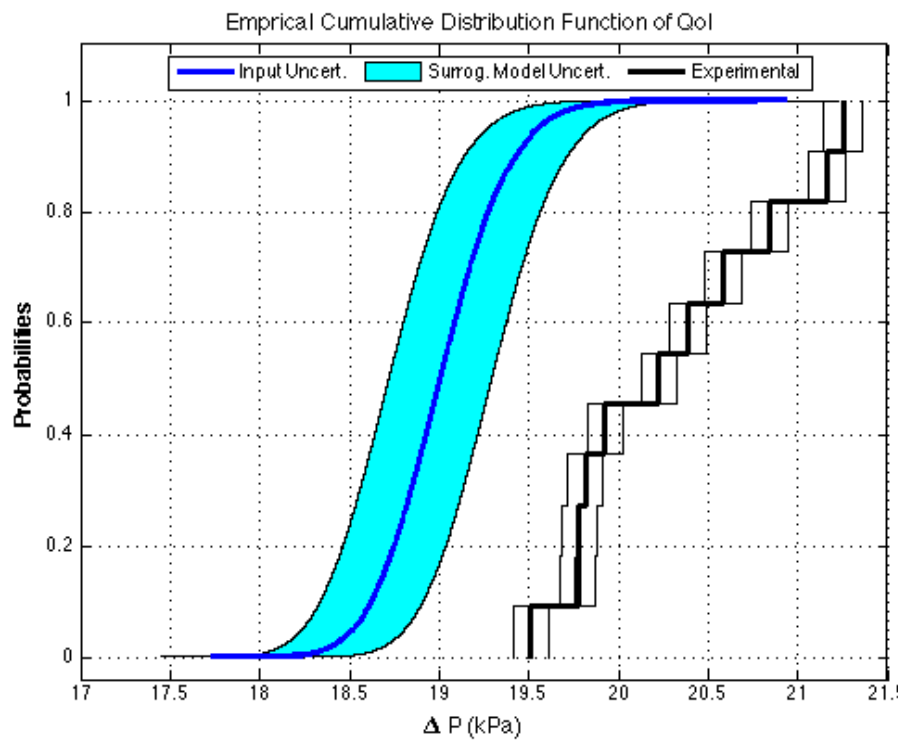
B22 riser schematic illustration

Publication Reference:
Gel, A., Li, T., Gopalan, B., Shahnam, M., Syamlal, M., "Validation and Uncertainty Quantification of a Multiphase CFD Model", ***Industrial & Engineering Chemistry Research*****, (2013) http://pubs.acs.org/doi/abs/10.1021/ie303469f.**

Case A: 3D Transient Fluidized Bed Riser Simulation (in collaboration with T. Li, M. Shahnam, B. Gopalan, M. Syamlal)

– **Model Form Uncertainty Assessment:**

- **Disagreement between simulation empirical CDF (blue) and experimental measurement empirical CDF (black line)**
- **Surrogate model uncertainty needs to be taken into account (cyan colored region)**
- **Experimental measurement uncertainty also shown (thin black lines between both sides)**



Estimated Model Form Uncertainty Interval:
0.992 kPa < Model Form Uncertainty < 1.566 kPa

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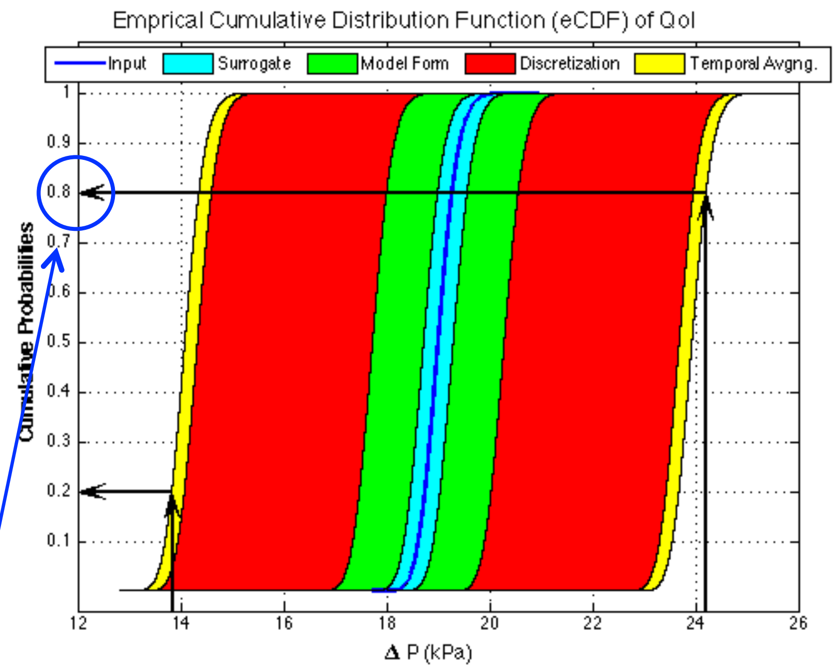
Case A: 3D Transient Fluidized Bed Riser Simulation (in collaboration with T. Li, M. Shahnam, B. Gopalan, M. Syamlal)

- Predictive Total Uncertainty Quantification: Accounts for various sources of uncertainties with the UQ framework
- Empirical CDF plot generated could be used to answer questions like:

  Given the uncertainties what is the probability of achieving a pressure drop > 24.2 kPa?

