Applying Uncertainty Quantification to Multiphase Flow CFDs

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Acknowlegment: The CCSI Technical Team

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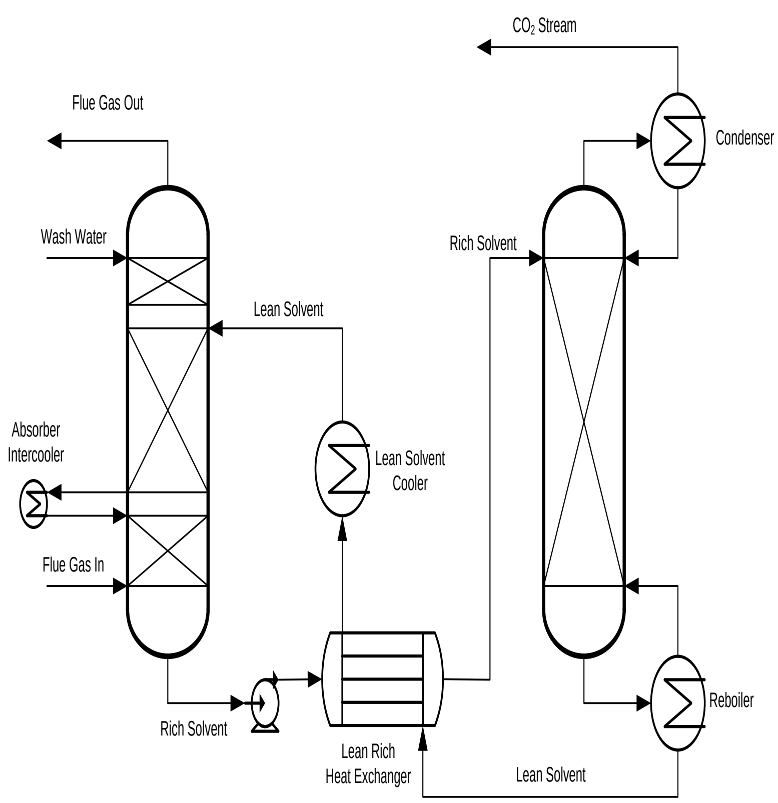
Presentation Outline

- Brief Introduction to Uncertainty Quantification & Analysis
- Introduction to UQ Toolkit, PSUADE
- Preliminary Results for Demonstration of Non-intrusive UQ Analysis for MFIX Simulations:
  - Gasification
  - DES Fluidized Bed
- Summary

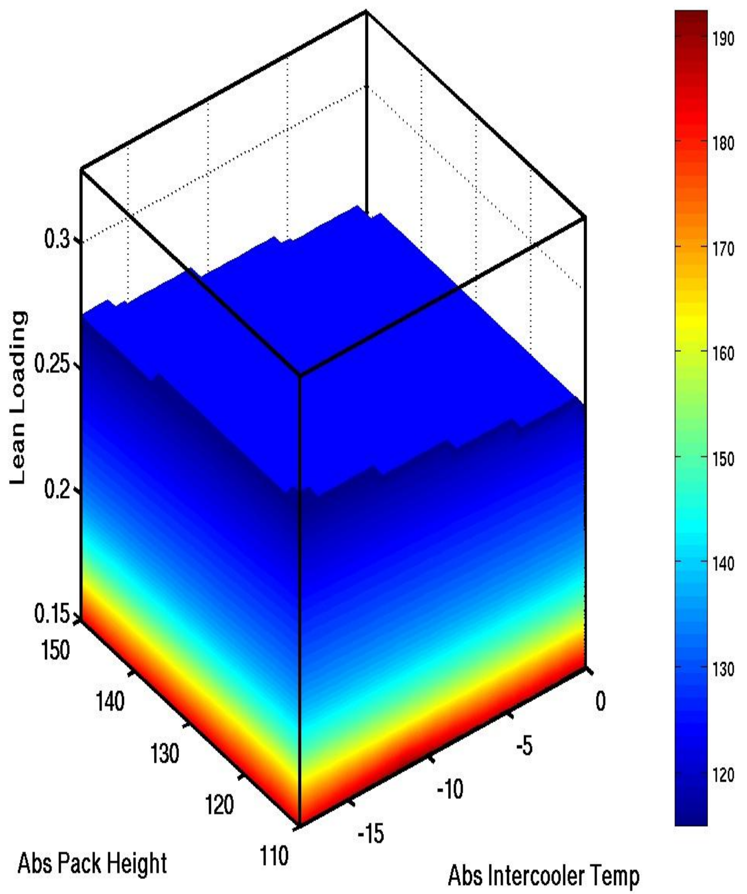
Let's use an example to illustrate the need for UQ



Variable	Min	Max	Units
Lean Loading	0.15	0.33	mol CO_2/mol MEA
Lean Solvent Feed Temperature	110	150	°F
Rich Solvent Feed Temperature	205	214	°F
Absorber Packing Height	15	40	ft
Absorber Intercooler Temperature Change	-18	0	°F
Regenerator Packing Height	10	30	ft
Regenerator Condenser Pressure	20	24	psia
Regenerator Condenser Temperature	110	150	°F
Compressor Intercooler 1 Temperature	110	140	°F
Compressor Intercooler 2 Temperature	110	140	°F

Objective: minimize the levelized cost of electricity while keeping carbon capture at above 90%

Optimization results using surrogate models



Optimal solution:

Lean solution = 2.66e-01
Abs packing height = 2.78e+01
Regen packing height = 1.95e+01
Abs Intercooler delta T= -1.11e+01
Lean Solvent Feed T = 1.29e+02
Rich Solvent Feed T = 2.14e+02
Regen Condenser P = 2.00e+01
Regen Condenser T = 1.29e+02

Which gives 90% CO_2 capture and LCOE ~ 113

However, it is known that some of the parameters in the model are uncertain: for example, reaction parameters

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- Scope: MEA equilibrium reactions

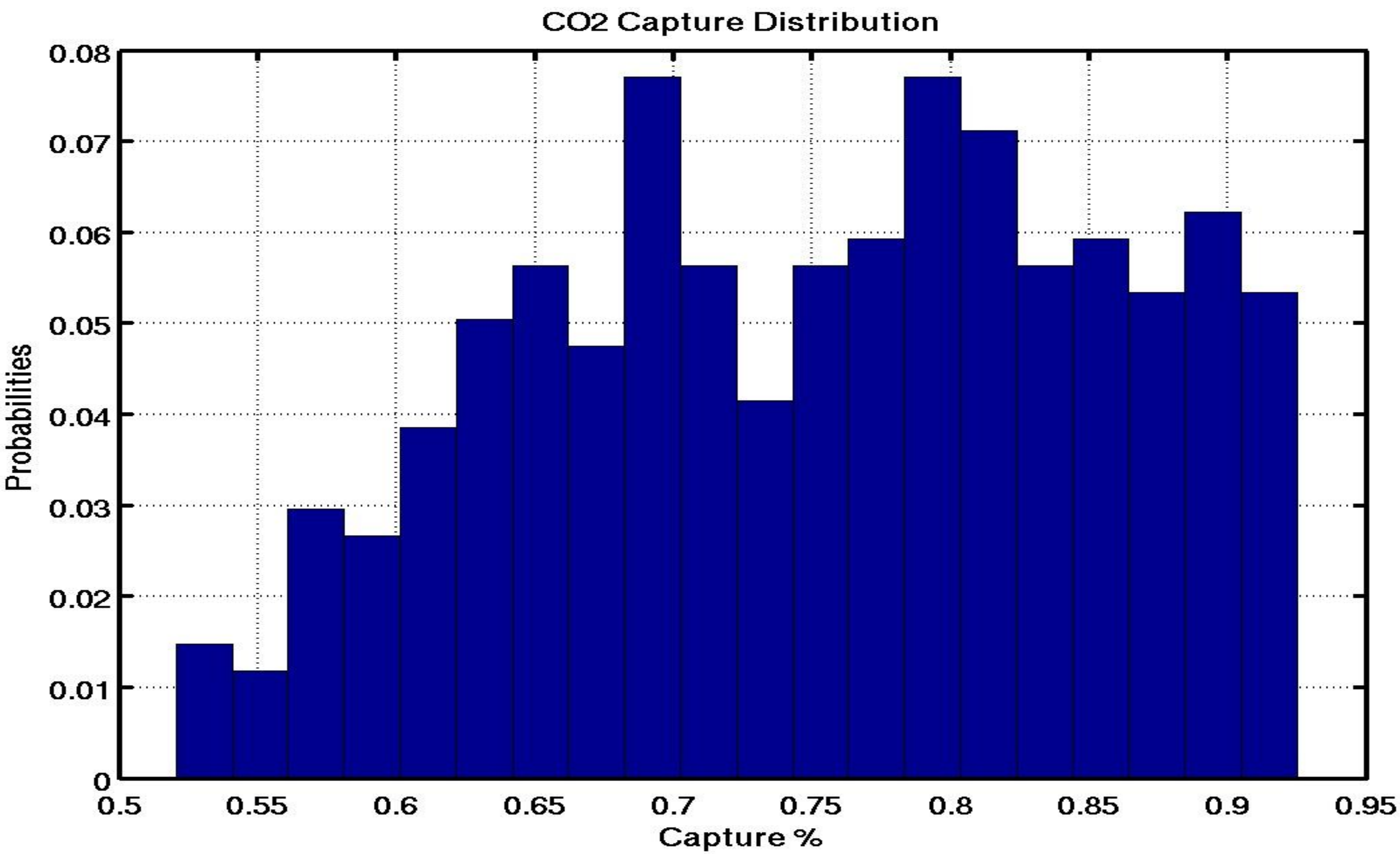
$H_2O + MEAH^+$	$\leftrightarrow$	$H_3O + MEA$	(Reaction 1-2)
$CO_2 + OH^-$	$\leftrightarrow$	HCO_3^-	(Reaction 2-2)
$H_2O + HCO_3^-$	$\leftrightarrow$	$H_3O^+ + CO_3^{2-}$	(Reaction 3-2)
$MEACOO^- + H_2O$	$\leftrightarrow$	$MEA + HCO_3^-$	(Reaction 4-2)
$2H_2O$	$\leftrightarrow$	$H_3O^+ + HO^-$	(Reaction 5-2)

$$\ln K_{eq} = A + \frac{B}{T} + C \ln T + DT$$

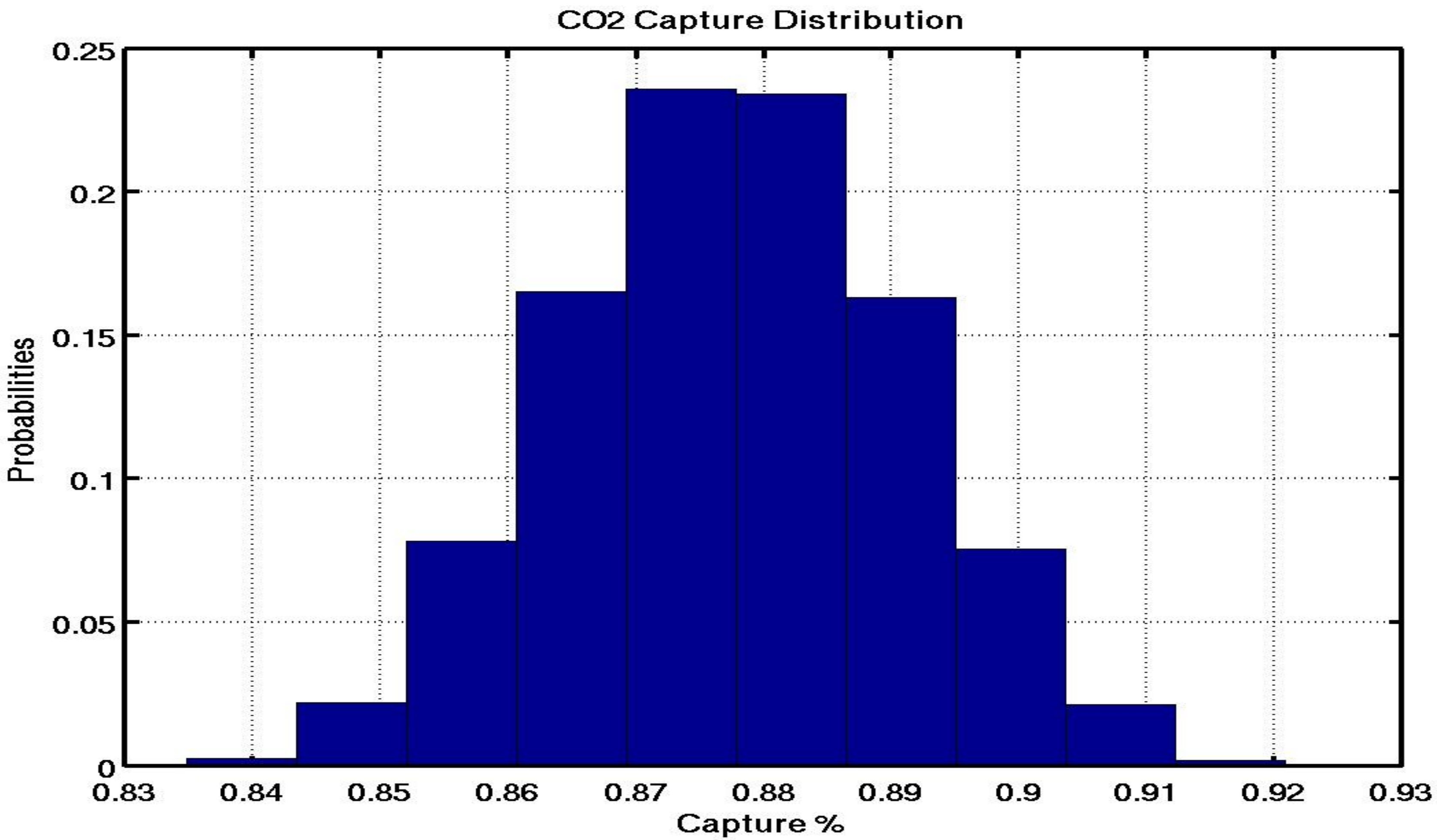
Reaction	A	B	C	D
1-2	0.7996	-8094.81	0.0	-0.007484
2-2	98.566	1353.8	-14.3043	0.0
3-2	216.049	-12431.7	-35.4819	0.0
4-2	1.282562	-3456.179	0.0	0.0
5-2	132.899	-13445.9	-22.4773	0.0

Other sources of uncertainties: mass transfer, equilibrium model, Flue gas composition, boundary conditions, …

As a result of parametric uncertainties, we have an uncertainty distribution for the CO2 capture %



The distribution may be unrealistic due to loose prescription of uncertainty bounds, adding data into the analysis, for example, gives



calibration

Questions we may ask about these uncertainties

- What is the uncertainty of the CO2 capture % as a result of these uncertainties?
- What other parameters in the systems are uncertain?
- Which parameters have the most effect on the output uncertainties?
- If I have more data, how much do they help in narrowing the output uncertainties?
- As a result of uncertainties, what is the probability that the CO2 capture falls below 90%?
- I am using an approximate process model, what is the effect of approximation on the accuracy of the solution?
- How do uncertainties affect the system design?

Welcome to the world of UQ

What is uncertainty quantification? One possible definition

Uncertainty quantification is the

- **identification (where the uncertainties are),**
  - **- Physics model, boundary conditions, data, …**
- **characterization (what form they are),**
  - **- Parametric (bounds, PDF, beliefs), model form**
- **propagation (how they evolve, forward/inverse),**
- **analysis (what are the impacts, quantitative) , and**
  - **- Sensitivity analysis, risk analysis, …**
- **reduction**

of uncertainties (all?) in simulation models.

