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Uncertainty Quantification Analysis in Multiphase Flow CFD Simulations With Application to Coal Gasifiers

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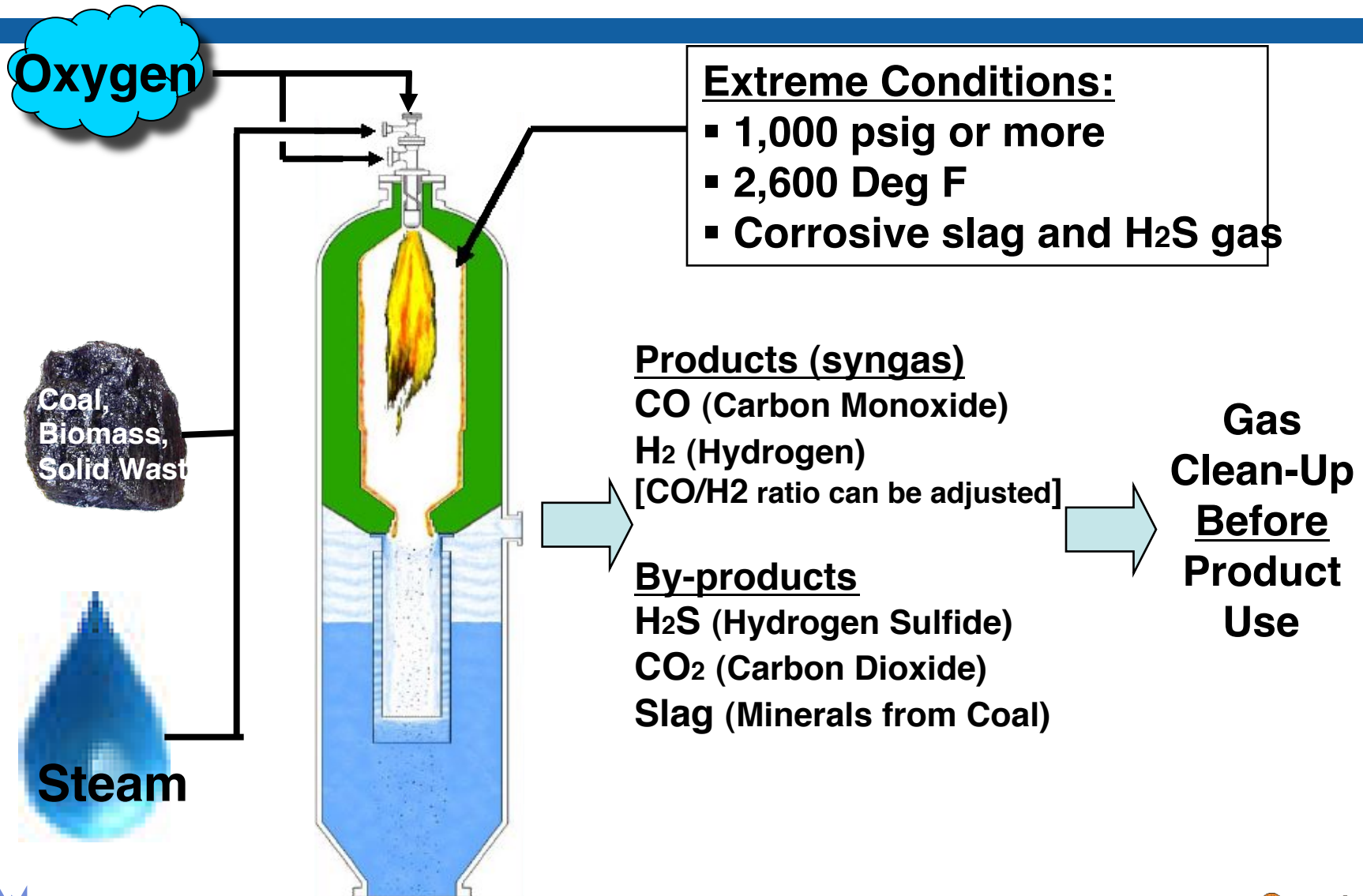
Presentation Outline

- Gasification
- Overview of Uncertainty Quantification Framework
- Preliminary Results for Demonstration of Non-intrusive UQ Analysis :
 - Gasification simulations
 - C3M – PCCL simulations
- Summary & Conclusions
- Future Direction

Gasification

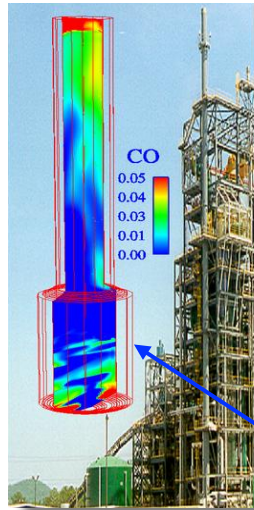
- Over 40% of electricity worldwide is generated through the use of coal
- New environmental regulations, mandating reduction on green house gases and other pollutants will impact coal-based power plants
- Coal gasification technology promises to generate power with reduced environmental impact

What is Gasification?



Challenge: How can we design commercial scale gasifiers for optimized operation?

Use validated computer models for answering scale up questions

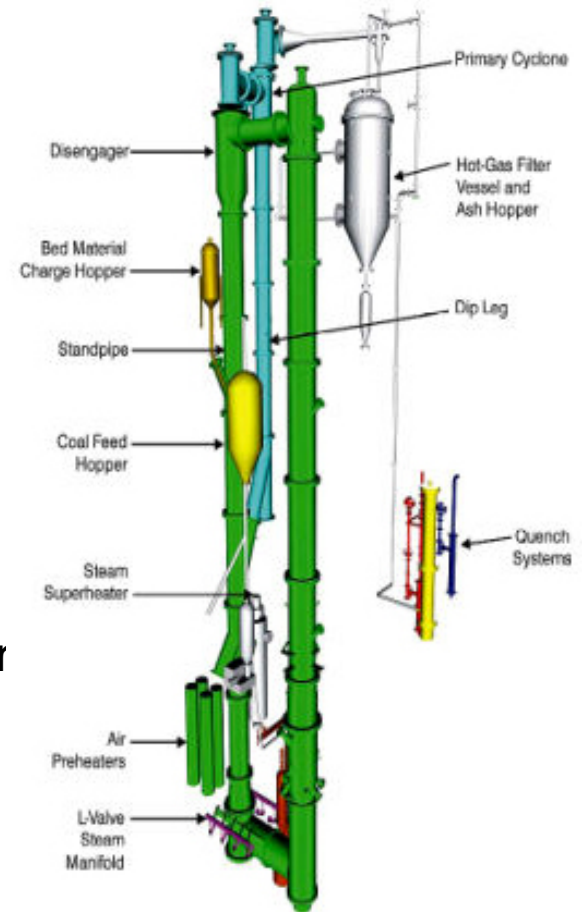


MFIx simulation of pilot scale **13 MW transport gasifier** at Wilsonville, AL. Validation of the computer model with prototype system
C. Guenther et al (2003)

Parametric Study

- Length/Diameter
- Coal feed rate
- Solids circulation rate
- Recycled syngas
- Coal jet penetration

Simulation Based Engineering by employing computational models with Computational Fluid Dynamics (CFD)



Commercial Scale Gasifier

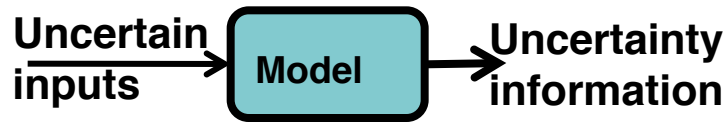


Source: Advanced coal gasifier designs using large-scale simulations, Syamlal et al. (2009)