  =(1-0.8) => at most 20 %

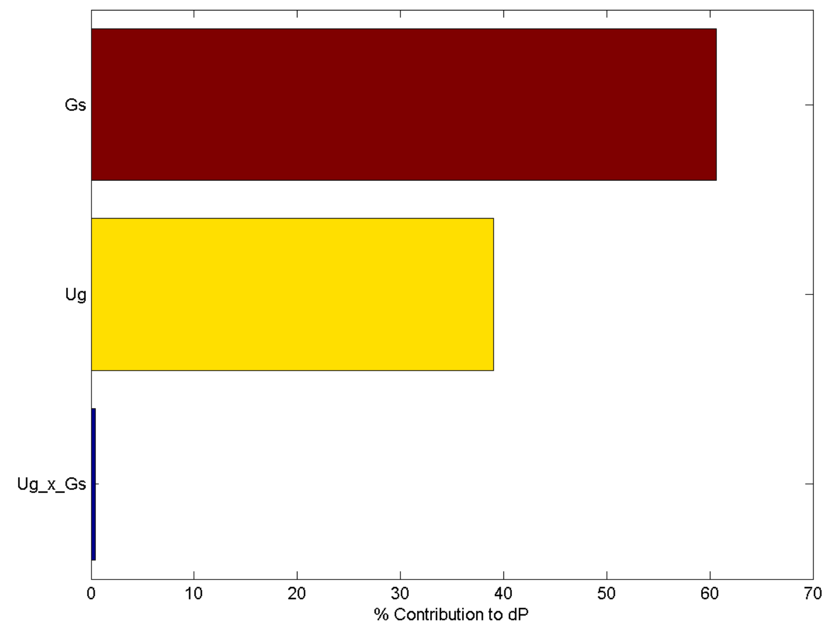


Total uncertainty quantification performed in validation domain

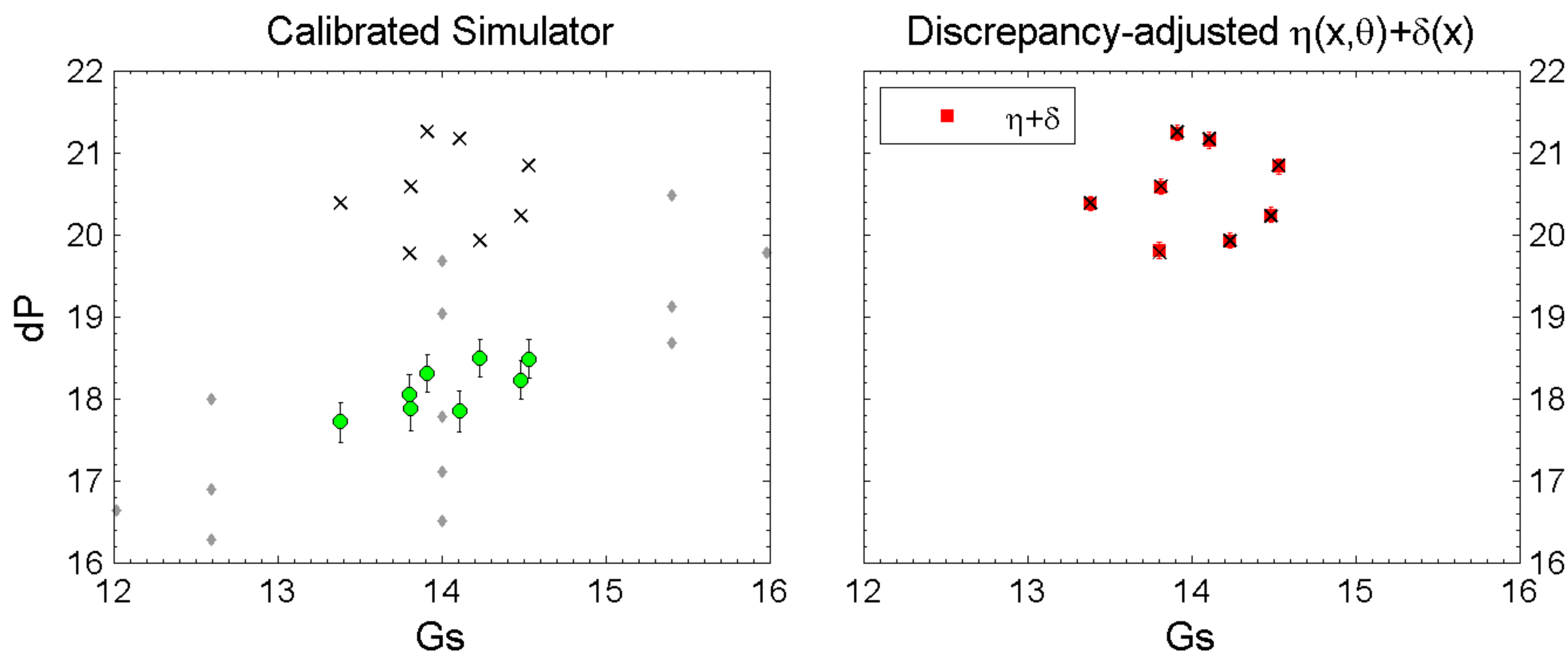
Preliminary Results of Alternate UQ framework for Same Data
Bayesian Analysis for Case A: Global Sensitivity Analysis

- **Which input parameter contributes most to the variability observed in the quantity of interest, dP?**
  - **Gs ~ 60%**
  - **Ug ~ 39%**
  - **Interaction of Gs & Ug < 1%**

- **Primarily main effects**



Bayesian Analysis for Case A: Bayesian Calibration



- MFIX Simulations (13 runs based on CCD sampling)
- Emulator prediction of experiments (η) without model discrepancy
- Experiments (only 8 out of 11 used)
- Emulator prediction of experiments (η) including model discrepancy (δ)

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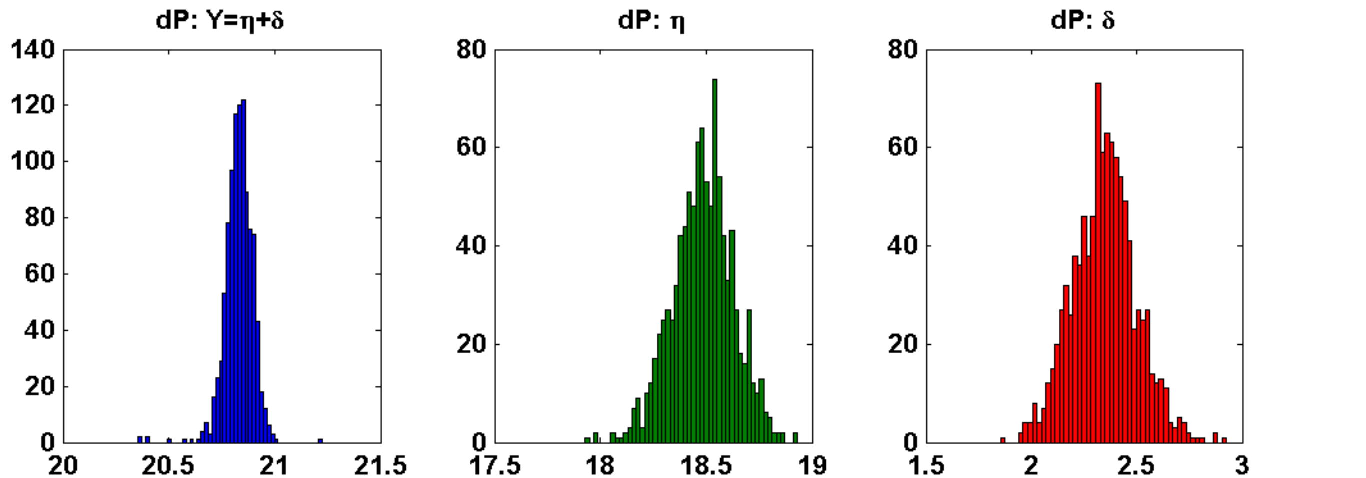
Bayesian Analysis for Case A: Bayesian Calibration - 2

Predictions for Experimental Data Point # 1

(Ug = 7.572 m/s, Gs = 14.5318 kg/s => dP = 20.839 kPa)



Emulator prediction of Experiment # 1 (η) including model discrepancy (δ)

Emulator prediction of Exp. # 1 (η) without model discrepancy

Model discrepancy (δ)

Summary and Conclusions

- Exploring different UQ techniques to identify those that are best suited for reacting multiphase flows.
- Non-intrusive UQ enables black box treatment of the application code but requires adequate samples to achieve the necessary accuracy by reducing sampling error.
- Typically 80% of effort spent goes into constructing an adequate surrogate model.
- Bayesian methods appears to offer various favorable features such as quantification of model discrepancy and inclusion of prior information, which can be used effectively to alleviate lack of data.