How do we put these into practice? → a UQ process

1. Define the objective of the UQ study (e.g. quantify risk)
2. Problem specification (model, assumptions, QOI, data)
3. Preliminary parameter identification and selection
4. Characterize parameter uncertainties (literature, expert)
5. Integrate data into models (Data Fusion Methodology)
6. Parameter screening (Dimension Reduction Methodology)
7. Build surrogates (Response Surface Methodology)
8. Uncertainty/Sensitivity analysis (Global SA methodology)
9. Sensitivity/Risk analysis and predictability assessment
10. Expert reviews, documentation

Identifying relevant sources of uncertainties is a very important first step in a UQ study

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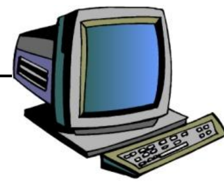
Mathematical model/simulation code



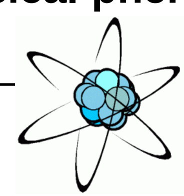
Design parameters → **Model responses**

Uncertainties in:
- Design parameter values
- initial/boundary conditions
- Measurement errors
- surrounding environment

Uncertainties in:
- Physics sub-models
  * imprecise/simplified physics
  * data-driven empirical models
- Sub-model couplings
- Missing physics
- Model implementation
- Roundoff errors
- Algorithmic errors (e.g. MC)
- Discretization errors

- Measurement errors
- Data scarcity
- Noisy data

Physical phenomenon



Experiments → **Observations**

Proper characterization of uncertainties is key to accurate propagation of uncertainties

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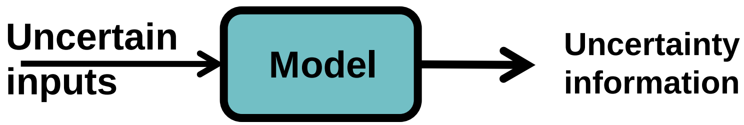
- **Aleatoric (known probability distributions)**
- **Epistemic**
  - **unknown probability distributions**
  - **use intervals or belief functions**
  - **missing physics (will give systematic errors)**
- **Mixed aleatoric/epistemic**
  - **known pdfs, unknown means and/or standard deviations**
- **Model form uncertainties**
  - **many possible equations to represent the submodels**
  - **each sub-model may have its own aleatoric/epistemic uncertainties**
- **Errors (considered as uncertainties?)**
  - **discretization errors, roundoff errors, algorithmic errors**

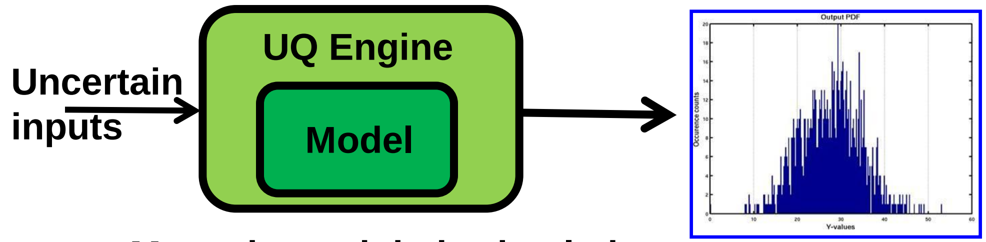
Different approaches to propagate uncertainties

- **Intrusive approach**



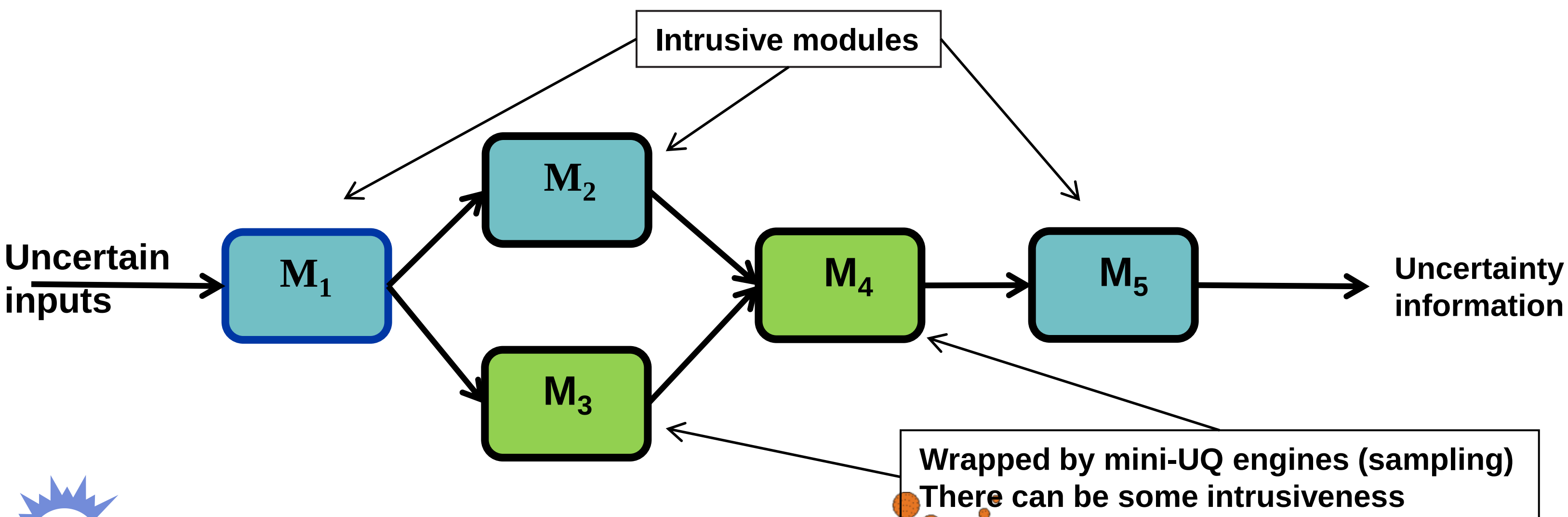
Stochastic simulation (UQ embedded in the model)

- **Non-intrusive approach**



Many deterministic simulation

- **hybrid approach for multi-physics (one scenario)**



Uncertainty propagation can be challenging for complex physics models due to

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- Models may be expensive to evaluate (hours on many processors)
- Nonlinear (may be discontinuous) input-output relationships
- High-dimensionality of the uncertain parameters (10’s -100’s)
- Complex correlation between uncertain parameters
- Mostly epistemic uncertainties (maybe mixed aleatoric/epistemic)
- Model form (structural) uncertainties
- Different types of data at different physics modules/subsystems
- Data scarcity
- Model operating at different regime than experiments (extrapolation)
- Uncertainties mixed with numerical errors in operator splitting
- Unknown unknowns (unknown processes, unknown couplings

PSUADE (A Problem Solving environment of Uncertainty Analysis and Design Exploration) is a software library of UQ tools

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- Confidence interval analysis
- Orthogonal arrays
- Cross validation
- Principal component analysis
- Correlation analysis
- Latin hypercube
- Kolmogorov Smirnov test
- Nonparametric testing
- Gaussian process
- Space-filling designs
- Screening designs
- Graphical analysis
- Derivative-based methods
- Delta test
- Constrained optimization
- Probability distributions
- Support vector machines
- Factorial design
- Second order sensitivity indices
- Manifold mapping optimization
- Sobol' decomposition
- Multivariate splines
- Main effects
- Adaptive response surfaces
- Total sensitivity indices
- Sparse grids
- Markov chain Monte Carlo
- Reliability analysis
- Fourier amplitude sampling test
- Artificial neural networks
- Bayesian Sensitivity analysis
- Regression analysis
- Analysis of variance

PSUADE is a toolkit for facilitating different UQ methodologies

- **Methodologies/methods: (arbitrary input inequality constraints)**
  - several dimension reduction methods
  - classical uncertainty analysis methods
  - many response surface methods (including adaptive)
  - several global sensitivity analysis methods
  - some basic risk assessment methods
  - numerical/stochastic optimization methods
  - hypothesis testing, principal component analysis
- **A job execution environment (to support automation)**
  - synchronous and asynchronous modes
  - dependency and chain modes (suitable for psub/moab)
  - multiple single-processor, multiple multiple-processor (intrusive)
- **An interactive user interface**
  - many ways of visualizing uncertainties

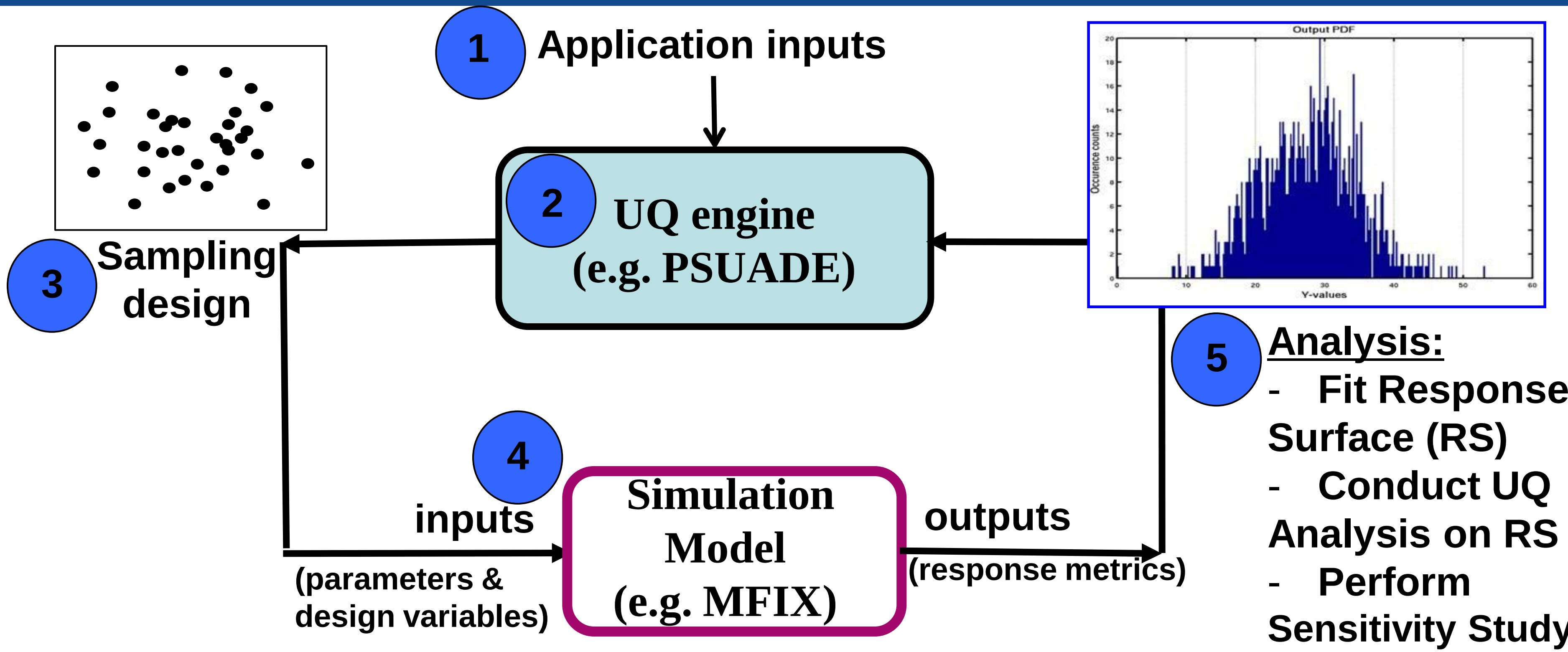
Preliminary Results for Demonstration of Non-intrusive Uncertainty Quantification Study with MFIX Simulations:

- Sample Problem # 1: DES Fluidized Bed
- Sample Problem # 2: Gasification

How Uncertainty Quantification Can Be Used in Our Community?

- What impact do parameter/model uncertainties have on model outputs? Establish confidence levels & quantitative quality assessment in simulation results.
- Which parameters cause the most output uncertainties? [Sensitivity Analysis]
- How do output uncertainties affect input uncertainties? [Inverse UQ]
- How to use observed data to calibrate system parameters? [Calibration]
- In view of uncertainty, how to quantify risk? [Risk analysis]

Non-intrusive Uncertainty Quantification



- 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

MFIX, Open Source Multiphase Flow Code

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MFiX

http:/mfix.netl.doe.gov

Mass conservation for phase m (m=g for gas and s for solids)

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \nabla\cdot(\varepsilon_m \rho_m \vec{v}_m) = \sum_{l=1}^{N_m} R_{ml}$$

Momentum conservation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m \vec{v}_m) + \nabla\cdot(\varepsilon_m \rho_m \vec{v}_m \vec{v}_m) = \nabla\cdot\overline{\overline{S}}_m + \varepsilon_m \rho_m \vec{g} + \sum_n \vec{I}_{mn}$$

Granular energy conservation (m ≠ g)

$$\frac{3}{2}\varepsilon_m \rho_m \left(\frac{\partial \Theta_m}{\partial t} + \vec{v}_m \cdot \nabla\Theta_m\right) = \nabla\cdot\vec{q}_{\Theta_m} + \overline{\overline{S}}_m : \nabla\vec{v}_m - \varepsilon_m \rho_m J_m + \Pi_{\Theta_m}$$

Energy conservation

$$\varepsilon_m \rho_m C_{pm}\left(\frac{\partial T_m}{\partial t} + \vec{v}_m\cdot\nabla T_m\right) = -\nabla\cdot\vec{q}_m + \sum_n \gamma_{mn}(T_n - T_m) - \Delta H_{rm}$$

Species mass conservation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{ml}) + \nabla\cdot(\varepsilon_m \rho_m X_{ml}\vec{v}_m) = R_{ml}$$

R&D 100

R&D100 Award 2007

FLC Federal Laboratory Consortium for Technology Transfer

Excellence in Technology Transfer Award 2008 for C3M

Federal Laboratory Consortium FLC Mid-Atlantic Region

Tech-Transfer Award 2006

- Syamlal et al. "MFIX Documentation, Theory Guide,“ DOE/METC-94/1004, NTIS/DE94000087 (1993)
- Benyahia et al. “Summary of MFIX Equations 2005-4”, From URL http://www.mfix.org/documentation/MfixEquations2005-4-3.pdf, July 2007.