Quick Overview of Uncertainty Quantification (UQ) Methods

Intrusive UQ



**Stochastic simulation
(UQ embedded in the model)**

Several Available Methods:

- Polynomial Chaos Expansions (PCE)
- Stochastic Expansion

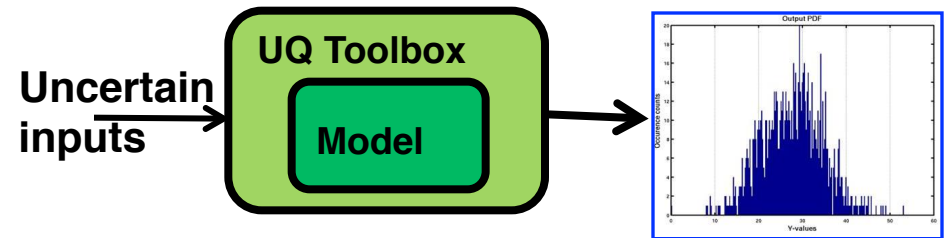
Pros:

- Quick prediction

Cons:

- Surgery in the code and long development time

Non-Intrusive UQ



Many deterministic simulations

Several Available Methods:

- Bayesian Techniques
- PCE
- Surrogate Model + Monte Carlo

Pros:

- Short development time

Cons:

- Sampling error

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

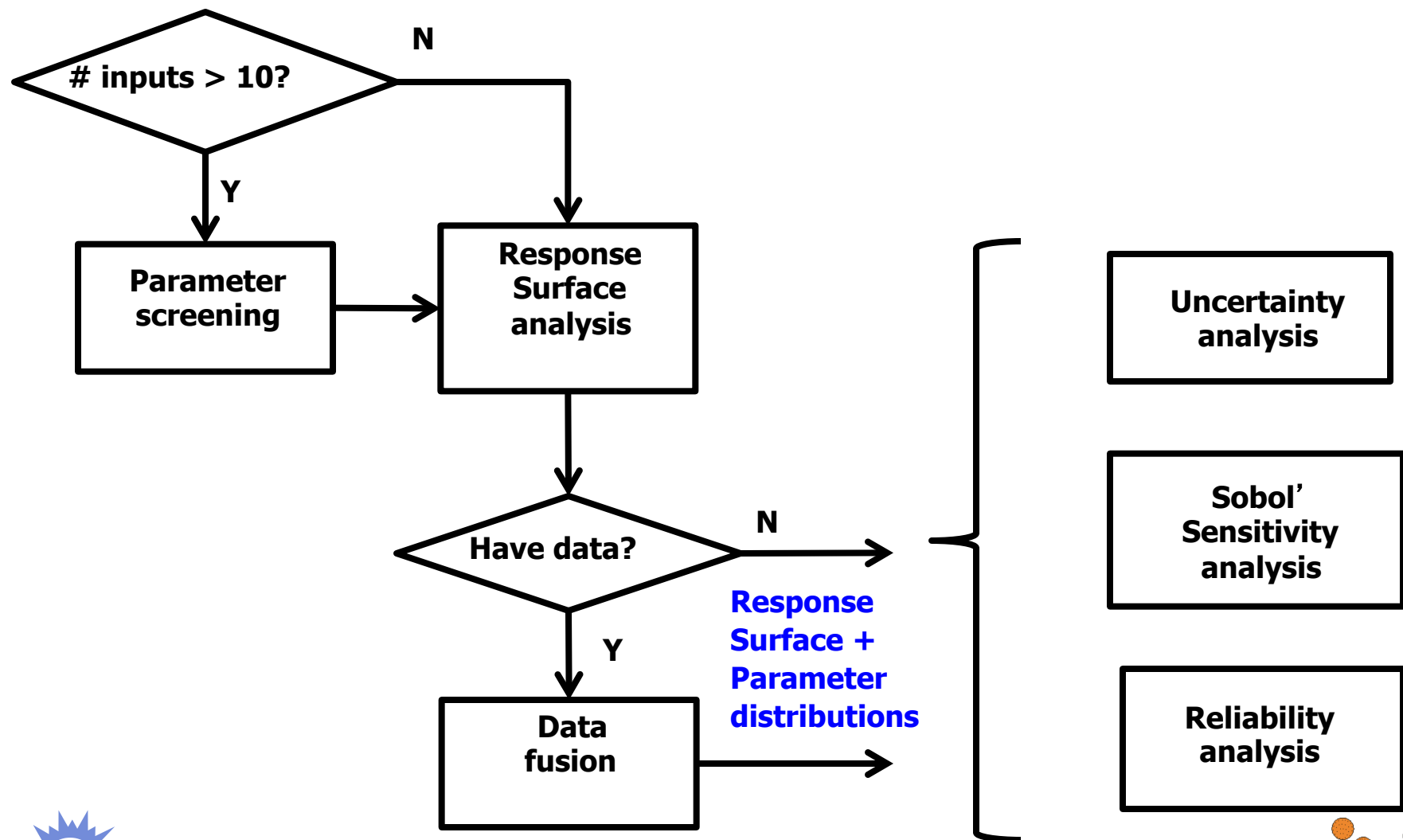
- What parameters have uncertainty and how to represent these uncertainties adequately?
- What impact do parameter uncertainties have on model outputs? Establish confidence levels & quantitative quality assessment in simulation results.
- Which parameters cause the most output uncertainties?
[Sensitivity Analysis]
- How do output uncertainties affect input uncertainties?
[Inverse UQ]
- How to use observed data to calibrate system parameters? [Data Fusion and Calibration]
- In view of uncertainty, how to quantify risk? E.g. given input uncertainties what is the probability of achieving carbon conversion below certain level? [Risk analysis]

Survey To Identify Various Parametric Sources of Uncertainties and Their Mathematical Characterization