Future Work:
Case C: 3D Transient Fluidized Bed Gasifier
(in collaboration with J. Musser, J. Dietiker, R. Spiteri & S. Karimipour)

Uncertainty Quantification Study Properties:

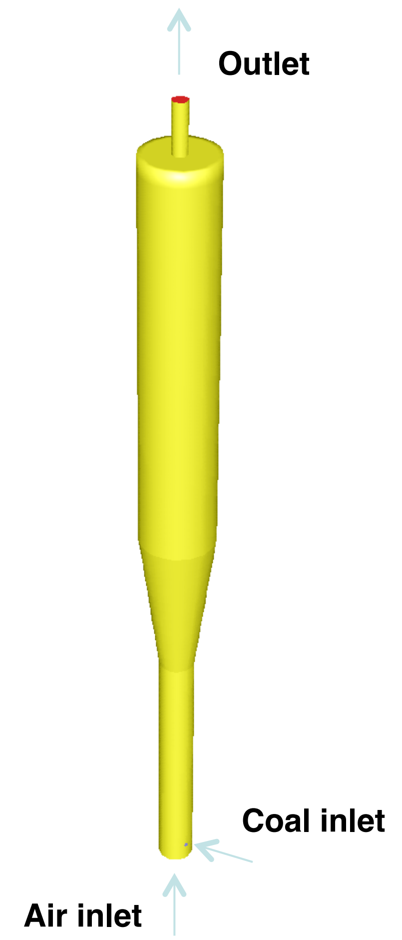
Input parameters with Uncertainty [min-max range]:
(1) Coal Flow Rate
(2) Particle Size
(3) H_2O / O_2 ratio

Quantities of Interest:
(1) Carbon Conversion
(2) Gas Yield
(3) Efficiency
(4) H_2/CO
(5) CH_4/H_2

Experimental Sampling Method: Central Composite Design (CCD)
Sample Size = 15 + 5 replications

Run #	Coal flow rate (g/s)	Particle size (µm)	Steam / O2 ratio in feed
1	0.0495	285	0.75
2	0.0495	285	0.75
3	0.0495	285	0.75
4	0.036	70	1
5	0.036	285	0.75
6	0.0495	285	1
7	0.0495	285	0.75
8	0.0495	285	0.5
9	0.063	70	1
10	0.063	285	0.75
11	0.063	500	0.5
12	0.063	500	1
13	0.063	70	0.5
14	0.0495	500	0.75
15	0.036	500	0.5
16	0.0495	285	0.75
17	0.0495	285	0.75
18	0.0495	70	0.75
19	0.036	500	1
20	0.036	70	0.5

Reference:
Karimipour S, Gerspacher R, Gupta R, Spiteri RJ. Study of factors affecting syngas quality and their interactions in fluidized bed gasification of lignite coal. Fuel. 2013; 103: 308-320



Fluidized Bed Gasifier Model

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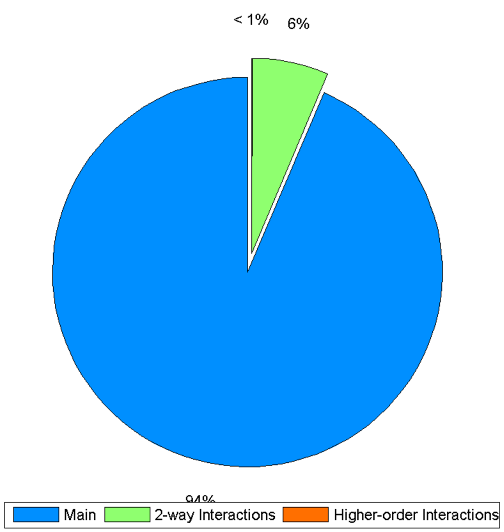
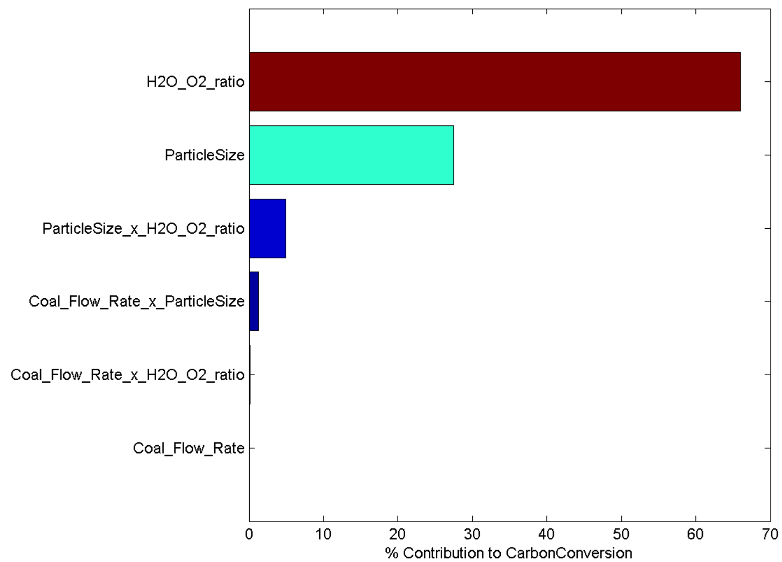
Case C: 3D Transient Fluidized Bed Gasifier
(in collaboration with J. Musser, J. Dietiker, R. Spiteri & S. Karimipour)

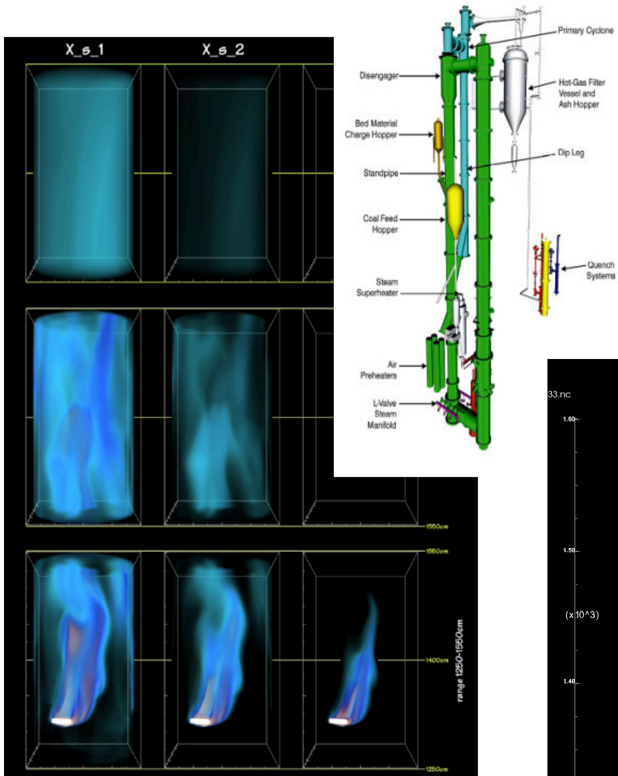
- Initial analysis of the experimental results with Bayesian framework performed