Demonstration Problem for Parametric Non-Intrusive UQ: Gasification

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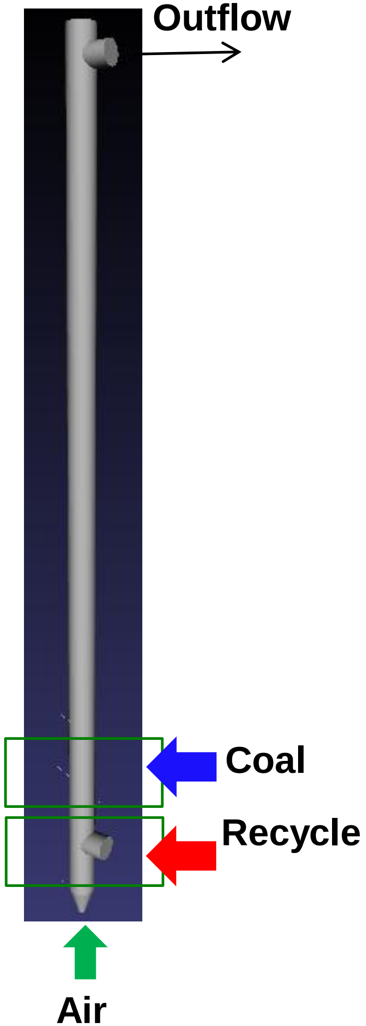

Problem Setup and Properties:
Solids: Rosebud coal with D_p = 0.01 cm, ρ_p = 2.85 g/cm^3 Coal flow rate: 1 g/s, Recycled char :100 g/s
Gas: Air flow rate: 2.76 g/s
Geometric dimensions = 10 cm x 200 cm **Grid Resolution =** (10 x 200) cells **(2–D simulation)**
Governing Physics & Models: Multiphase flow hydrodynamics, heat transfer, chemical reactions.
Numerical Scheme: Spatial discr. : Upwind Temporal discr.: 1st order

Test problem provided by Dr.Tingwen Li

Demonstration Problem for Parametric Non-Intrusive UQ: Gasification (con't)

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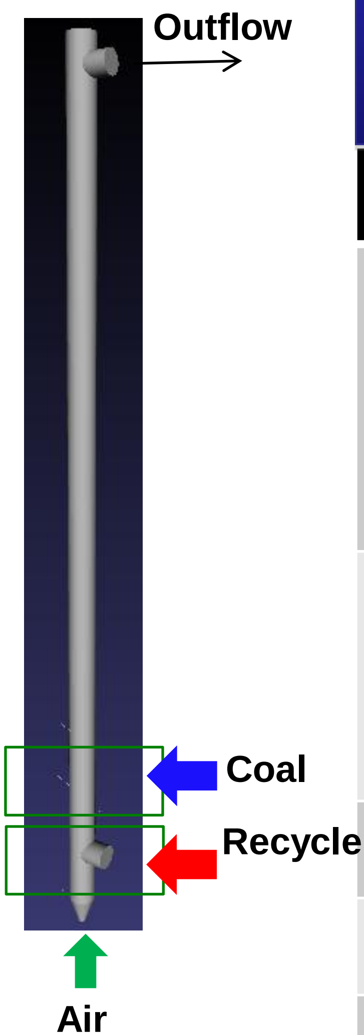

Objective: Determine the effect of uncertainty in reactions rates on the species mass composition at the outlet of the gasifier.

Uncertainty Quantification Study Properties:

Input parameters with Uncertainty (min-max range):
(1)Reaction rate constant for CO_2 gasification
C(6) : 0.1 – 10,100,1000.0 [Uniform distribution]
(2) Reaction rate constant for devolatilization
C(8) : 0.1 – 10,100,1000.0 [Uniform distribution]

Response Variables:
(1) CO species mass fraction at the outlet
(2) CH_4 species mass fraction at the outlet
(3) H_2 species mass fraction at the outlet

UQ Toolbox/Engine: PSUADE from LLNL

Sampling Method = LPTAU, **Sample Size = 100, 1024**

Computational Cost to simulate 40 seconds
Per sample: 1 to 1.5 hrs wallclock on single core

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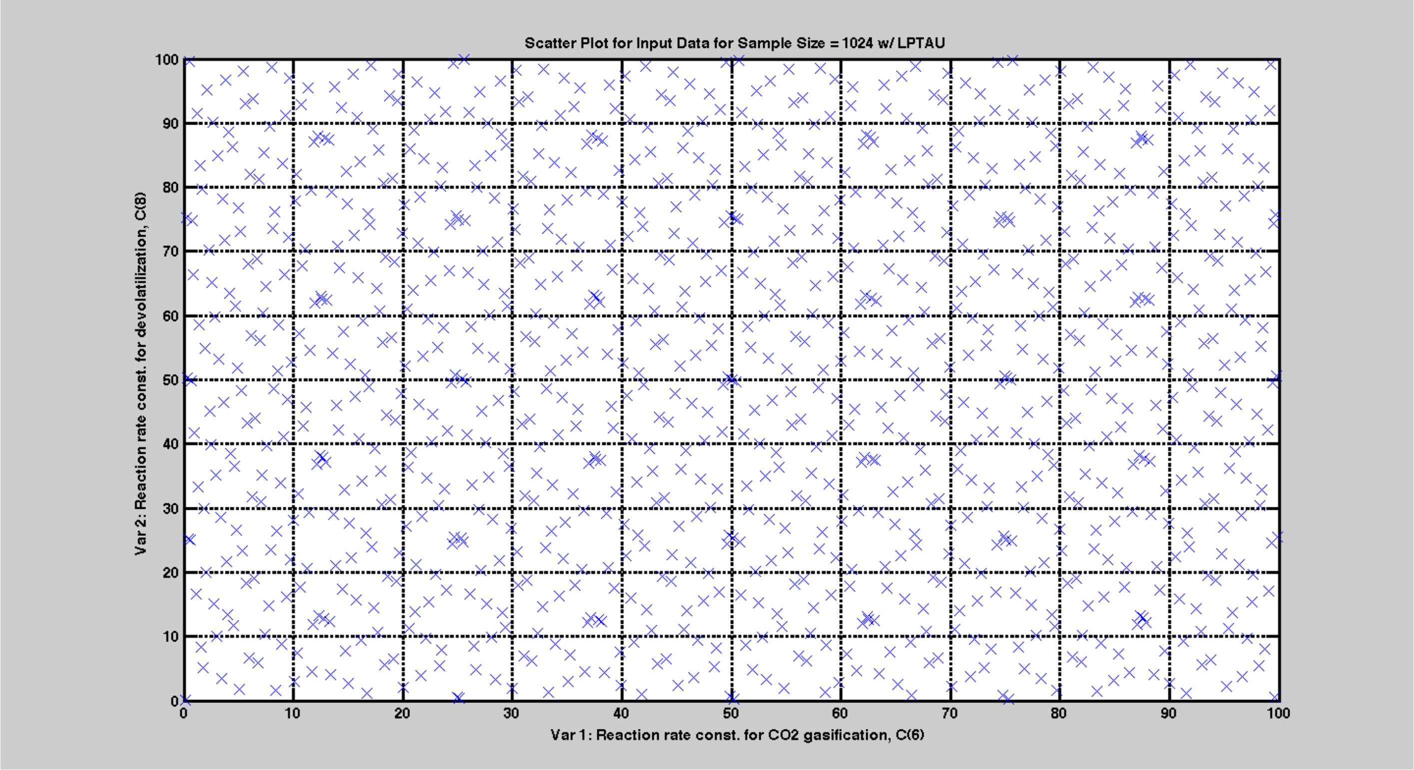
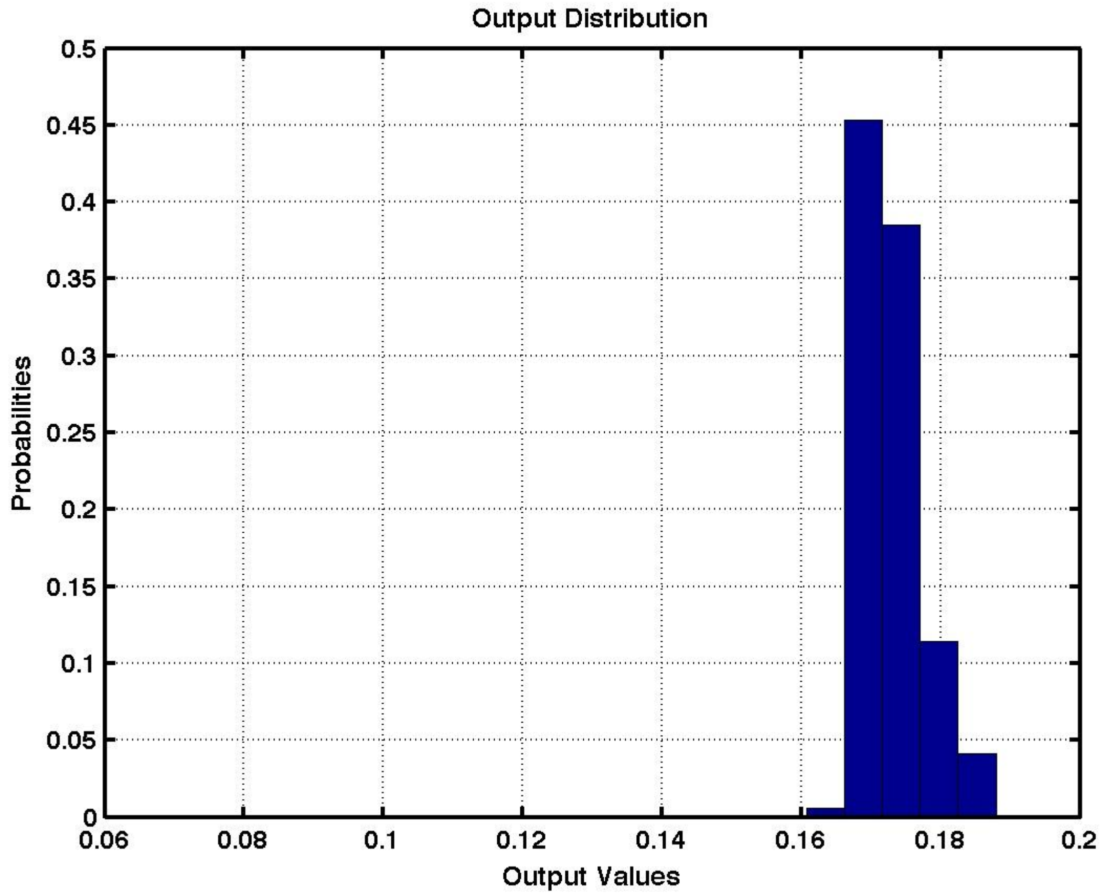
Demonstration Problem for Parametric UQ Study: Gasification

Sample size = 1024

Variables with uncertainty:	lower – upper bound
(1)Reaction rate constant for CO2 gasification, C(6) :	0.1 - 100
(2)Reaction rate constant for devolatilization, C(8) :	0.1 - 100



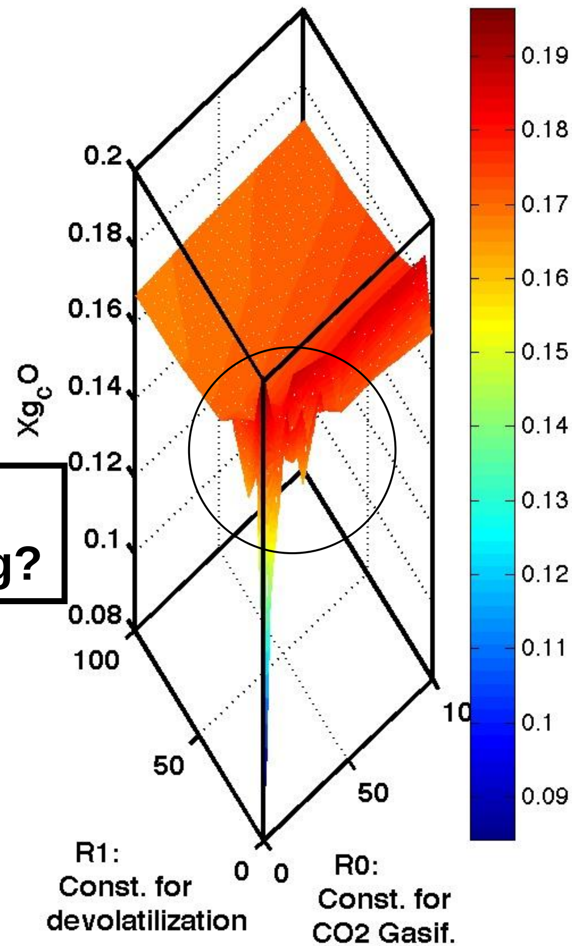
Histogram of Output 1 : CO mass fraction (Xg_CO)



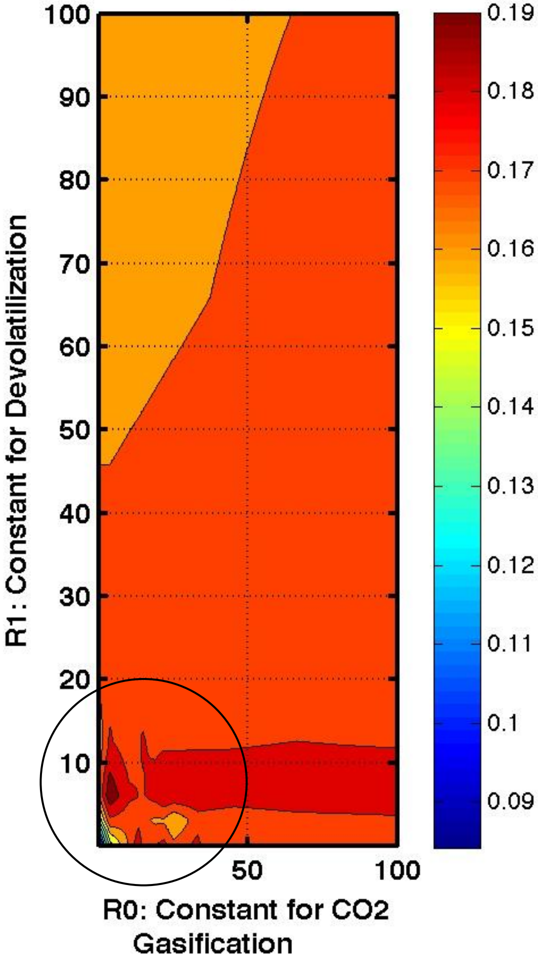
Sample mean = 1.7295e-01

Sample std dev = 5.0652e-03

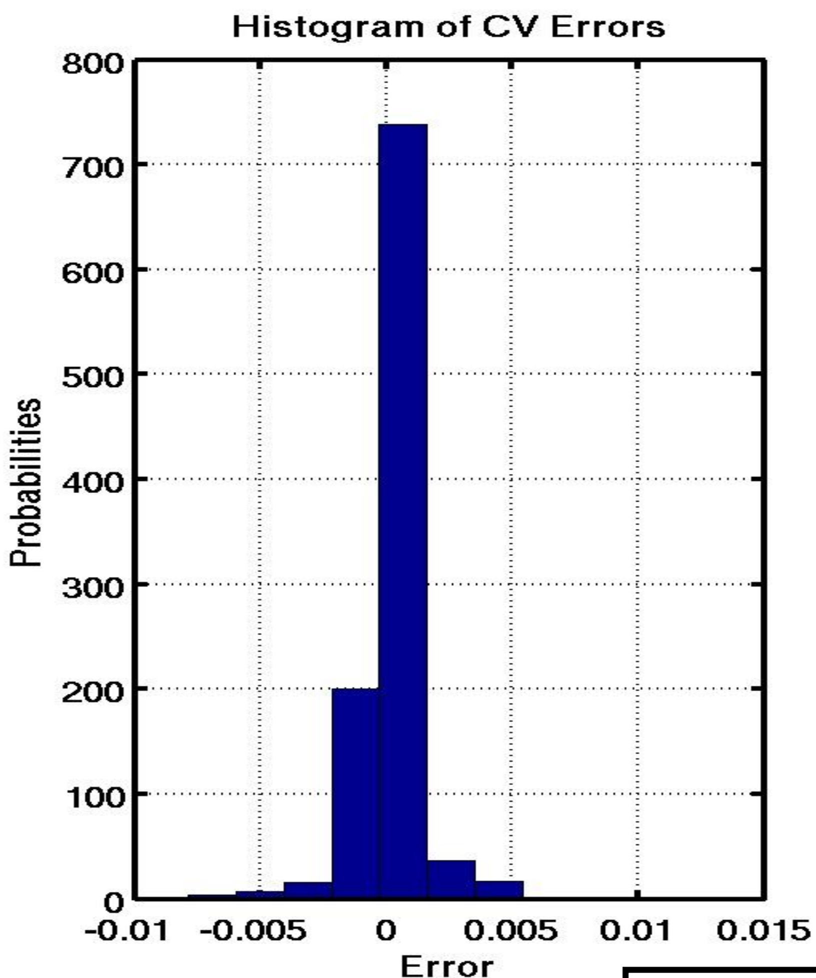
Response Surface for CO mass fraction (Xg_CO): Cubic splines based method (MARS)