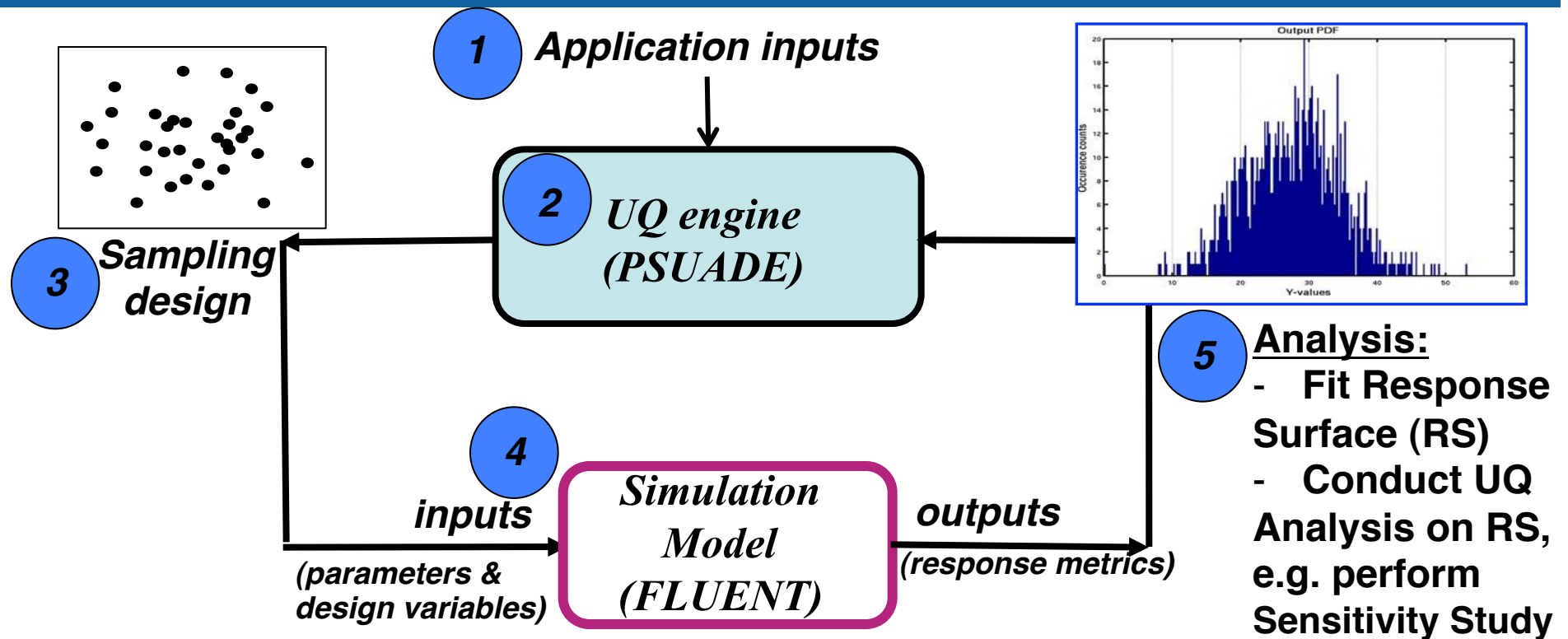
Columns: A B C D E F G H I J K L M N

Importance Rank (Select)	Sources of Uncertainty in Model Input or Uncertain Input Parameters	Symbol or Variable Name	Units	Enter either Nominal value ΔN (Min/Max values OR Min/Max %)				Justification for the provided "most likely value" and lower/upper bounds (Please provide reference citations)	Classification of Uncertainty (Select from list)	Characterize Uncertainty (Select from list)	if Aleatory, set Probability distribution & parameters	Is it correlated with any other source of uncertainty?	If correlated then specify input parameter & why
				The most likely value (n) or the Nominal value	Minimum value: (a) { (a) < (n) }	Maximum value: (b) { (n) < (b) }	Minimum value (% of n)	Maximum value (% of n)					
1	Mean solids circulation rate	Gs	kg/s	14			90	110.00%	Experimental data [1,2]	Aleatory (A)	PDF	N(13.97,0.34)	Fsl
2	Mean superficial gas velocity at bottom	Ug	m/s	7.58			95	105.00%	Experimental data [1,3]	Aleatory (A)	PDF	N(7.57,0.04)	Fsl
5	Gas flow rate from standpipe and L-valve	Fsl	SCMs	0.029			99.955	100.05%	Experimental data [1,3]	Aleatory (A)		N	
11	Temperature	T	K	293	287	299			Experimental data [1,3]	Aleatory (A)		N	
10	Pressure at top exit	P	kPa	105			99.996	100.00%	Experimental data [1,3]	Aleatory (A)		N	
6	Particle diameter	dp	um	802	784	820			Experimental data [1]	Aleatory (A)		N	
7	Particle density	rho	kg/m3	863			99.99	100.01%	Experimental data [1]	Aleatory (A)		N	
8	restitution coefficient	e	-	0.8					Literature [4]	Epistemic (E)		N	
9	sphericity (*)	phi	-	0.95					Experimental data [1]	Aleatory (A)		N	
3	wall boundary for solids phase (\$)	BC	-	partial-slip					Expert opinion [5]	Epistemic (E)		N	
4	Interphase drag (&)	beta	-							Epistemic (E)			

A Simple Workflow for Non-intrusive Parametric Uncertainty Quantification and Propagation:



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.

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

- Sample Problem # 1: 2D Gasification (Aleatory) *
- Sample Problem # 2: 2D Gasification (Mixed)
- Sample Problem # 3: C3M – PC Coal Lab (Aleatory)

* This work was presented at the 2012 ASME V&V Symposium in Las Vegas, Nevada, May 3rd, 2012.



Sample Problem # 1 for Parametric Non-Intrusive UQ Study: 2D Gasification (Aleatory Uncertainty only)

Objective: Determine the effect of uncertainty in mass flow rate and O₂ mass fraction on the species composition at the outlet of the gasifier.

Gasifier Model

Solids: PRB coal with $d_p = 0.015$ cm, $\rho_p = 2.93$ g/cm³

Geometric dimensions = 52 cm x 1300 cm

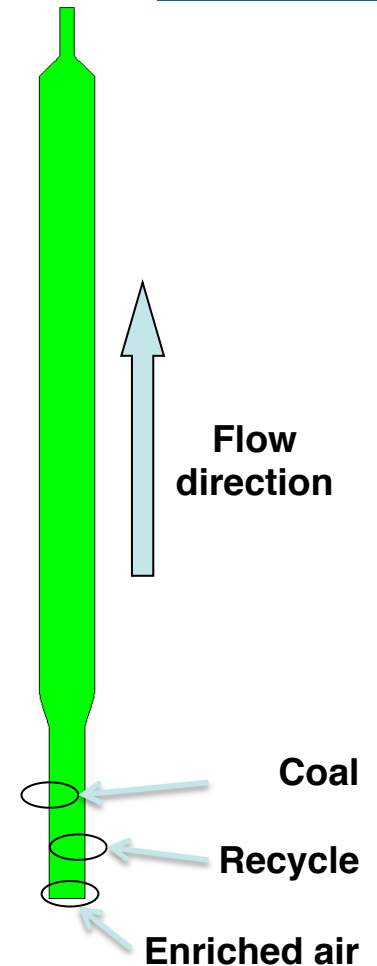
Grid Resolution = 4,579 cells

Governing Physics & Models: Multiphase flow (TFM) hydrodynamics, heat transfer, chemical reactions.

Spatial discretization: Second Order Upwind

Temporal discretization: 1st order

Computational time per simulation: ~ 2 weeks, 16 cores



Sample Problem # 1 for Parametric Non-Intrusive UQ Study: 2D Gasification (Aleatory Uncertainty only - cont'd)

Uncertainty Quantification Study Properties:

Input parameters with Uncertainty (min-max range):

- (1) Inlet mass flow rate (kg/s)
[1.575 – 2.424]
- (2) O₂ species mass fraction
[0.259 – 0.4]

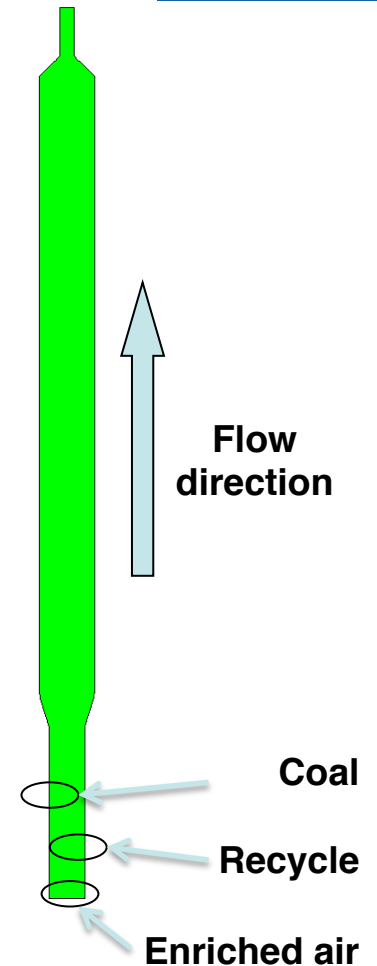
System Response Variables:

Time averaged mole fraction at the exit plane for species

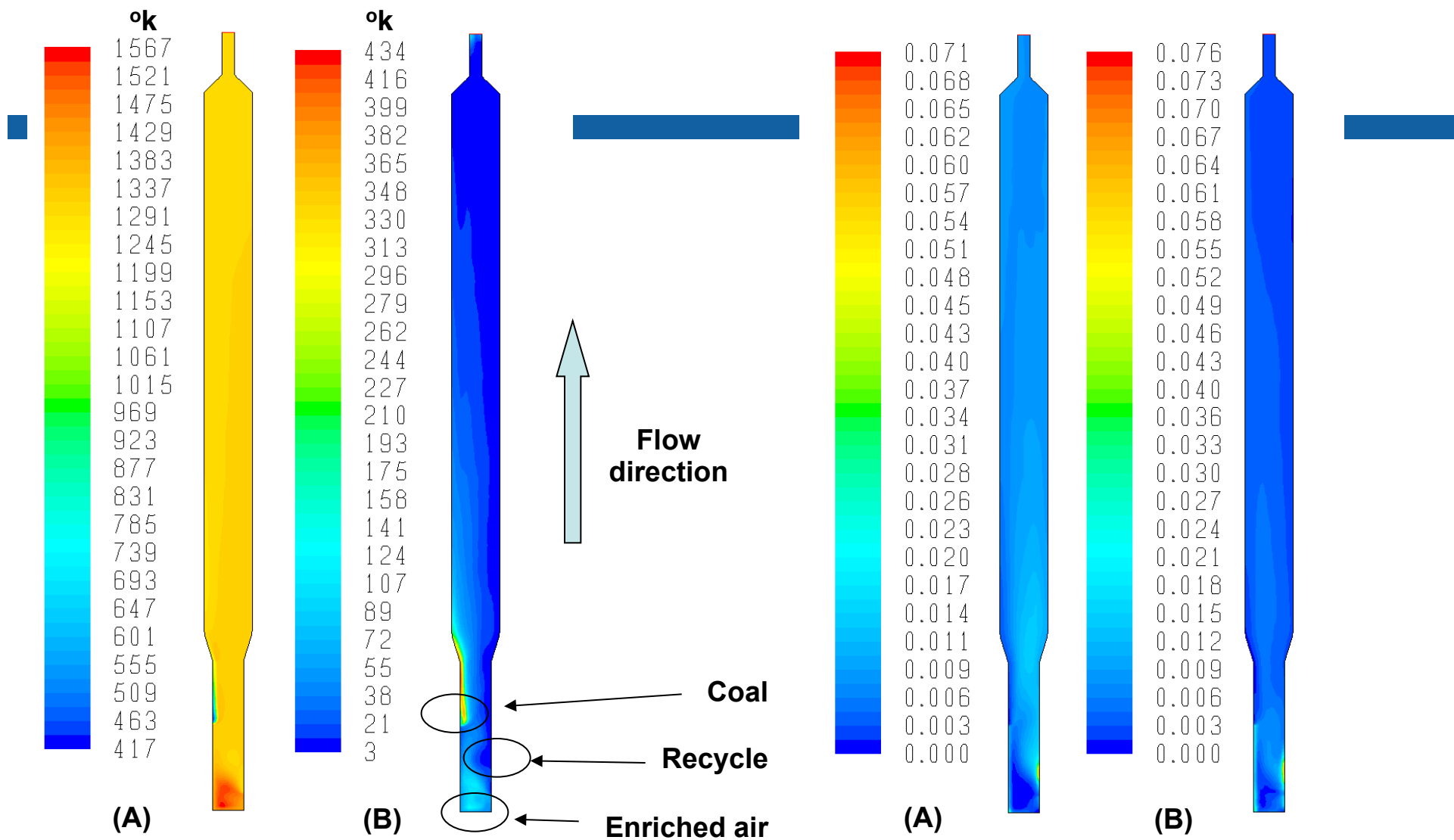
- (1) CH₄ (2) CO (3) H₂

Sampling Method: CCD, SparseGrid

Sample Size = 17 (CCD), 13 (SparseGrid)



* This work was presented at the 2012 ASME V&V Symposium, Las Vegas, Nevada, May 3rd, 2012.



Time averaged temperature (A) and its RMS value (B)

Time averaged CO mass fraction (A) and its RMS value (B)

Challenges in Multiphase Flow Simulation

- Typical 3D CFD simulation of a gasifier can take up to 6 to 8 weeks to reach a pseudo-steady state
- To expedite the process, a 2D transport gasifier is modeled using the Two-Fluid Multiphase model in ANSYS FLUENT version 14.0
- Coal pyrolysis, combustion, gasification along with H_2 , CO and CH_4 and soot combustion are modeled using 16 chemical reactions
- Total of 33 transport equations are solved

Surrogate Model Construction

- Non-intrusive UQ requires many samples, i.e.,
 - many simulations with the CFD code
- Computational cost per sample may prohibit UQ
 - On the average 30 days on 16 cores were employed to achieve converged solutions for the gasifier.
 - Other constraints such as license cost could be factor
- Need to construct a surrogate model
- Various surrogate models available:
 - Data-fitted surrogate models (Parametric polynomial response surfaces, Nonparametric MARS, GPM)
 - Reduced-order Models (ROM)
 - Stochastic collocation Models with Sparse Grid

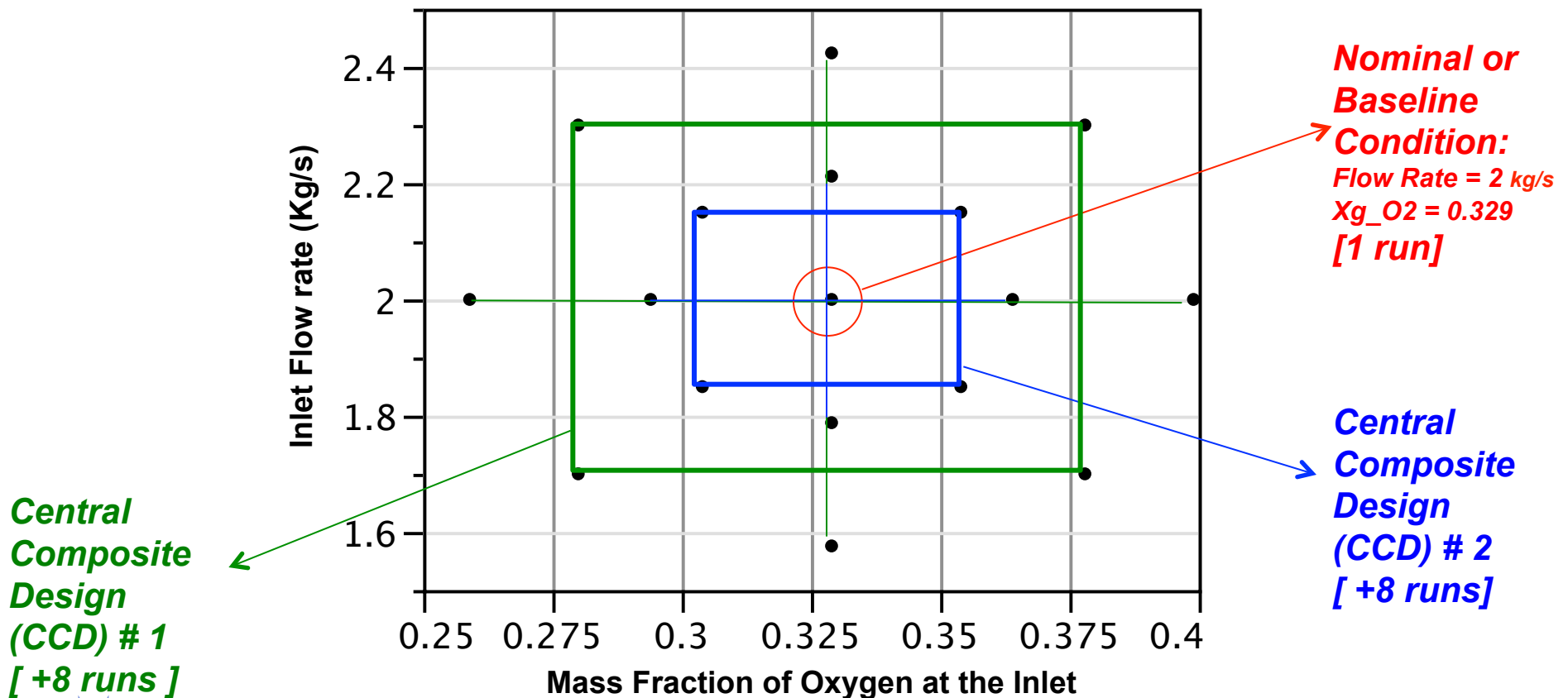
Surrogate Model Construction (cont' d)