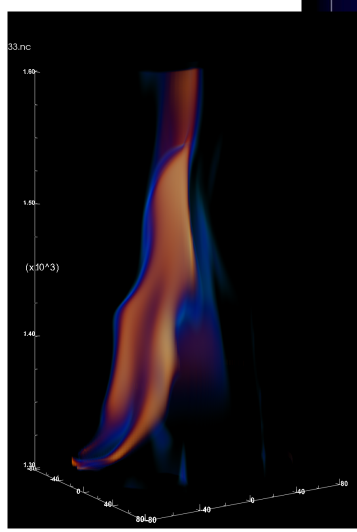
  E.g., global sensitivity analysis for Carbon Conversion

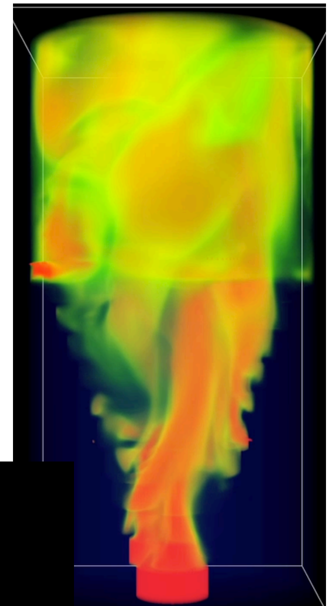


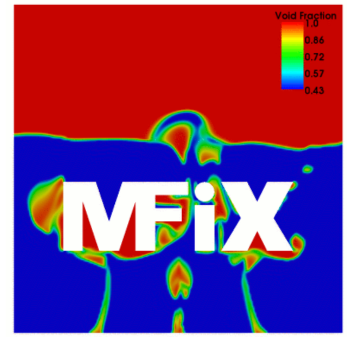


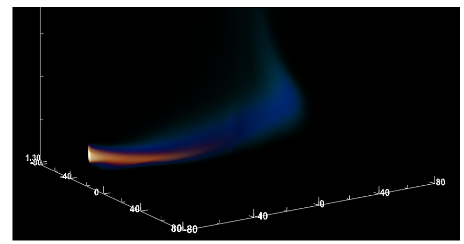
Thank you for your attention.
Questions?











Volume rendering visualizations of first-of-its-kind commercial scale gasifier simulation on Cray XT6 at OLCF by A. Gel.

Acknowledgments:

Dr. Charles Tong, CASC, Lawrence Livermore National Laboratory (LLNL).

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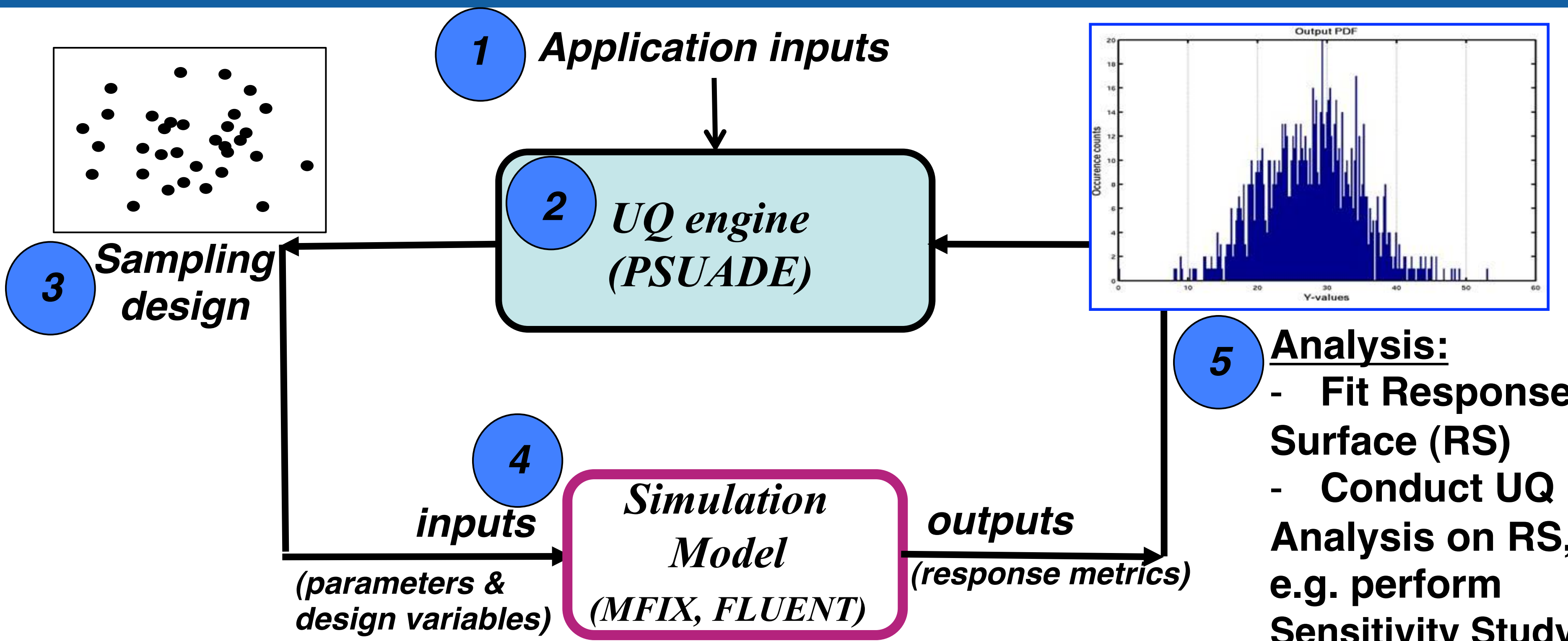
Additional Slides

Input Uncertainty Propagation and Quantification – Non-intrusive method



- *No need to modify simulation models: "black boxes"*
- *No need for analysis of the mathematical structures in the model*
- *May require large sample size for sufficient accuracy*
- *Model form uncertainty and numerical approximation uncertainty are disregarded.*