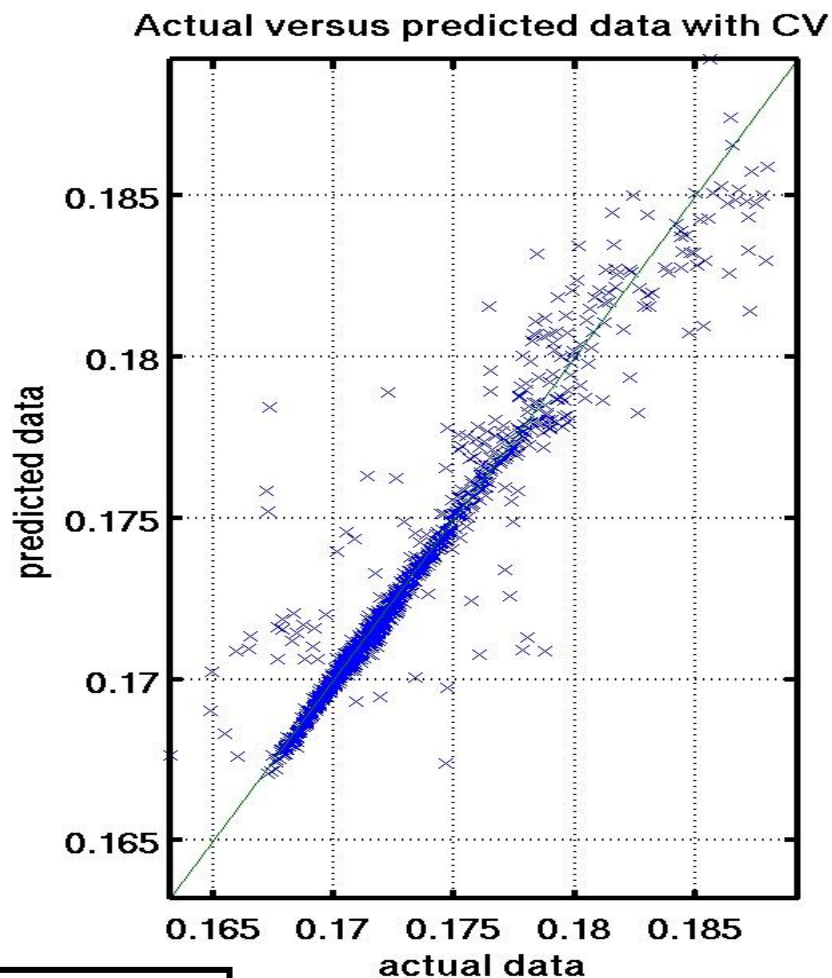


What is happening?



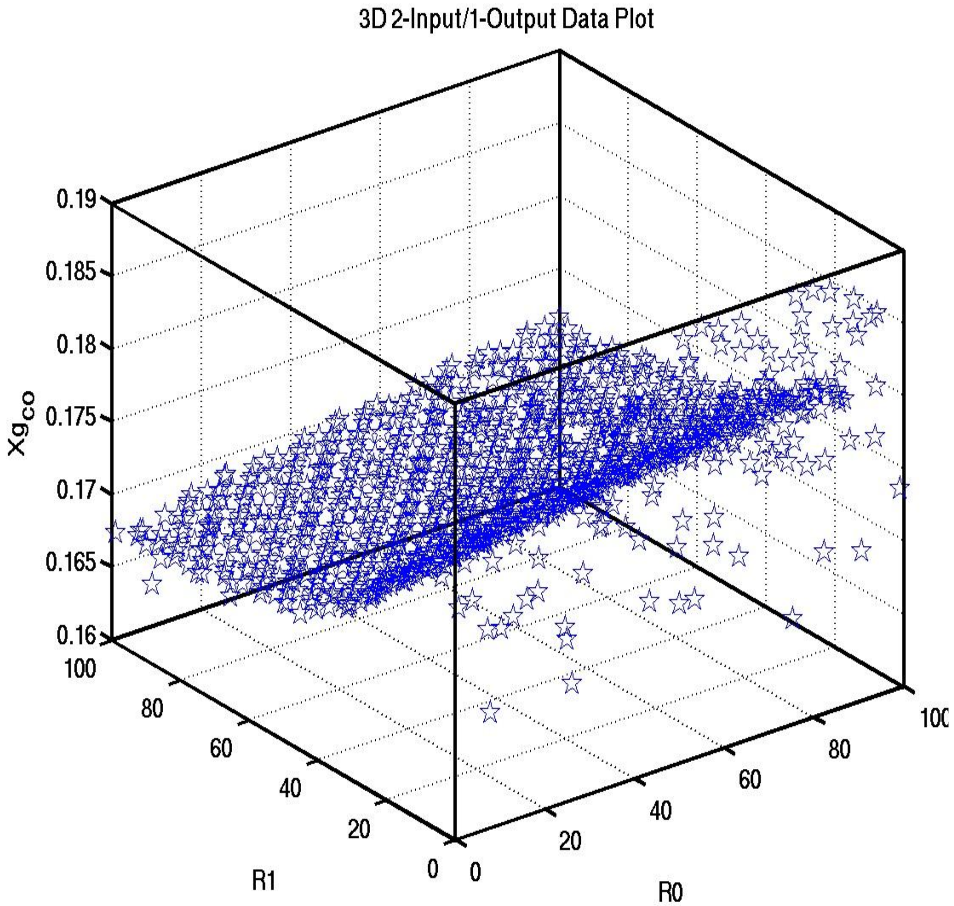
Response Surface Analysis (Xg_CO):

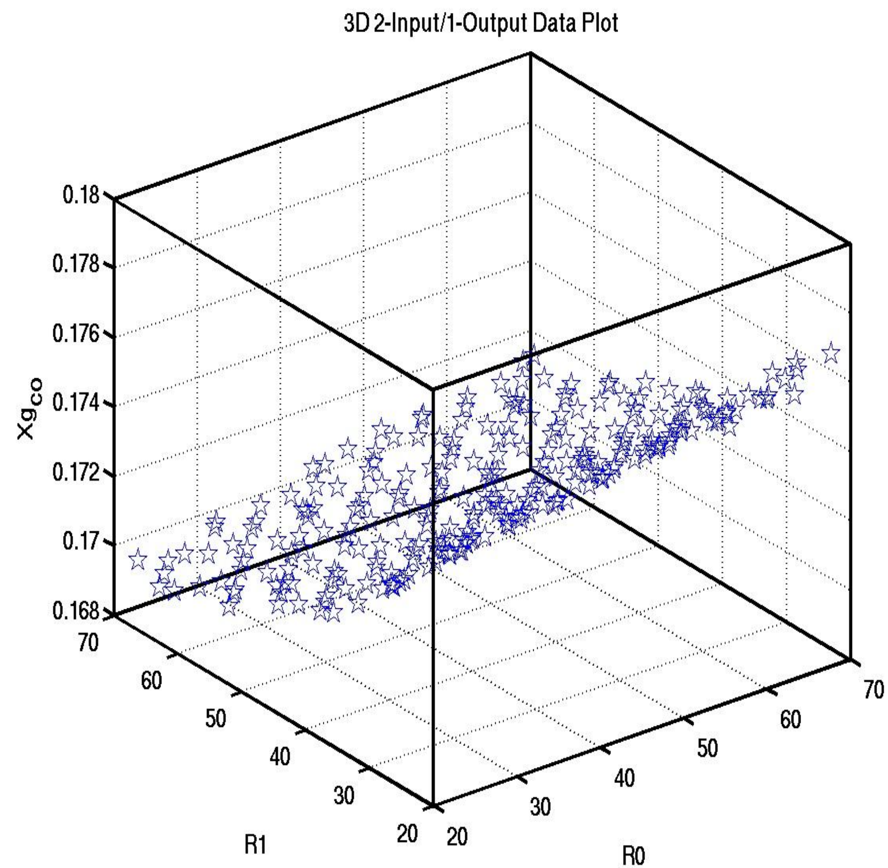




Not acceptable!!

What happened? Let's examine Xg_CO more closely.

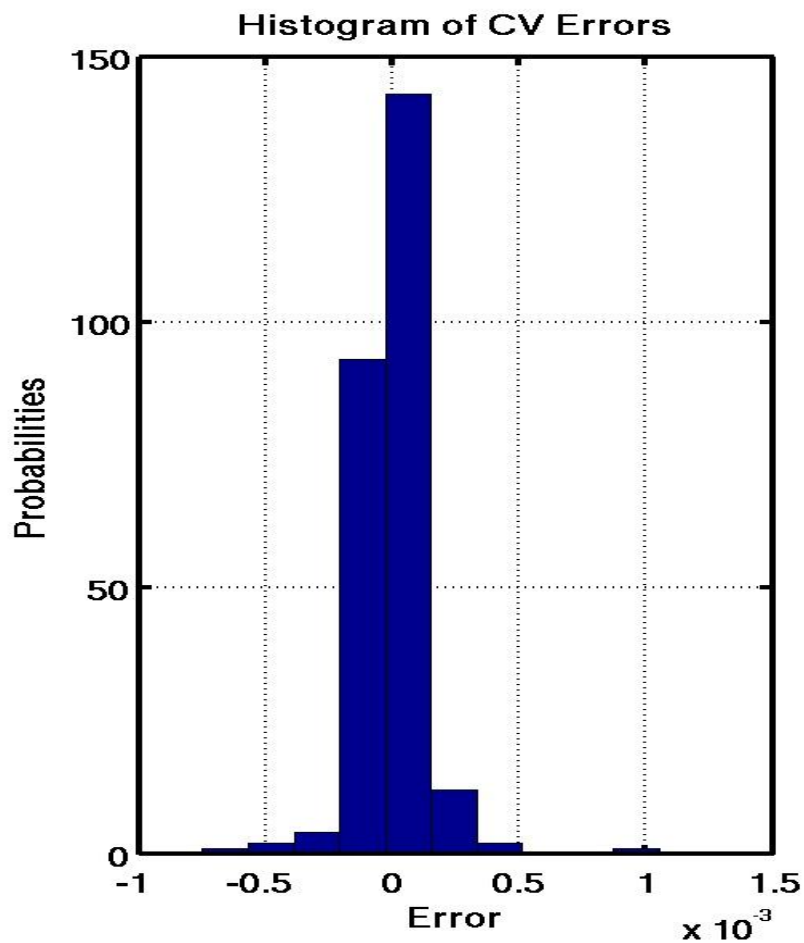


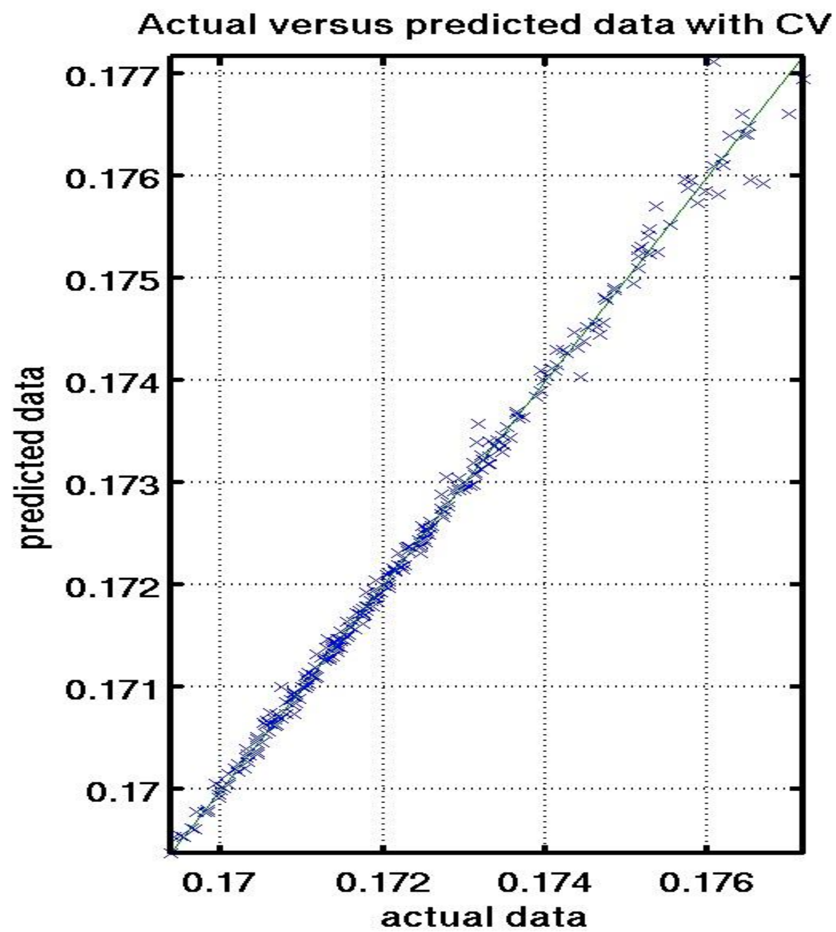


Many outliers on the edge

Alter the input range

Response Surface Analysis (on Xg_CO): on small range





Much more acceptable!!

Sensitivity Analysis for CO mass fraction:

- **Using the response surface for Xg_CO, we compute the global sensitivity indices for both input variables.**
- **Assume uniform distributions for input uncertainties.**
- **The sample mean is 0.173**
- **The sample standard deviation is 0.005**
- **For this specific example problem % of variance from each input is determined as:**
  - Input # 1: Reaction rate const. for CO2 gasification **~ 10%**
  - Input # 2: Reaction rate constant for devolatilization **~ 90%**

Summary

- UQ activities recently started within Multiphase Flow Group, work in progress.
- Several challenges to perform UQ in multiphase reacting flows:
  - Many uncertain parameters exist,
  - Highly nonlinear,
  - Transient behavior,
  - Computationally intensive simulations,
  - No assurance all samples will converge
- The trade-off between sample size and non-intrusive UQ analysis accuracy due to computational cost per sample.

Thank you! Questions ?