- Employed statistical design of experiments to sample
 - Computational cost constrained the sampling method choice.
 - Initially 9 simulations based on Central Composite Design (CCD) was employed. This analysis necessitated additional runs.
 - Initial run matrix was augmented with another 8-run CCD

Run No	Input Factors		Response Variables or Quantities of Interest						
	#1 Inlet Flow Rate	#2 Xg_O2	#1 CH4	#2 CO2	#3 CO	#4 H2	#5 H2O	#6 Soot	#7 wgs
1	1.700	0.280	0.0798	0.0145	0.0040	0.0828	0.5732	0.0804	0.5131
2	2.300	0.280	0.0752	0.0208	0.0051	0.0764	0.5434	0.0748	0.5568
3	1.700	0.378	0.0781	0.0199	0.0050	0.0798	0.5765	0.0775	0.5288
4	2.300	0.378	0.0743	0.0286	0.0065	0.0740	0.5489	0.0737	0.5789
5	1.576	0.329	0.0799	0.0160	0.0042	0.0827	0.5750	0.0803	0.5354
6	2.424	0.329	0.0779	0.0228	0.0055	0.0793	0.5597	0.0784	0.5742
7	2.000	0.259	0.0787	0.0155	0.0041	0.0814	0.5640	0.0796	0.5266
8	2.000	0.399	0.0791	0.0237	0.0058	0.0802	0.5705	0.0798	0.5651
9	2.000	0.329	0.0776	0.0198	0.0049	0.0793	0.5661	0.0775	0.5493
10	1.850	0.304	0.0783	0.0162	0.0042	0.0811	0.5658	0.0786	0.5445
11	2.150	0.304	0.0776	0.0180	0.0045	0.0796	0.5652	0.0778	0.5557
12	1.850	0.354	0.0789	0.0188	0.0046	0.0812	0.5716	0.0792	0.5632
13	2.150	0.354	0.0780	0.0215	0.0052	0.0797	0.5645	0.0785	0.5733
14	1.788	0.329	0.0781	0.0175	0.0045	0.0807	0.5679	0.0783	0.5376
15	2.212	0.329	0.0774	0.0206	0.0050	0.0794	0.5611	0.0778	0.5769
16	2.000	0.294	0.0781	0.0165	0.0042	0.0809	0.5645	0.0783	0.5538
17	2.000	0.364	0.0783	0.0199	0.0049	0.0803	0.5665	0.0787	0.5659

Surrogate Model Construction (cont' d)

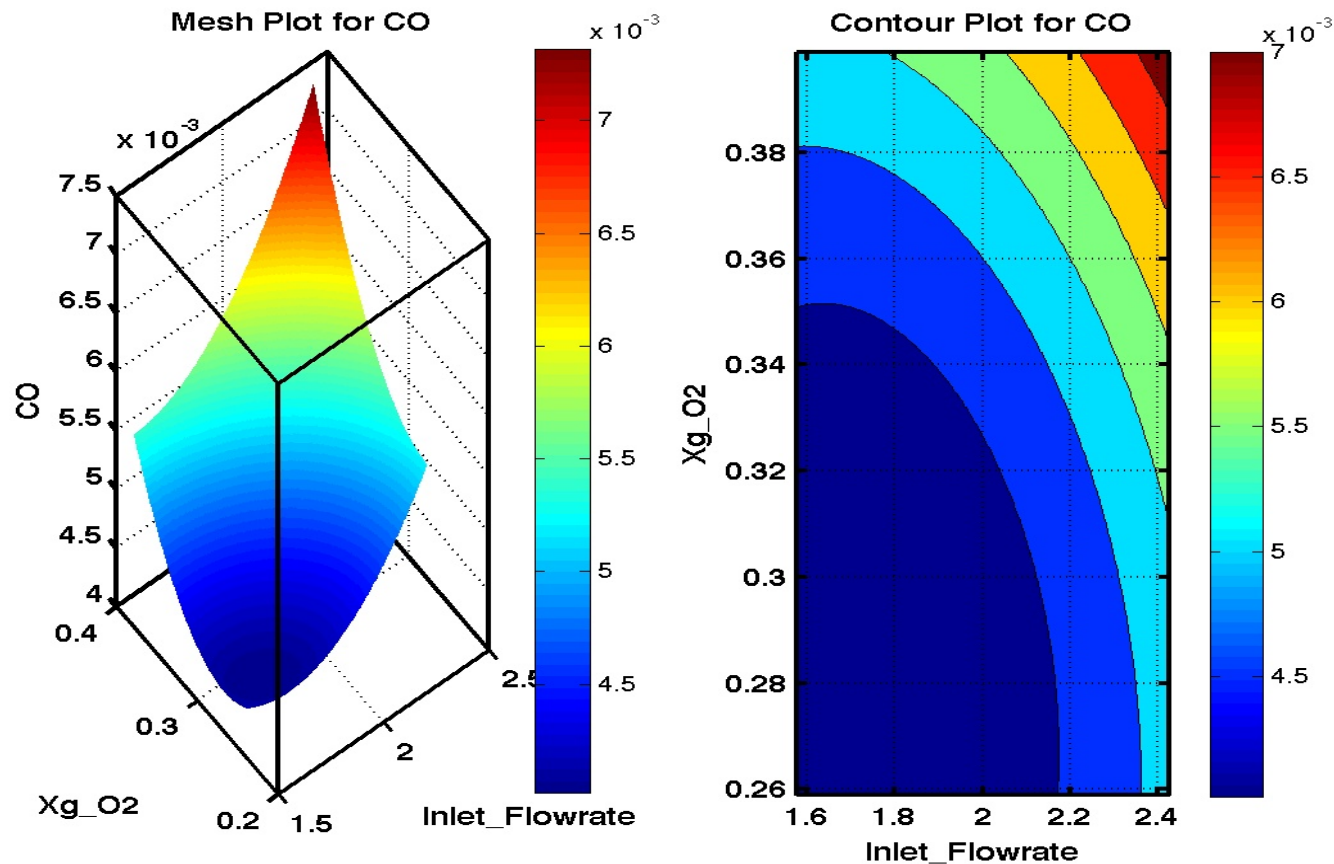
- Visual illustration of the sampling locations in the parameter space for two input parameters:



Surrogate Model Construction (cont' d)

Response # 3 mole fraction CO

- Quadratic polynomial regression based surrogate model



Surrogate Model Adequacy Check

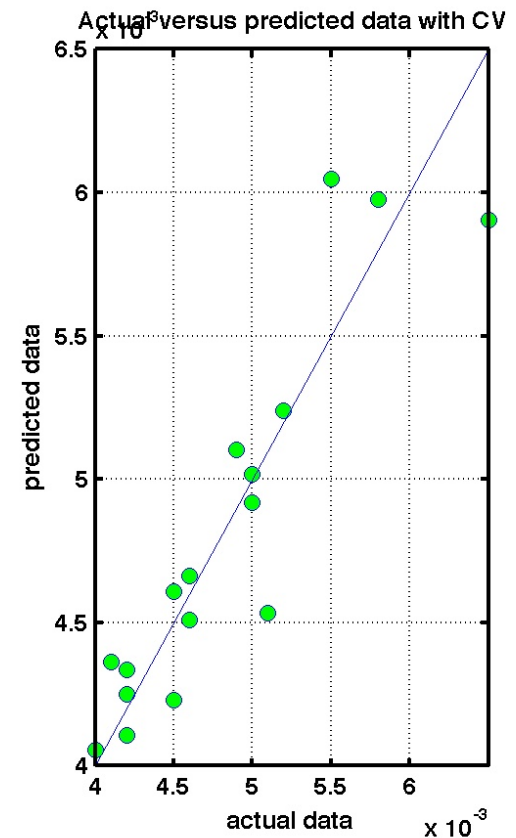
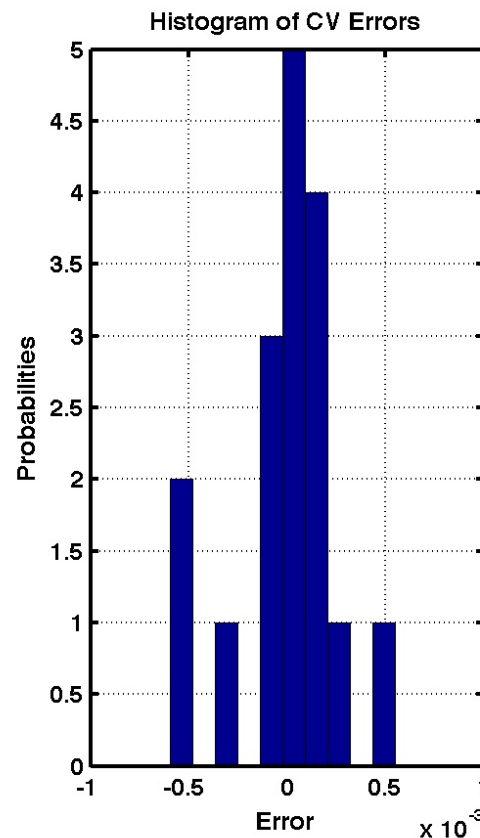
Response # 3 mole fraction CO

- Polynomial regression metrics:

Adj $R^2 = 95.5\%$

- Cross-validation errors:

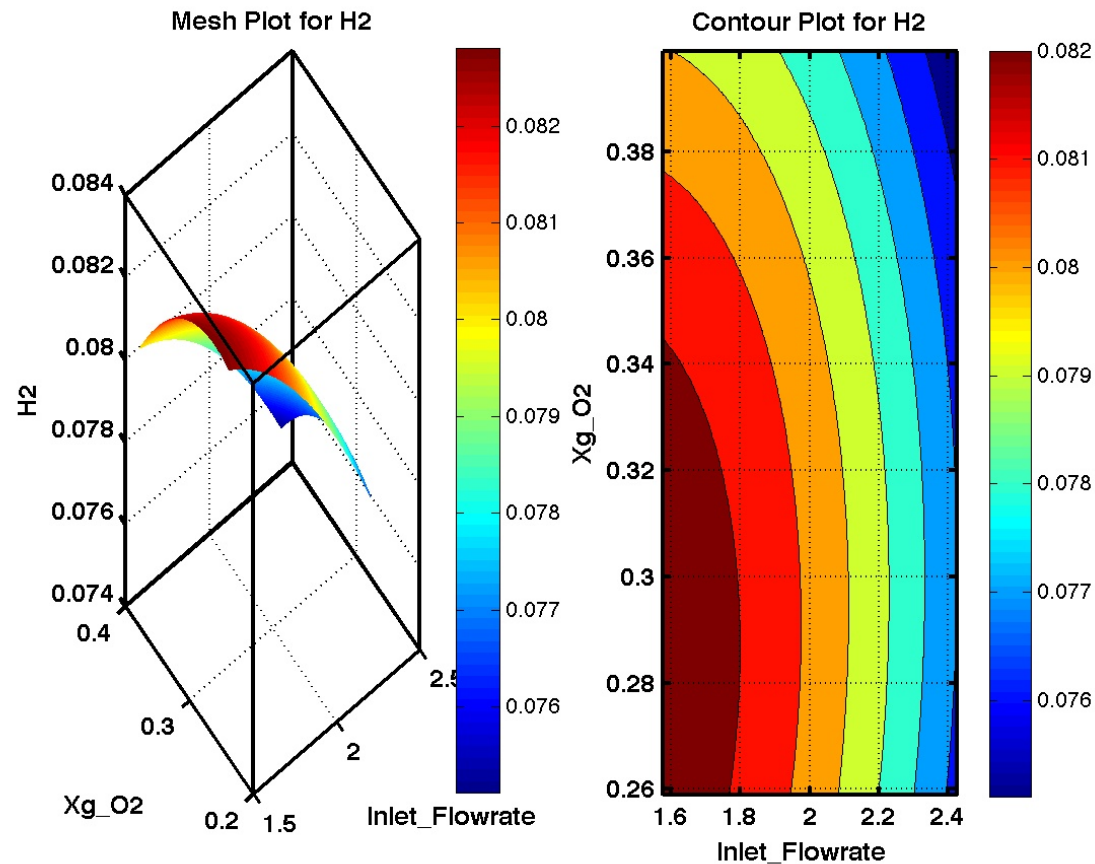
- No systematic bias error as mean CV error ~ 0
- Standard deviation of errors $\sim 2.8e-04$



Surrogate Model Construction (cont' d)

Response # 4 mole fraction H2 (iteration 1)