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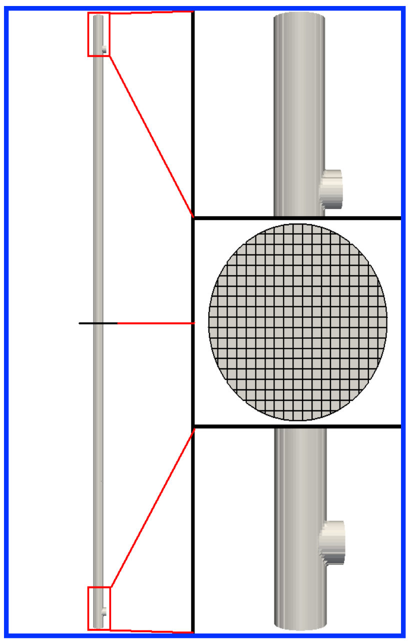
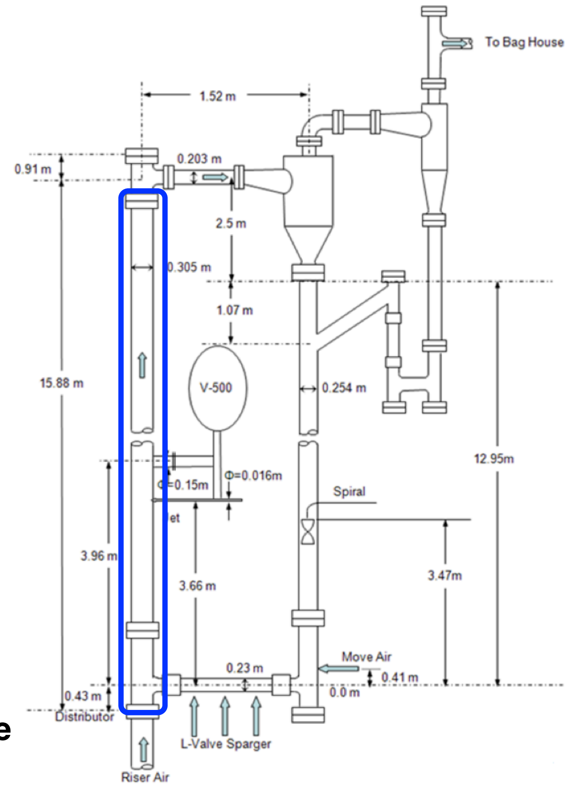
Accomplishments – UQ (Case A)

- Case A: 3D Transient Fluidized Bed Riser Simulation

  Objective: Assess total uncertainty using a comprehensive VUQ framework by Roy & Oberkampf



Enlarged view of the simulated section



B22 riser schematic illustration

Table 1. Basic experimental test conditions for challenge problem Case 5.

Test variable	Value	Test variable	Value
Gas	Air	Solids Material	HDPE
Superficial gas velocity[1] (m/s)	7.58	Solids circulation rate (kg/s)	14.0
Gas flow through distributor (SCMs)	0.640	Gas flow through standpipe and L-valve (SCMs)	0.029
Riser outlet pressure (kPa)	105	Temperature (K)	295

1. The superficial gas velocity is calculated based on the flow conditions at the riser bottom.

	Grid Resolution
Coarse	25 x 1050 x 19
Medium	35 x 1485 x 27
Fine	50 x 2100 x 38

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Accomplishments – UQ (Case A)

- Case A: 3D Transient Fluidized Bed Riser Simulation
  - Surrogate Model: Best fit quadratic regression model

	Input Parameters		System Response Quantity (SRQ)		%
Run	Input Fact. #1	Input Fact. #2	MFIX Simulation	Surrogate Model	error
#	U_g (m/s)	G_s (kg/s)	DP (kPa)	DP (kPa)	
1	7.20	12.60	17.999	18.112	0.63%
2	7.96	12.60	16.276	16.166	-0.68%
3	7.20	15.40	20.479	20.409	-0.34%
4	7.96	15.40	18.682	18.389	-1.57%
5	7.04	14.00	19.682	19.616	-0.34%
6	8.12	14.00	16.511	16.798	1.74%
7	7.58	12.02	16.636	16.737	0.61%
8	7.58	15.98	19.774	19.934	0.81%
9	7.58	14.00	17.781	17.807	0.15%
10	7.58	12.60	16.899	16.941	0.25%
11	7.58	15.40	19.128	19.202	0.39%
12	7.20	14.00	19.035	18.996	-0.20%
13	7.96	14.00	17.109	17.013	-0.56%

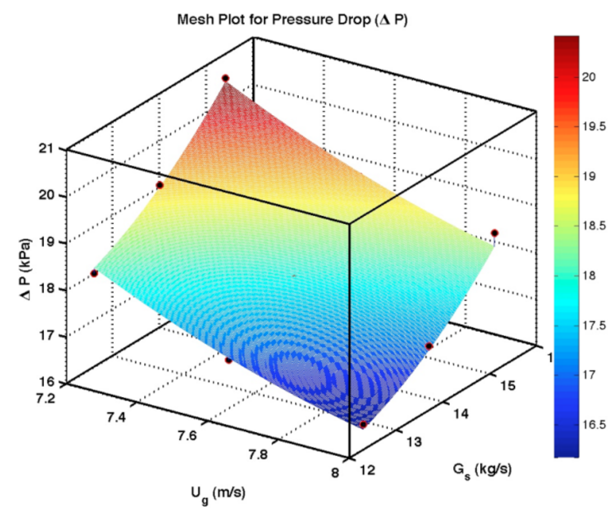
Performed 6 simulations in addition to existing 7 runs.
Each simulation takes 3 to 4 weeks on parallel processors.

Maximum discrepancy between surrogate model and MFIX simulation results. Additional checks based on statistical measures such as "adjusted R^2" used. Adj. R^2 shows 98 % of the variability observed can be explained with the surrogate model.

Also cross-validation errors were checked to determine adequacy of the surrogate model as compared other surrogate model choices.

Quadratic polynomial based surrogate model constructed

$$\Delta P = 127.72 - 22.89U_g - 27.032G_s - 0.34774U_gG_s + 1.3699U_g^2 + 0.13479G_s^2$$