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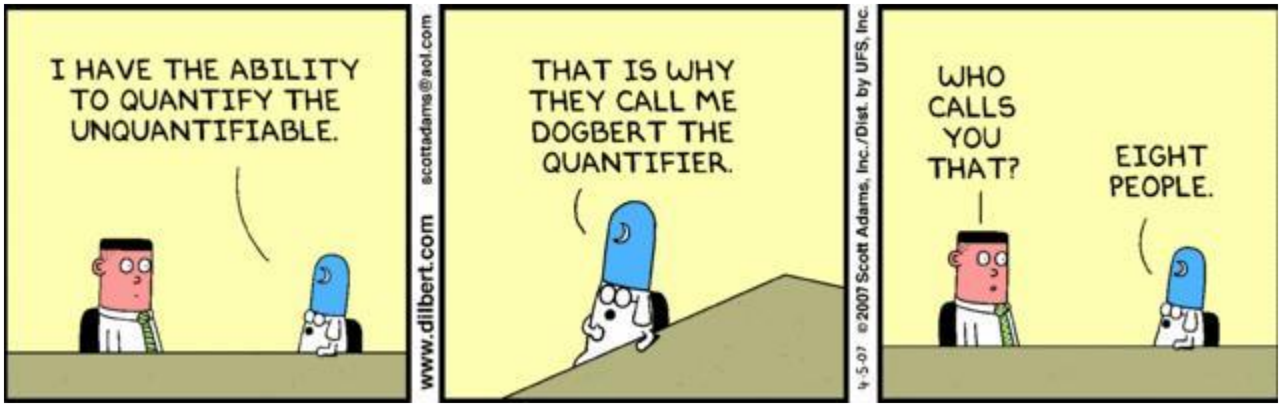

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APPENDIX

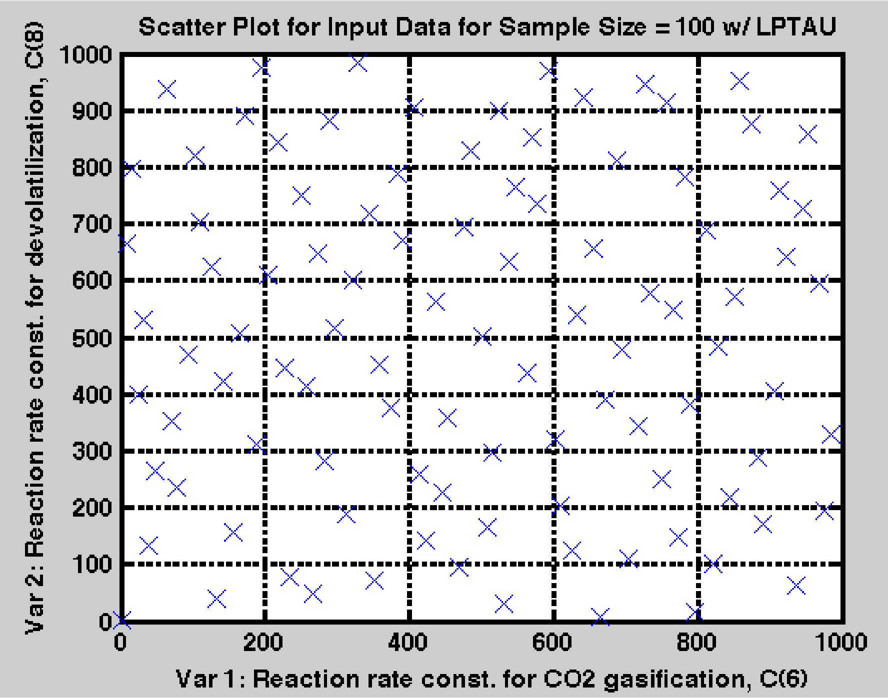
Does the Sample Size Matter? A Comparison.

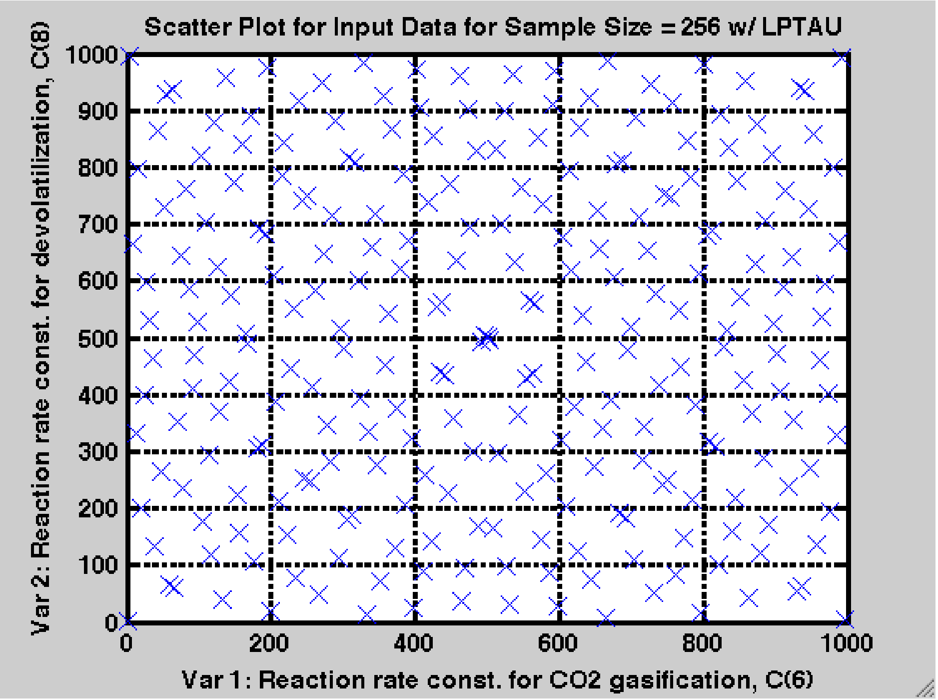
Sampling Method: LPTAU

Variables with uncertainty: lower – upper bound

(1)Reaction rate constant for CO2 gasification, C(6) : 0.1 - 1000

(2)Reaction rate constant for devolatilization, C(8) : 0.1 - 1000





Sample size = 100 **Sample size = 256**

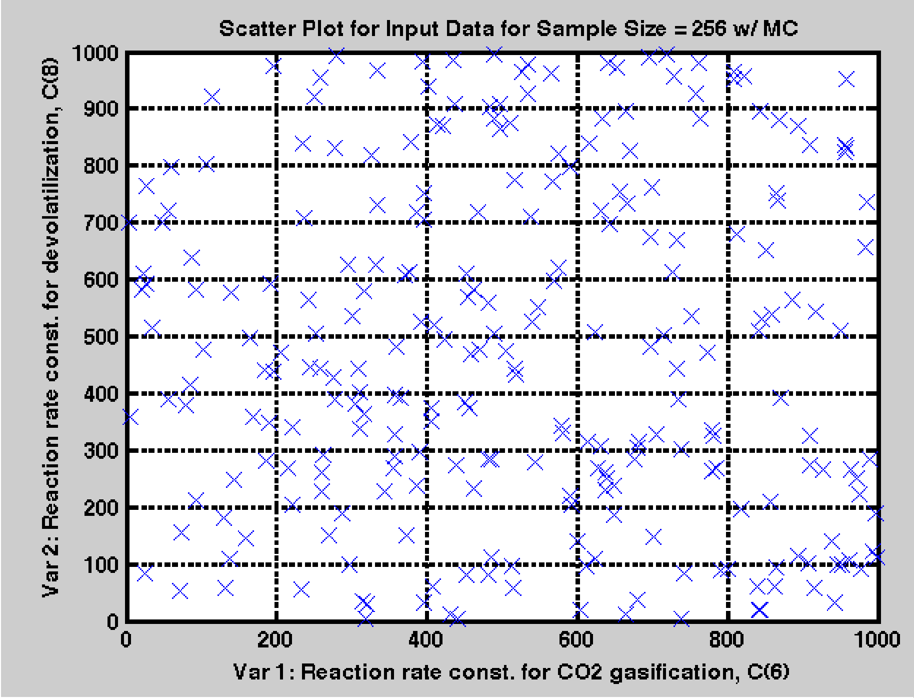
Does the Sampling Method Matter? A Comparison.

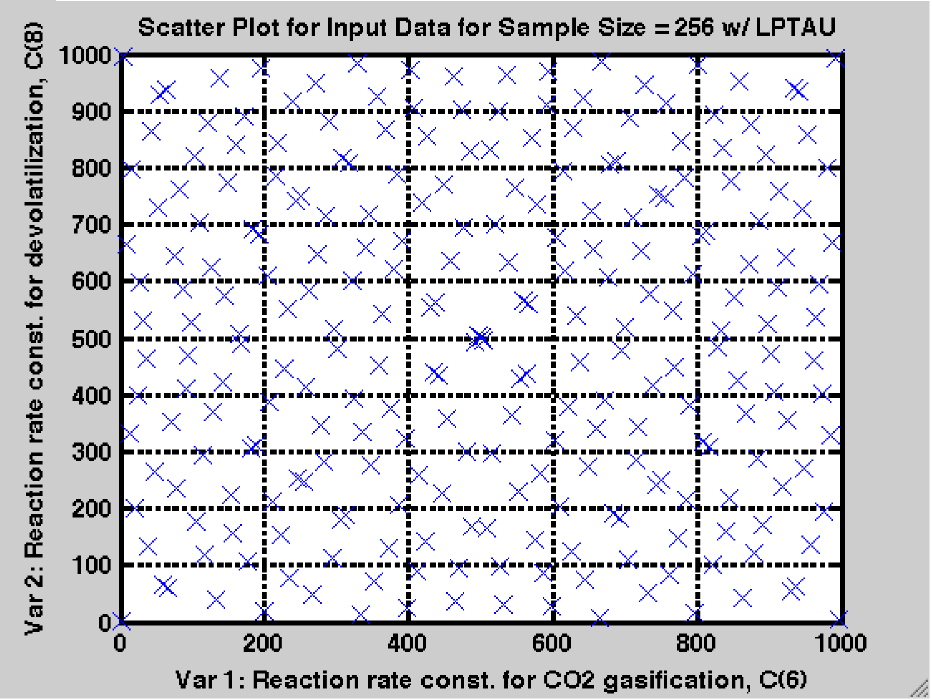
Sample size = 256

Variables with uncertainty: lower – upper bound

(1)Reaction rate constant for CO2 gasification, C(6) : 0.1 - 1000

(2)Reaction rate constant for devolatilization, C(8) : 0.1 - 1000





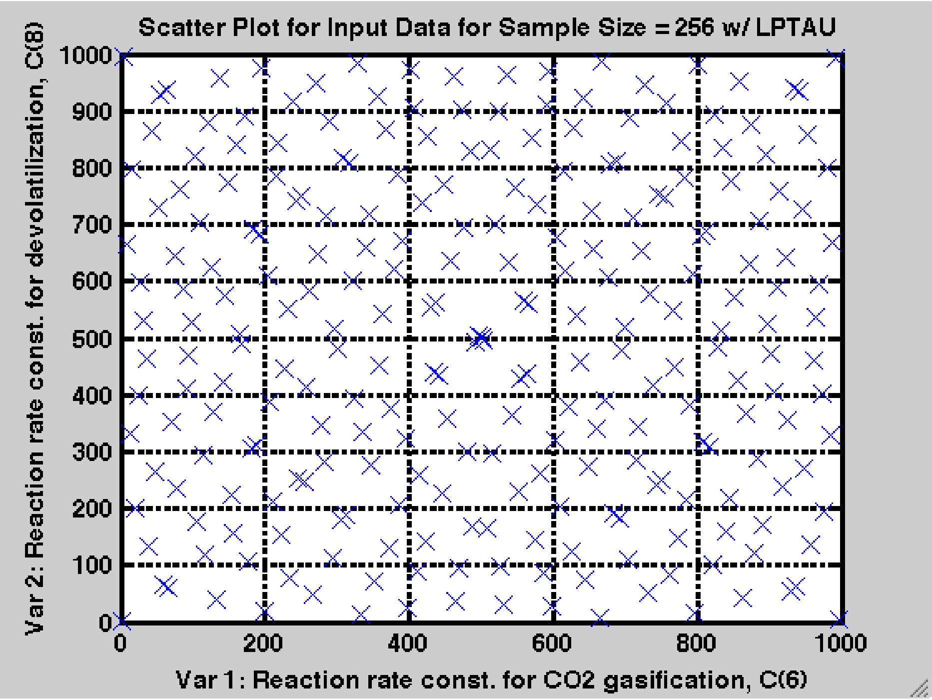
Monte Carlo Sampling (MC)

Quasi Random Sequence Generator Sampling (LPTAU)

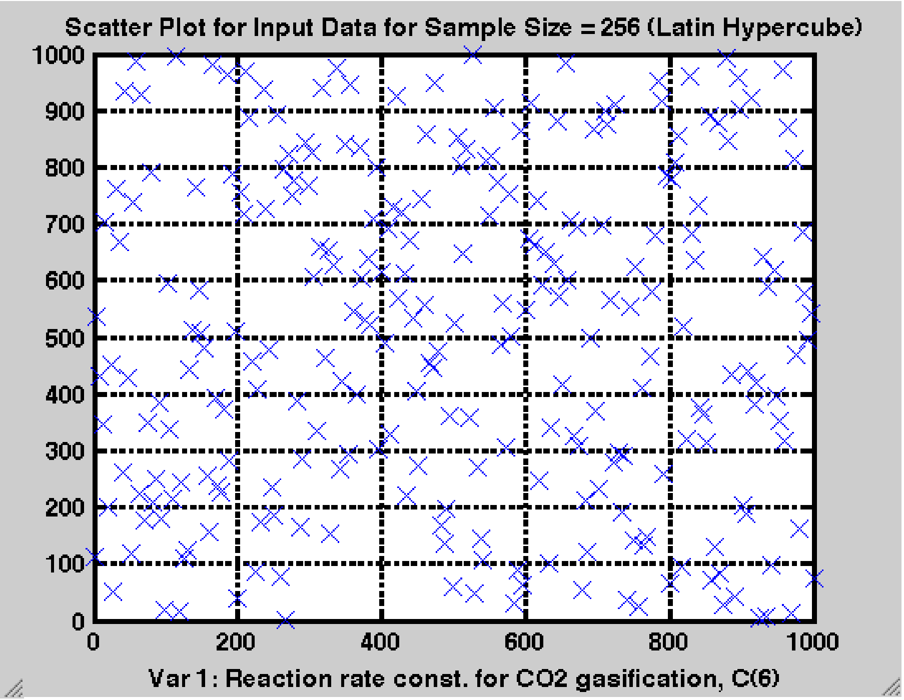
Does the Sampling Method Matter? A Comparison. (cont'd)

Sample size = 256

Variables with uncertainty:	lower – upper bound
(1)Reaction rate constant for CO2 gasification, C(6) :	0.1 - 1000
(2)Reaction rate constant for devolatilization, C(8) :	0.1 - 1000



Quasi Random Sequence Generator Sampling (LPTAU)



Latin Hypercube Sampling (LH)

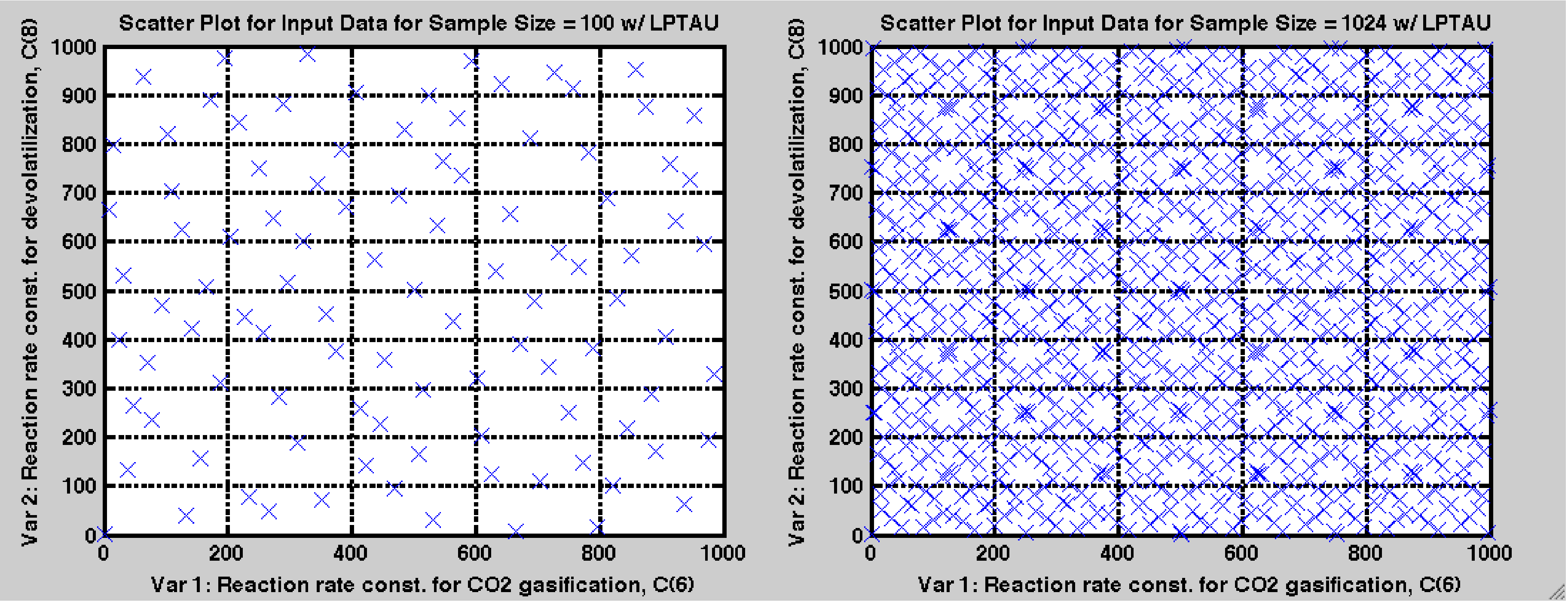
Does the Sample Size Matter? A Comparison. (cont'd)