- Quadratic polynomial regression based surrogate model



Surrogate Model Adequacy Check

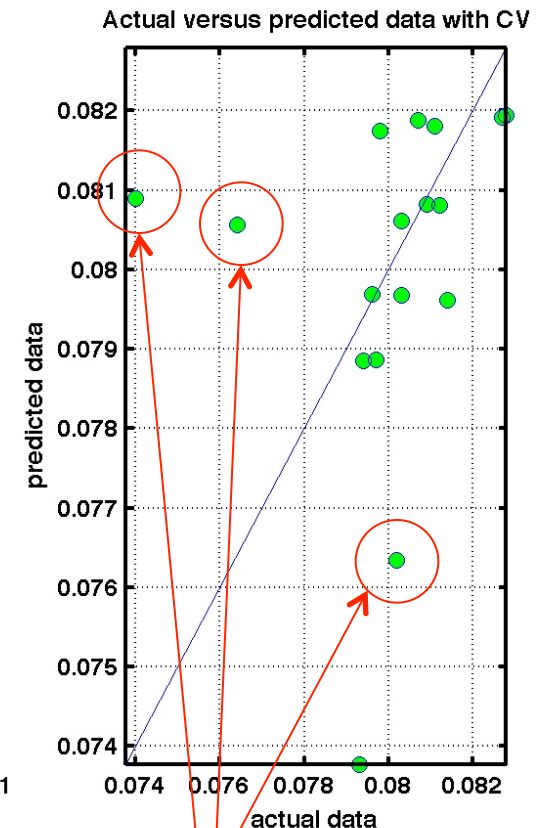
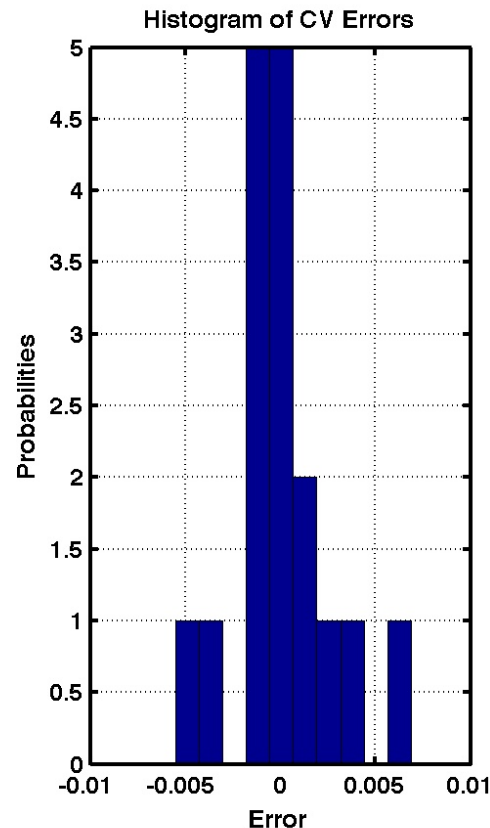
Response # 4 mole fraction H2 (iteration 1)

- Polynomial regression metrics:

Adj. $R^2 = 64.3\%$

- Cross-validation errors:
 - No systematic bias error as mean CV error ~ 0
 - Standard deviation of errors $\sim 2.8e-03$

Adjusted R^2 implies only 64 % of the variability observed in H2 mass fraction can be explained with the quadratic regression based surrogate model constructed!



Several outliers causing the degradation in the surrogate model

Surrogate Model Adequacy Check

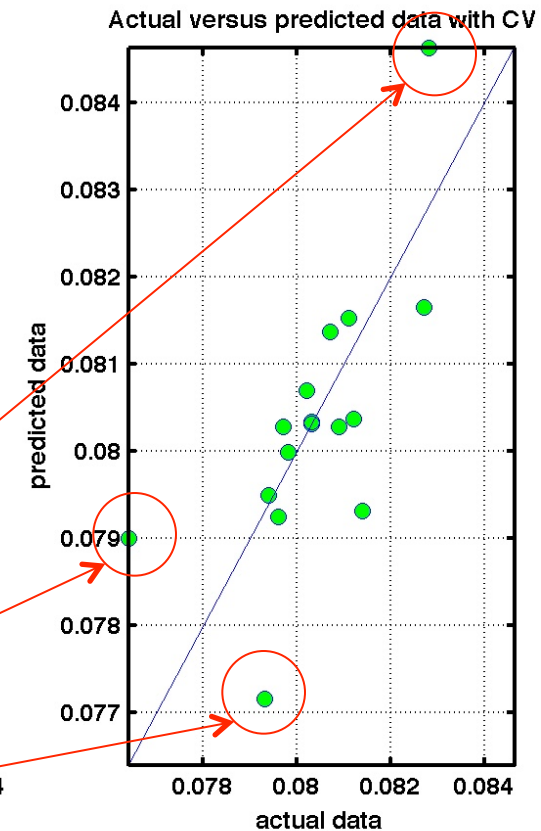
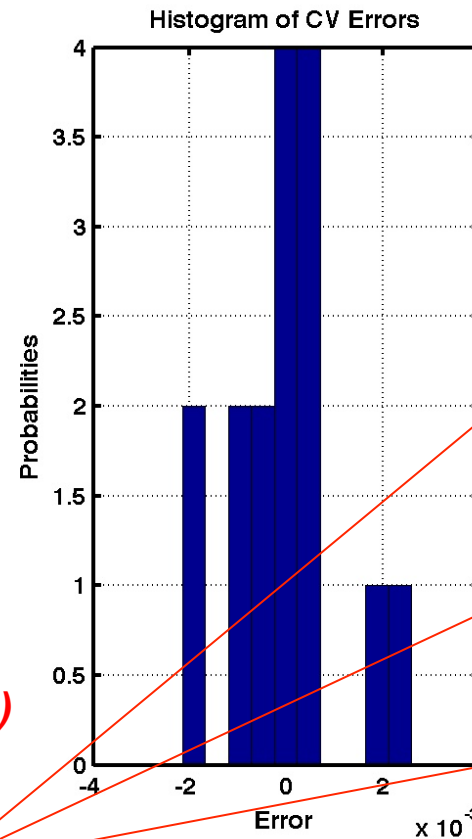
Response # 4 mole fraction H2 (iteration 2)

- Polynomial regression metrics:

$$\text{Adj } R^2 = 86.3\%$$

- Cross-validation errors:
 - No systematic bias error as mean CV error ~ 0
 - Standard deviation of errors $\sim 1.2\text{e-}03$

Adjusted R^2 improved by removing one outlier (Run # 4)