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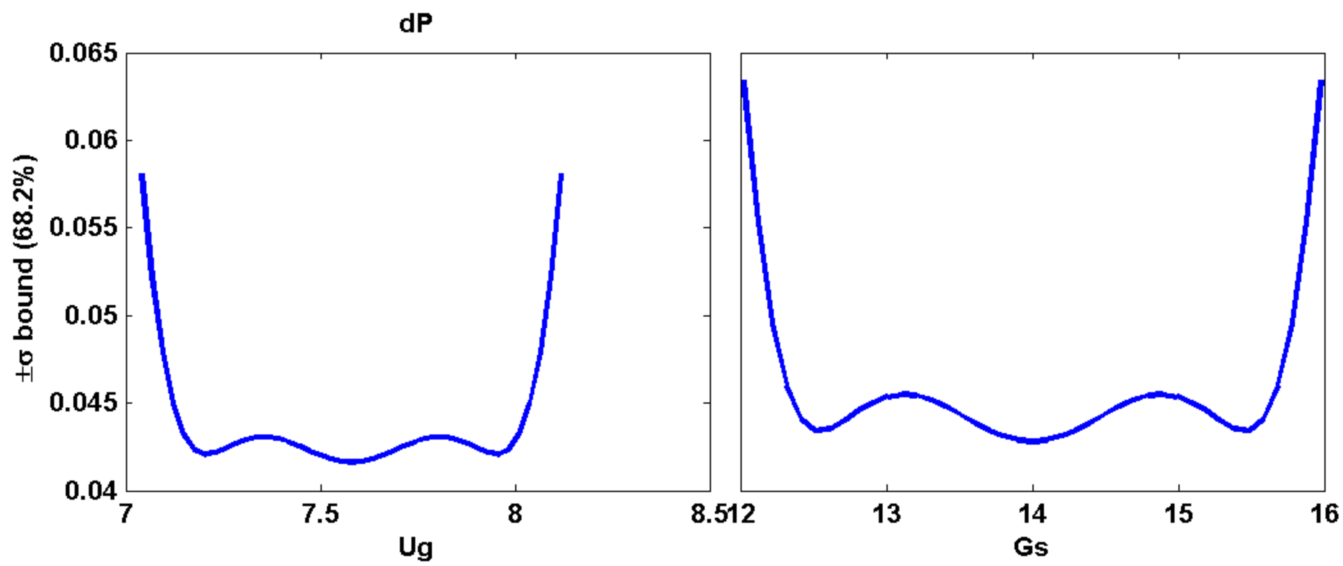
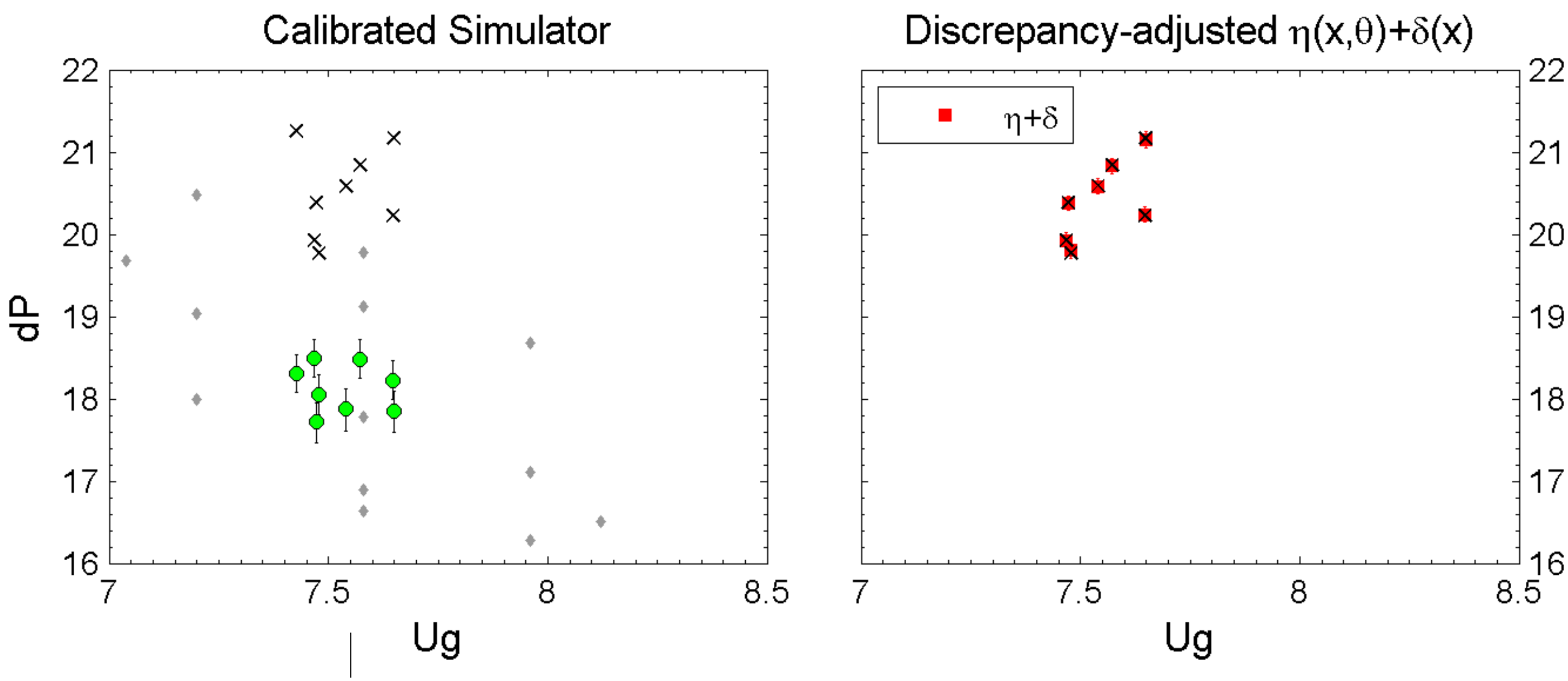
Bayesian Analysis for Case A: 1D Uncertainty w.r.t. Ug & Gs



– At any point of Ug, (e.g. Ug = 8 m/s) the plotted uncertainty in dP is due to variation in Gs over it's entire range, i.e., 12.02 – 15.98 kg/s, which is obtained by integrating along Gs.

Bayesian Analysis for Case A: Bayesian Calibration



- MFIX Simulations (13 runs based on CCD sampling)
- Emulator prediction of experiments (η) without model discrepancy
- Experiments (only 8 out of 11 used)
- Emulator prediction of experiments (η) including model discrepancy (δ)

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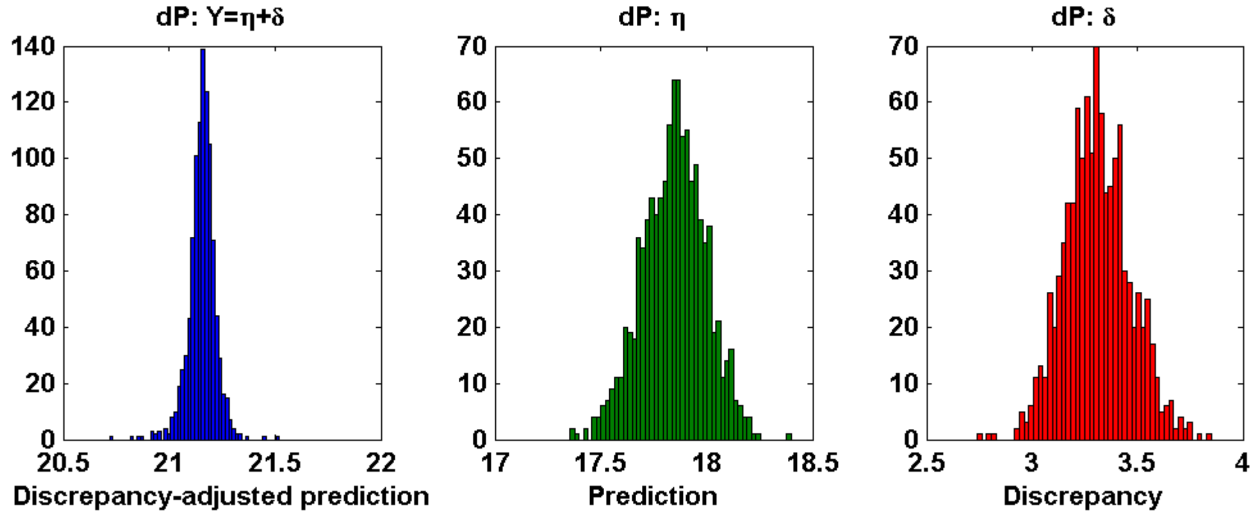
Bayesian Analysis for Case A: Bayesian Calibration - 3