Sampling Method: LPTAU

Variables with uncertainty: — **lower – upper bound**

(1)Reaction rate constant for CO_2 gasification, C(6) : 0.1 - 1000

(2)Reaction rate constant for devolatilization, C(8) : 0.1 - 1000



Sample size = 100 — **Sample size = 1024**

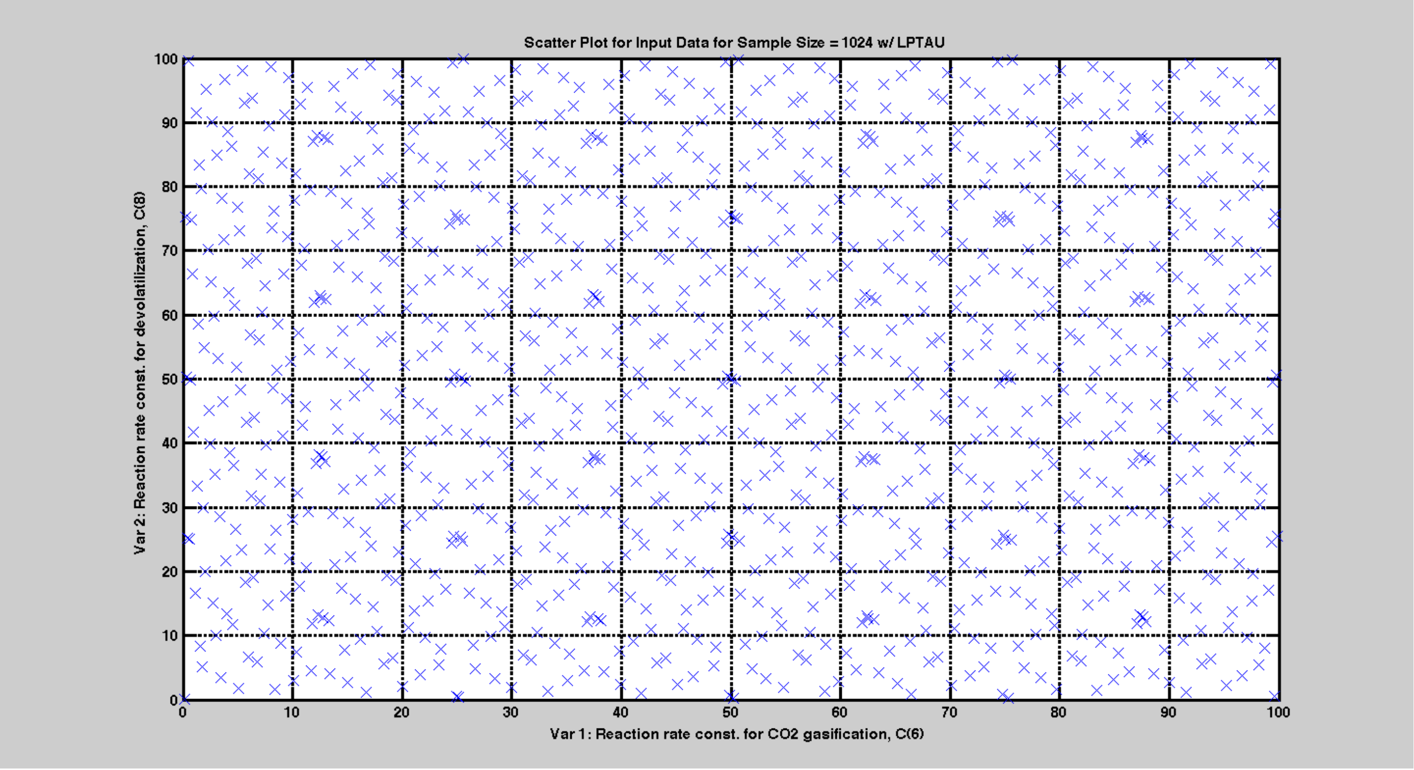
Sample Problem # 2 for Parametric UQ Study: Gasification

Sample size = 1024

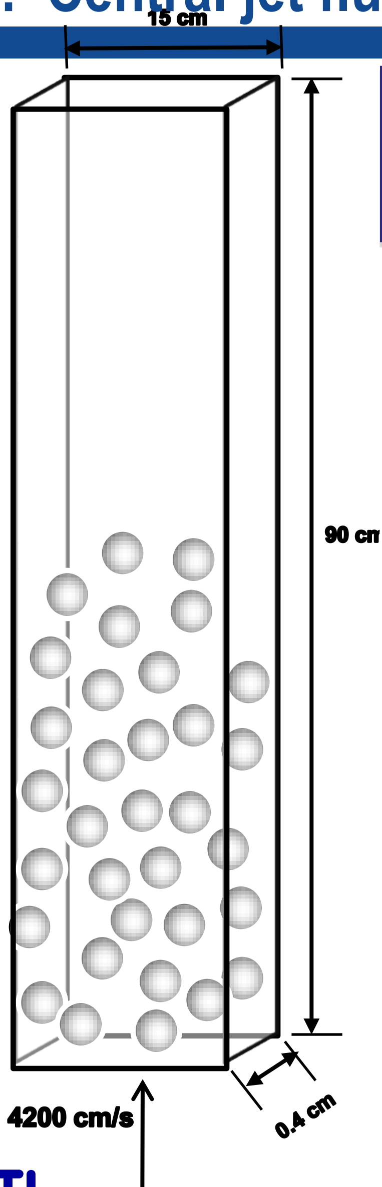
Variables with uncertainty: **lower – upper bound**

(1)Reaction rate constant for CO2 gasification, C(6) : 0.1 - 100

(2)Reaction rate constant for devolatilization, C(8) : 0.1 - 100



Sample Problem # 1 for Parametric Non-Intrusive UQ Study: Central jet fluidized bed



Objective: Determine the effect of uncertainty in coefficients of restitution and friction on bed expansion and bubbling behavior.

Problem Setup and Properties:

Solids: D_p = 0.4 cm, ρ_p = 2.7 g/cm^3
Initial solid volume fraction: 0.4 up to height of 20 cm
5 parcels per cell

Gas: Air at standard conditions
Fluidization velocity = 4200 cm/s with no slip BC at walls

Geometric dimensions = (15 x 90 x 0.4) cm^3
Grid Resolution = (15x45) cells **(2–D simulation)**

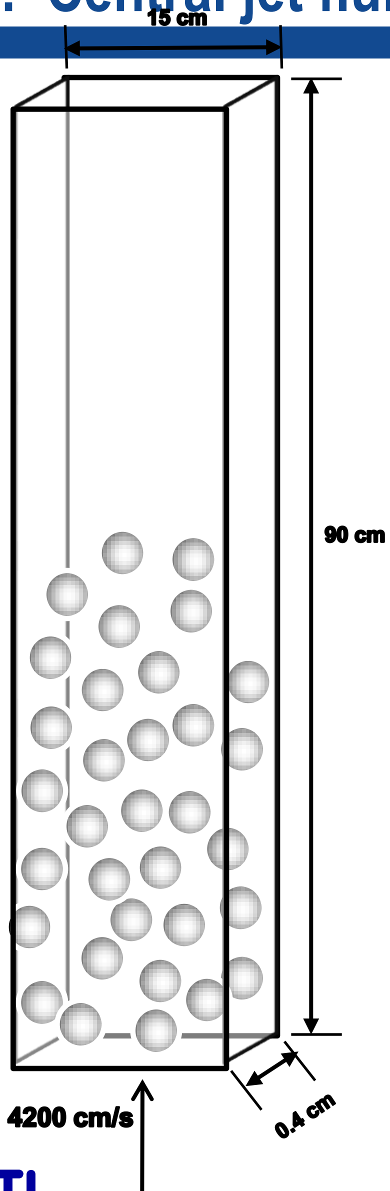
Governing Physics & Models: Multiphase flow hydrodynamics with DEM, Drag model: Wen &Yu/Ergun,

Numerical Scheme: Δt_{max} = 1.E-03. , First order upwind

Test problem provided by Dr. Rahul Garg

Sample Problem # 1 for Parametric Non-Intrusive UQ Study: Central jet fluidized bed (cont'd)

CCSI Carbon Capture Simulation Initiative



Objective: Determine the effect of uncertainty in coefficients of restitution and friction on bed expansion and bubbling behavior.

Uncertainty Quantification Study Properties:

Input parameters with Uncertainty (min-max range):

(1)Particle-particle coefficient of restitution

e_n = 0.6 – 1.0 [Uniform distribution]

(2) Particle-wall coefficient of restitution

e_n = 0.6 – 1.0 [Uniform distribution]

Response Variables:

(1)Average bed expansion height (cm?)

(2)Average pressure drop (??)

UQ Toolbox/Engine: PSUADE from LLNL

Sampling Method = LPTAU, **Sample Size = 24, 100**

Computational Cost to simulate 20 seconds

Per sample: 2 to 2.5 hrs wallclock on single core

Test problem provided by Dr. Rahul Garg

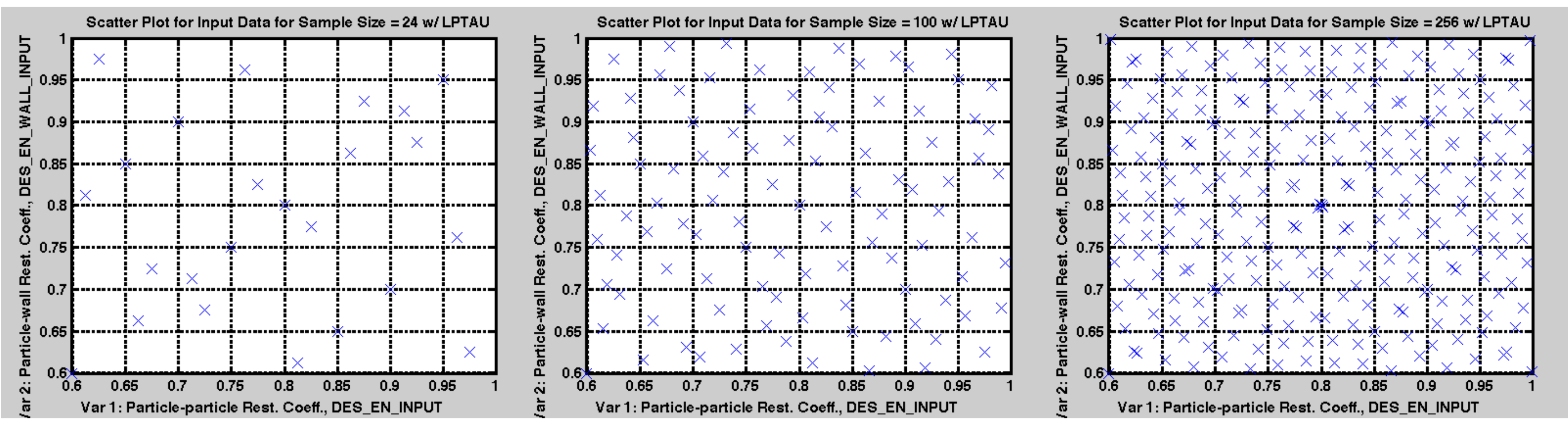
Does Sample Size Matter?

Quasi Random Sequence Generator Sampling (LPTAU)

Variables with uncertainty: lower – upper bound

(1)Particle-particle Restitution Coeff., DES_EN_INPUT : 0.6 - 1.0

(2)Particle-wall Restitution Coeff., DES_EN_WALL_INPUT: 0.6 - 1.0

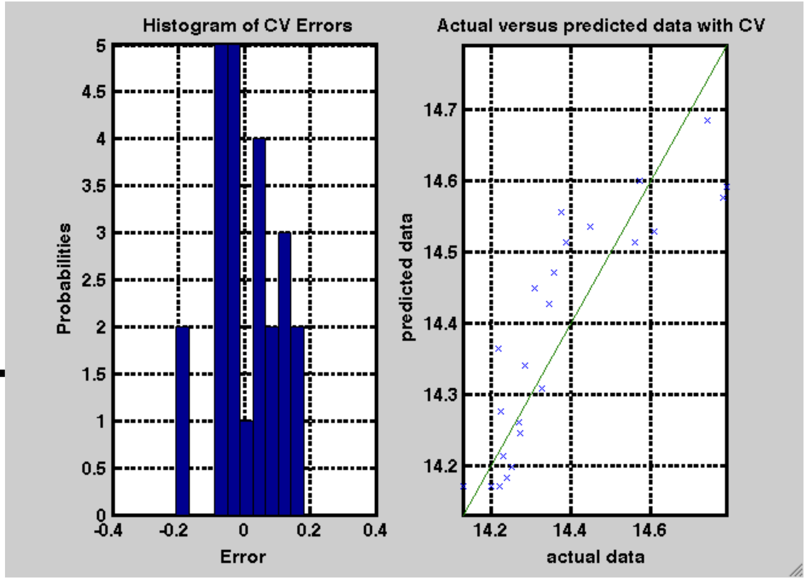


Sample size = 24 **Sample size = 100** **Sample size = 256**

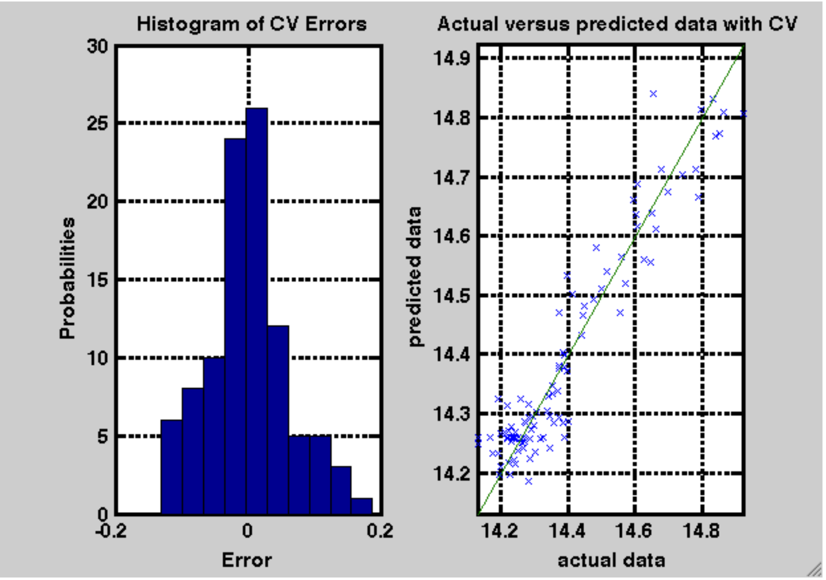
Comparison of Fitness Quality of Response Surface for Output 1: Avg. Bed Height for different sample size runs:

Carbon Capture Simulation Initiative

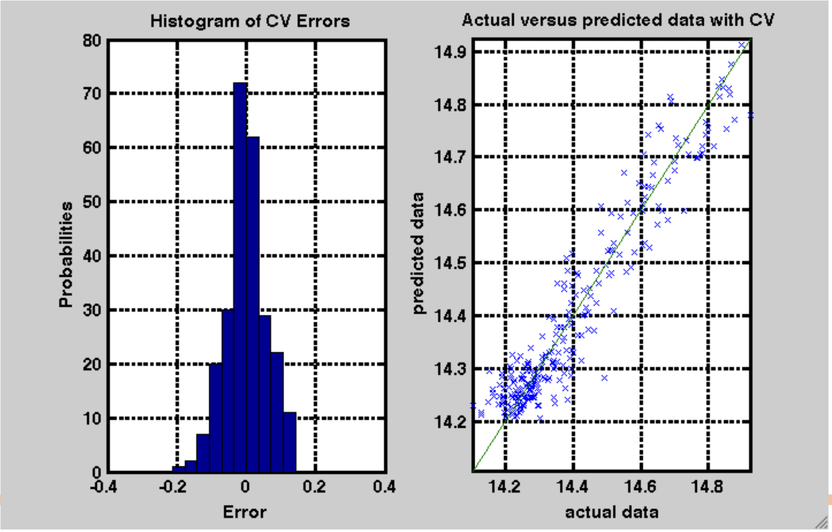
Sample Size = 24



Sample Size = 100



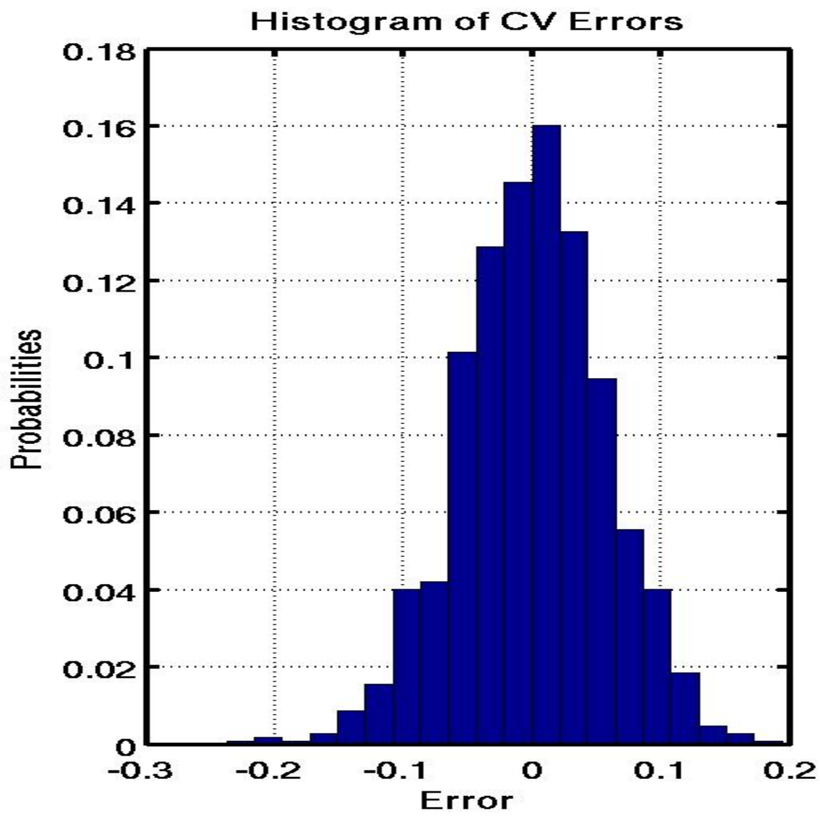
Sample Size = 256

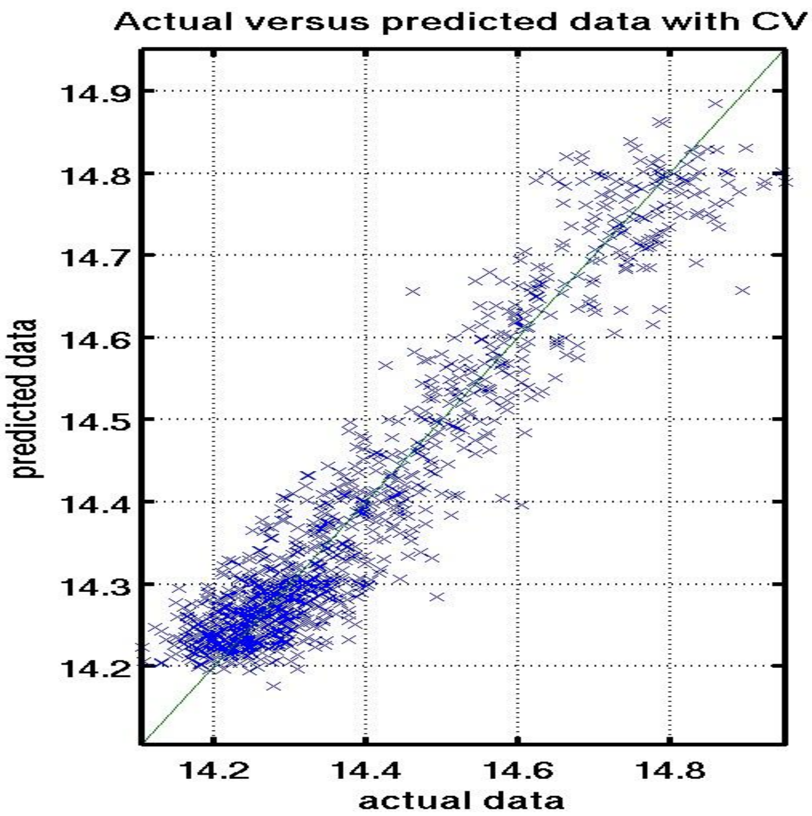


Response Surface Method: Multivariate Adaptive Regression Splines (MARS)

Fluidized Bed Data Analysis (Avg_h)

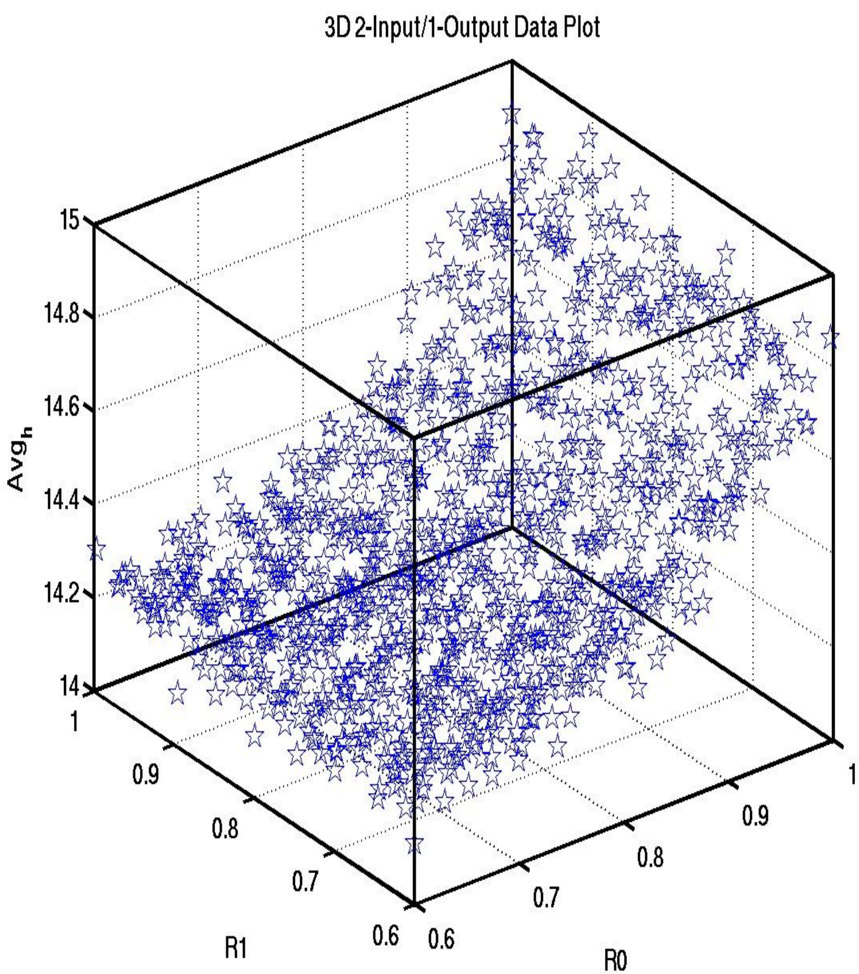
- response surface analysis using cubic splines gives

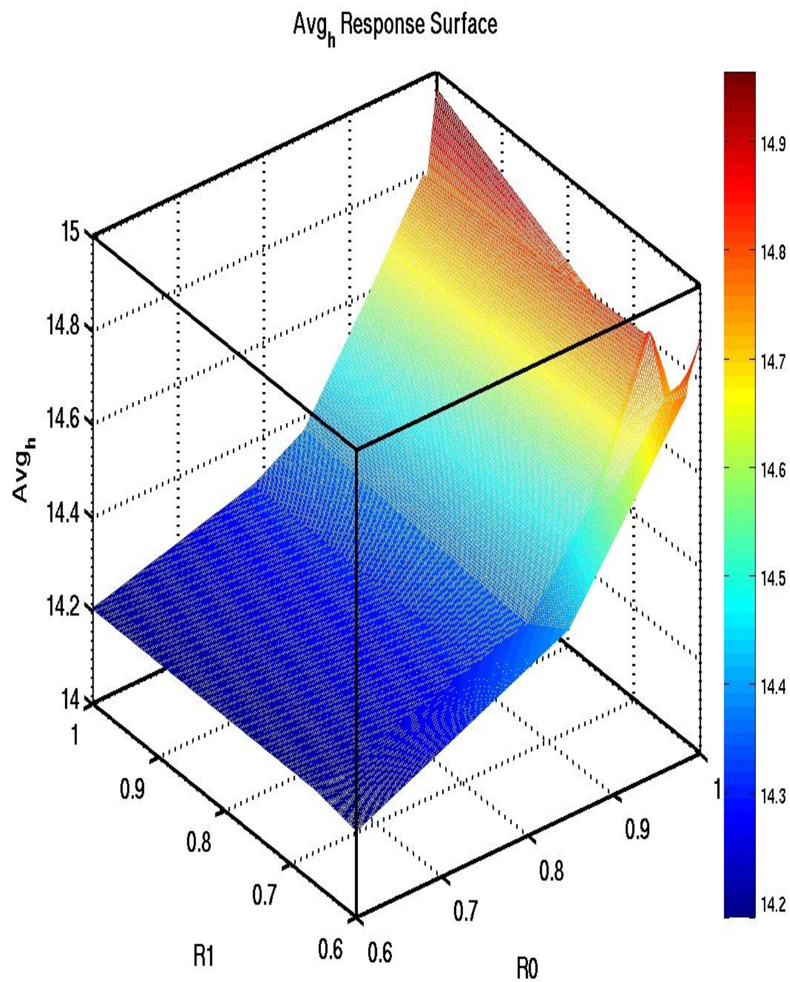




- max prediction uncertainty ~ 0.2 (<2%)
- but it is large relative to the output range (0.7)

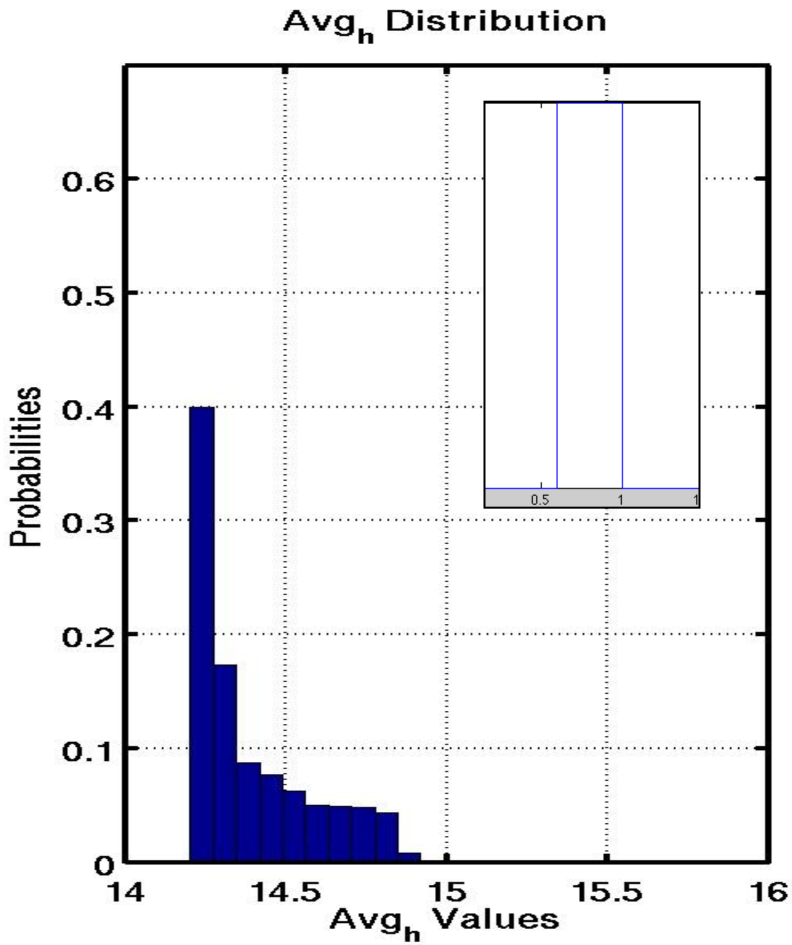
Comparing data and response surface (Avg_h)



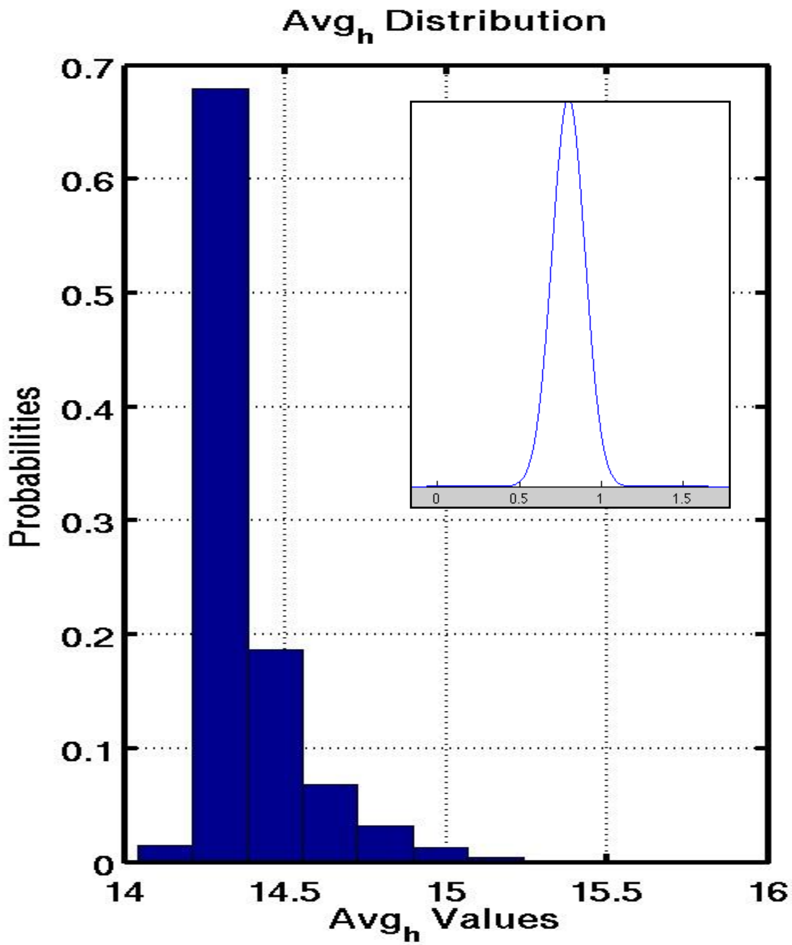


Q: is Avg_h smoothly varying with R0 and R1?