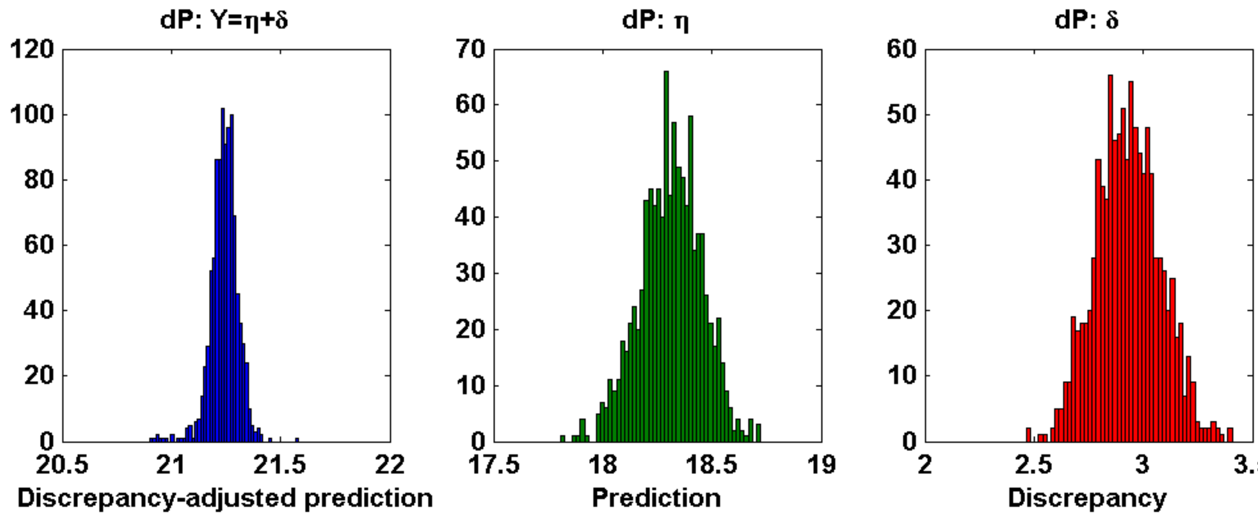
Predictions for Experimental Data Point # 2

(Ug = 7.649 m/s, Gs = 14.1075 kg/s : dP = 21.1647 kPa)



Predictions for Experimental Data Point # 3

(Ug = 7.427 m/s, Gs = 13.913 kg/s : dP = 21.2529 kPa)



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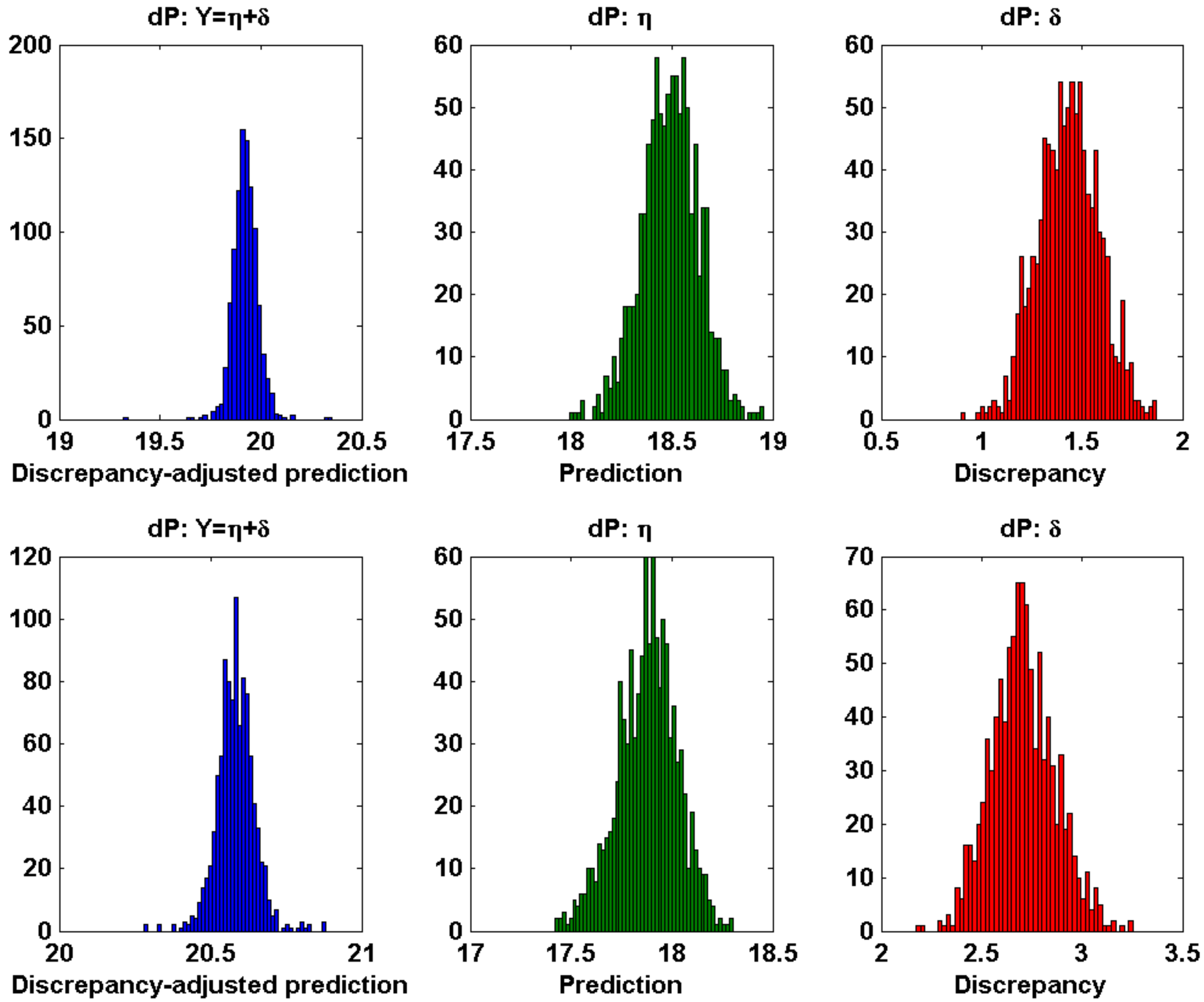
Bayesian Analysis for Case A: Bayesian Calibration - 3

Predictions for Experimental Data Point # 4

(Ug = 7.648 m/s, Gs = 14.2348 kg/s : dP = 19.9257 kPa)

Predictions for Experimental Data Point # 5

(Ug = 7.54 m/s, Gs = 13.813 kg/s : dP = 20.5865 kPa)



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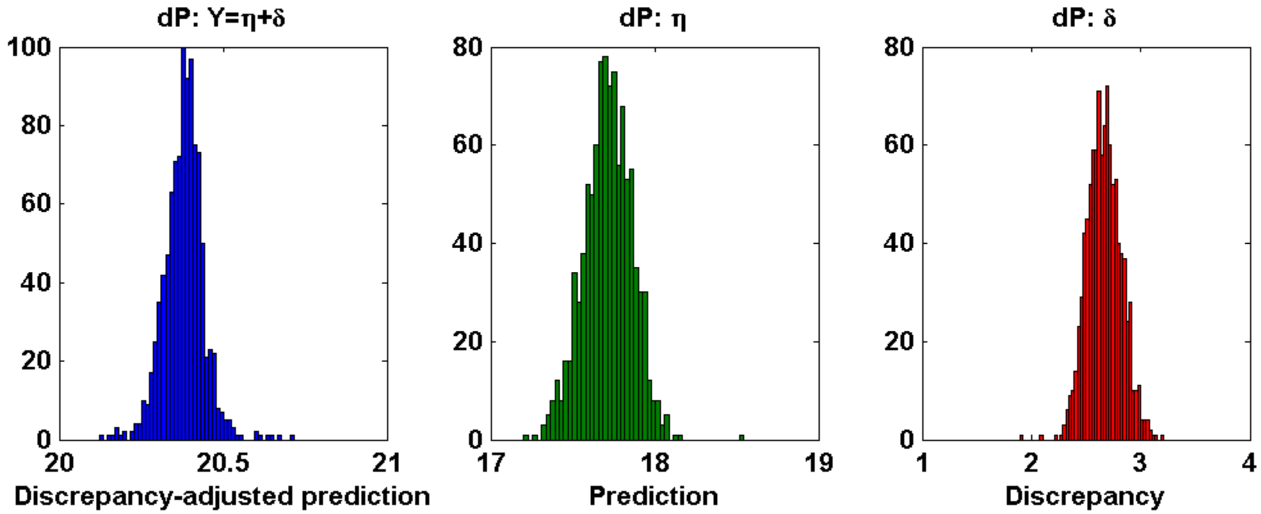
Bayesian Analysis for Case A: Bayesian Calibration - 3

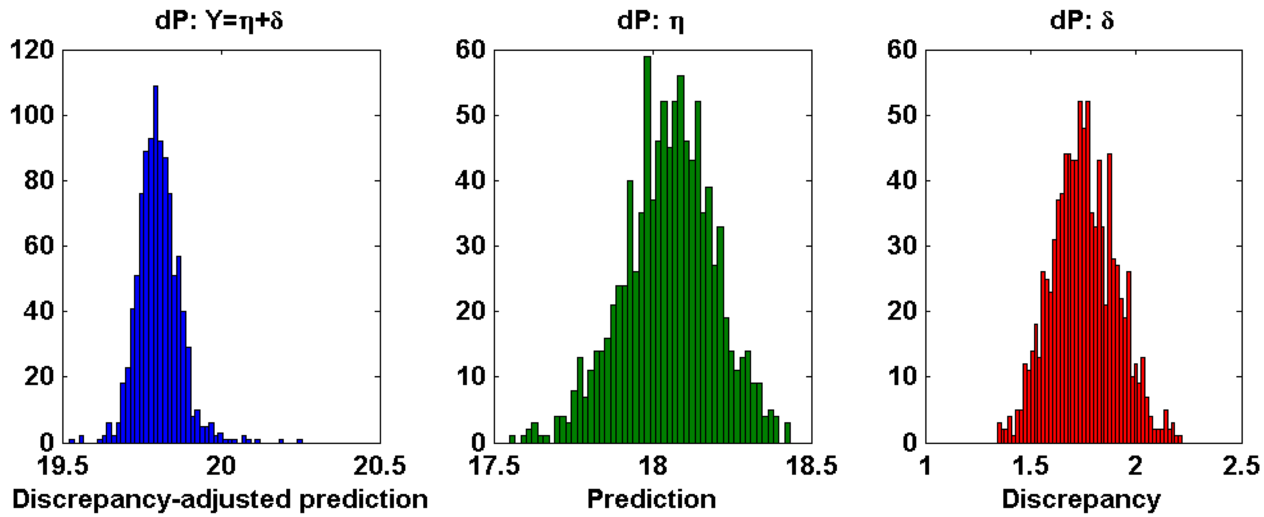
Predictions for Experimental Data Point # 6

(Ug = 7.472 m/s, Gs = 13.3843 kg/s : dP = 20.3883 kPa)



Predictions for Experimental Data Point # 7

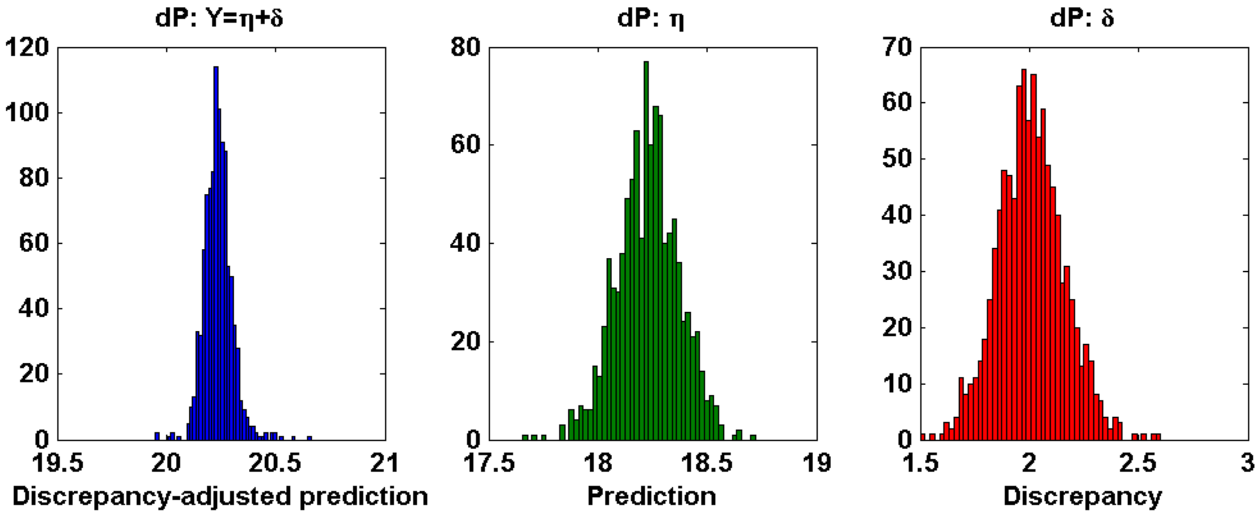
(Ug = 7.479 m/s, Gs = 13.8039 kg/s : dP = 19.7741 kPa)



Bayesian Analysis for Case A: Bayesian Calibration - 3

Predictions for Experimental Data Point # 8

(Ug = 7.647 m/s, Gs = 14.4833 kg/s : dP = 20.2264 kPa)



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