If R0 and R1 are uncertain, the output is also uncertain

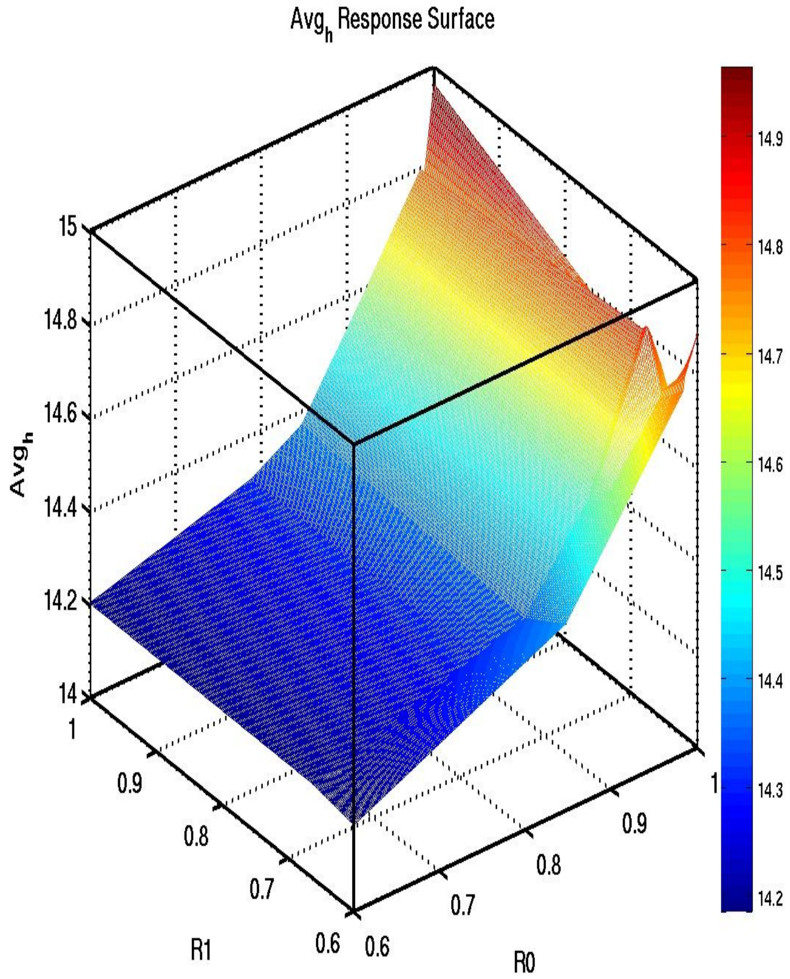


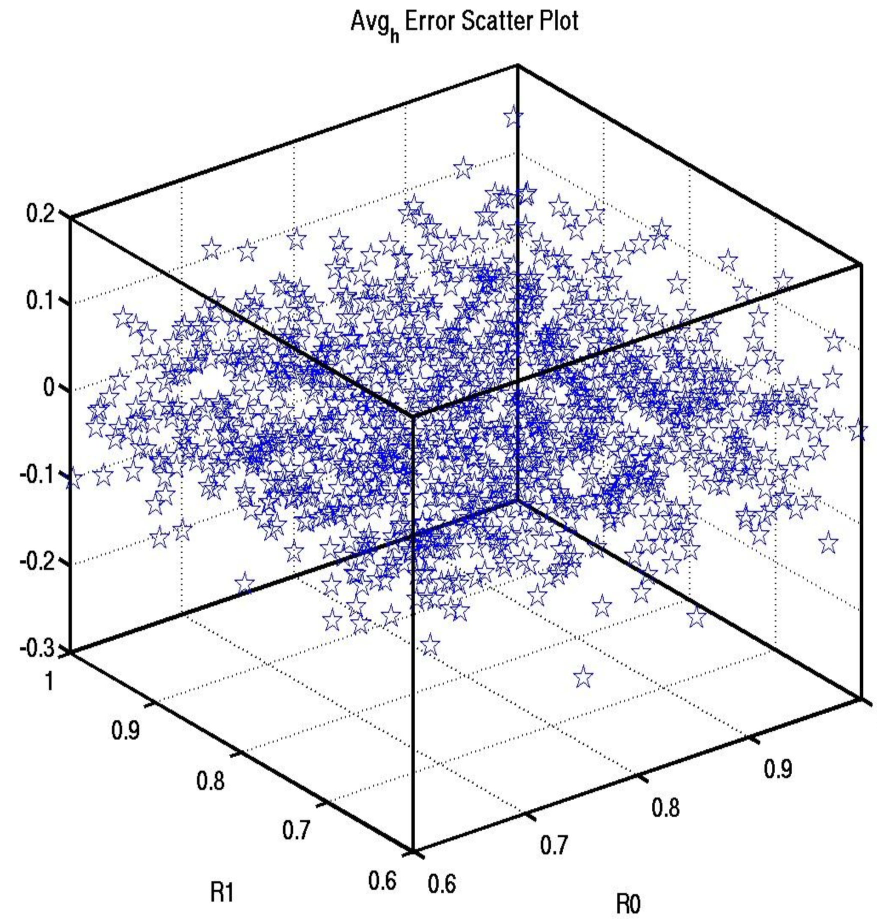
R0, R1 ~ Uniform(0.6, 1.0)



R0, R1 ~ Normal(0.8, 0.1)
(give more weight to center)

What happened? Let's examine Avg_dp more closely.

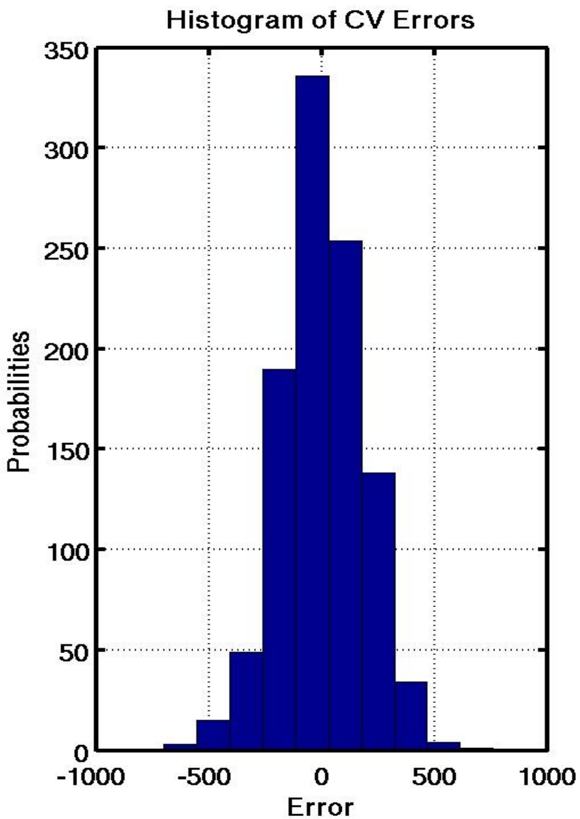


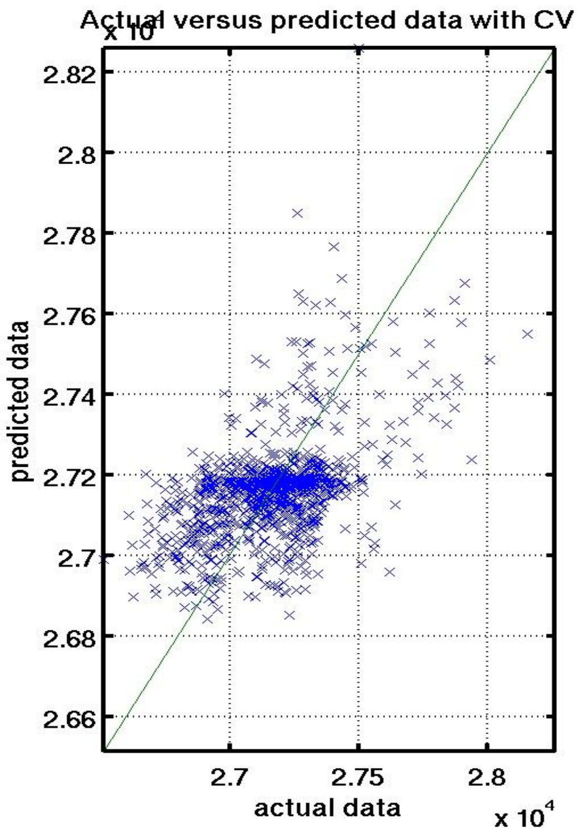


Interpolation errors all over – locally smooth?

Fluidized Bed Data Analysis (Avg_dP)

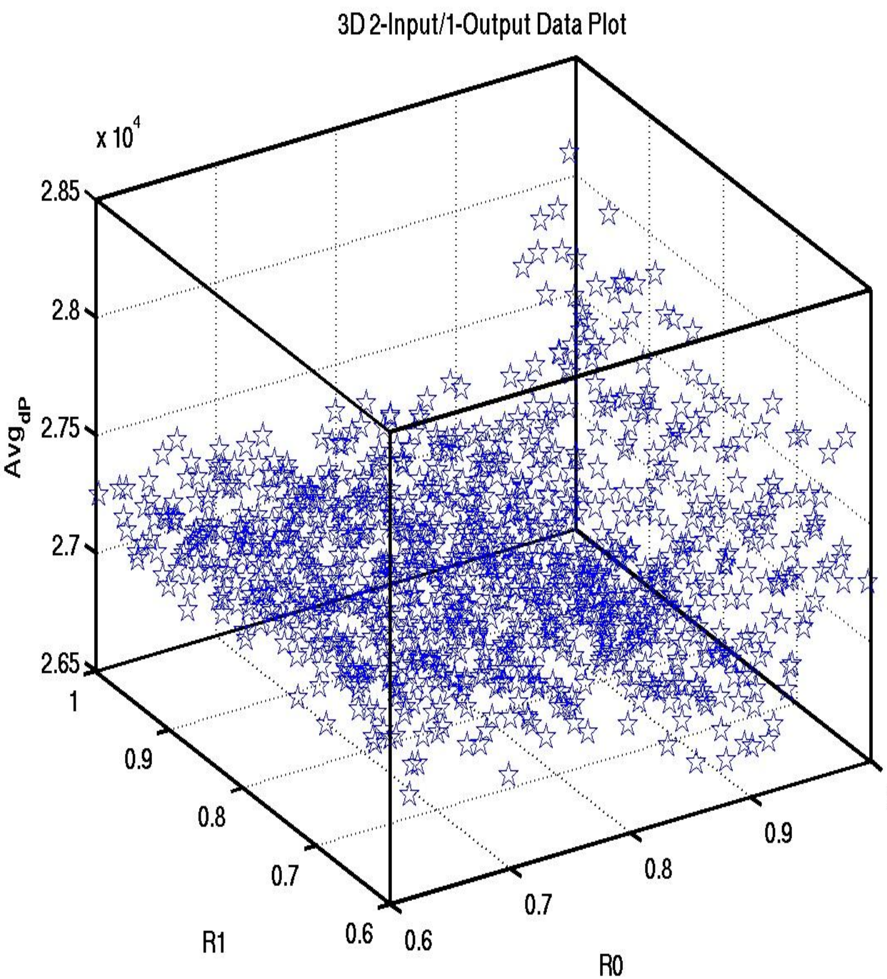
- response surface analysis using cubic splines gives

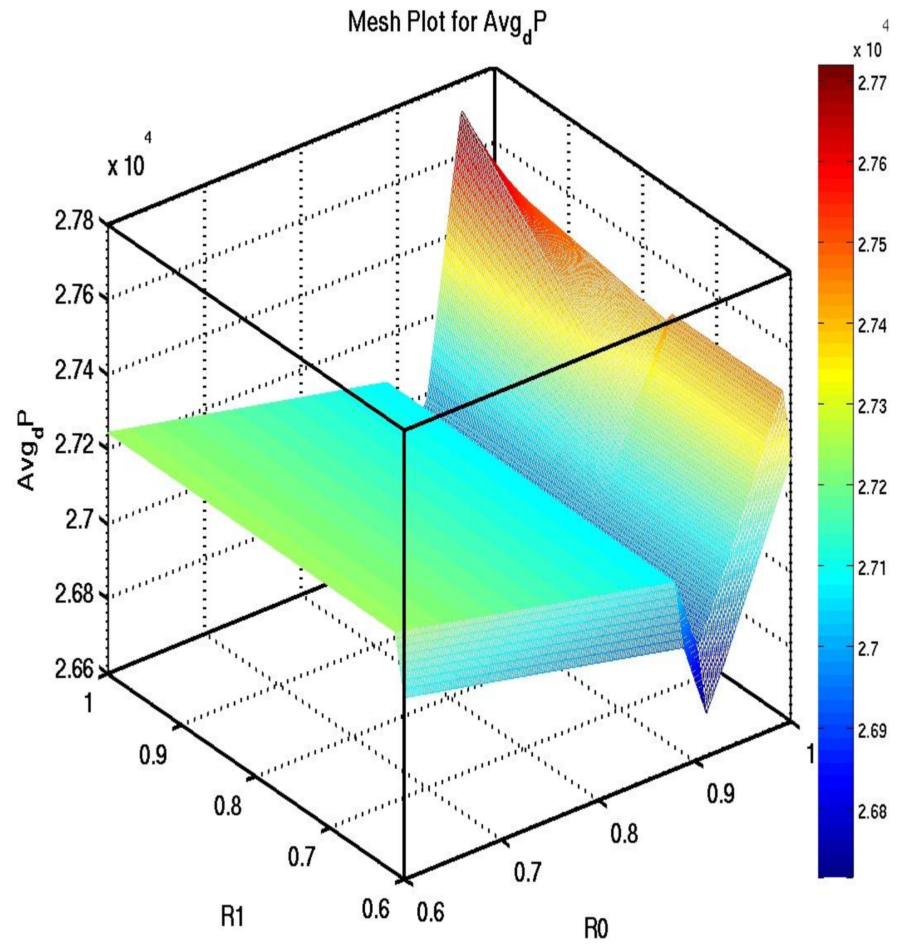




- Errors ~ output range ➔ not acceptable

What happened? Let's examine Avg_dp more closely.





Abrupt changes: physical?