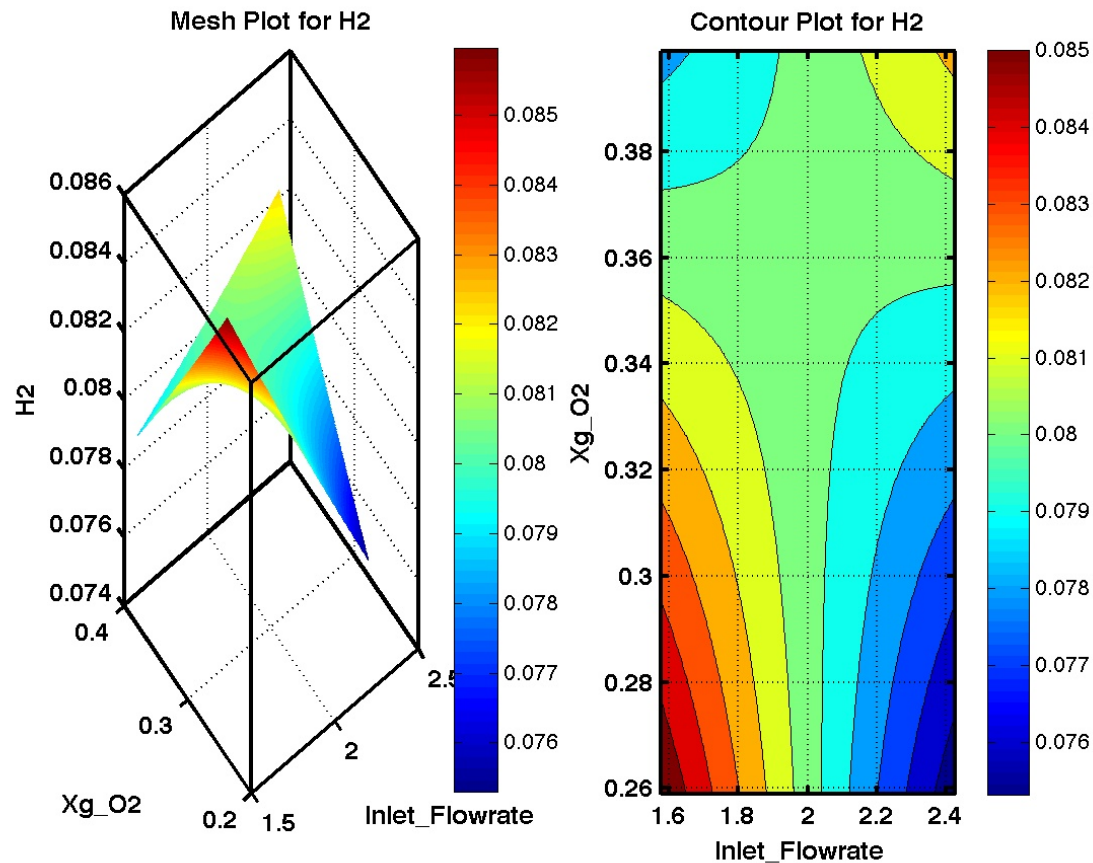


Still several outliers causing problems but we have limited number of samples so assumed the surrogate model to be adequate for the purposes of this study.

Surrogate Model Construction (cont' d)

Response # 4 mole fraction H2 (iteration 2)

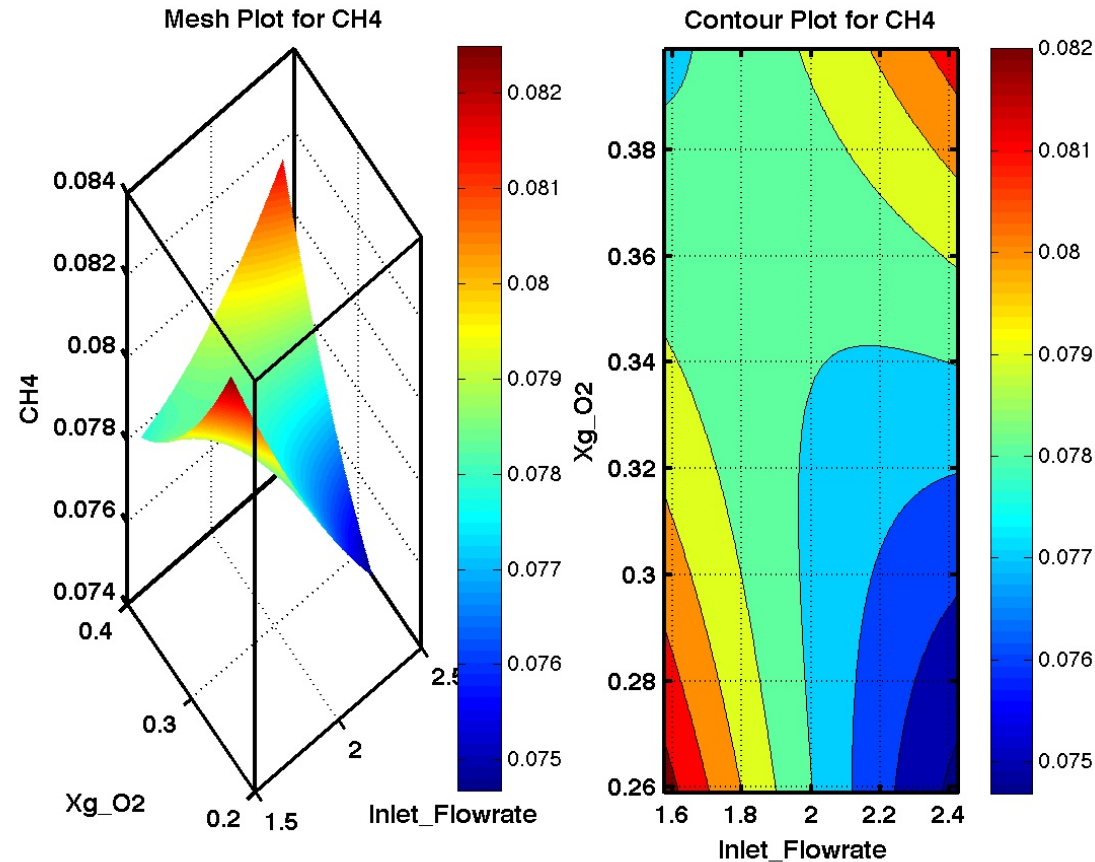
- Quadratic polynomial regression based surrogate model



Surrogate Model Construction (cont' d)

Response # 1 mole fraction CH4 (iteration 2)

- Quadratic polynomial regression based surrogate model



Surrogate Model Adequacy Check

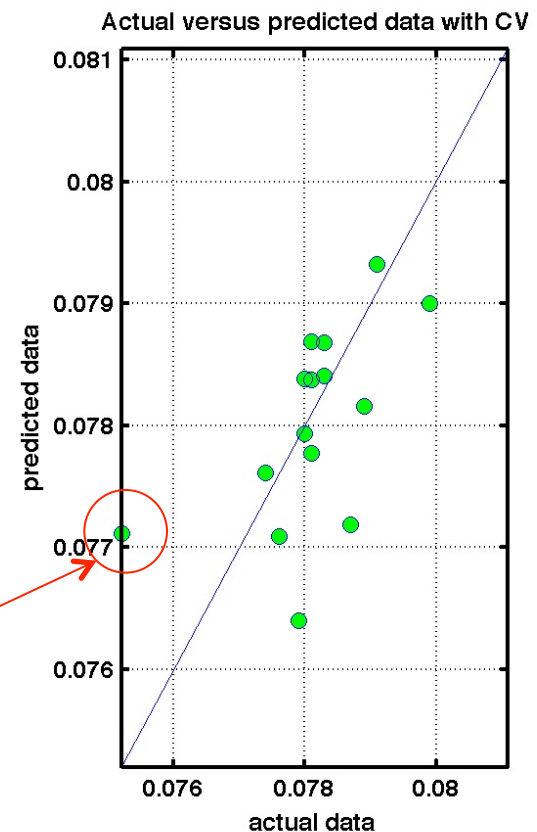
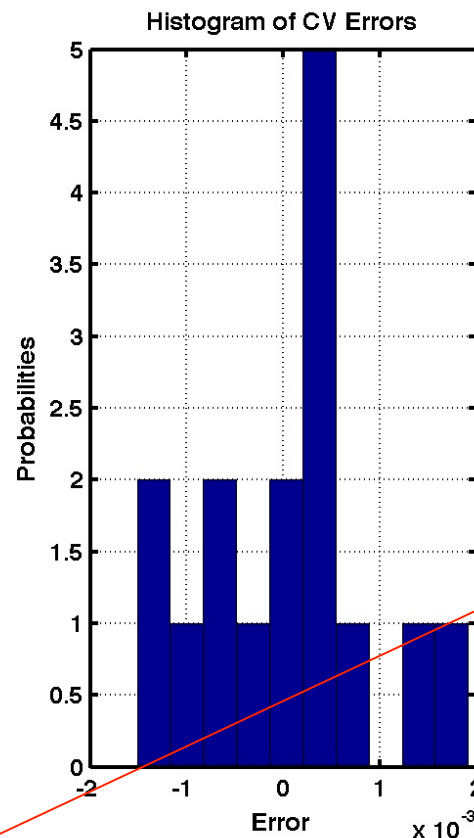
Response # 1 mole fraction CH4 (iteration 2)

- Polynomial regression metrics:

Adj $R^2 = 84\%$

- Cross-validation errors:
 - No systematic bias error as mean CV error ~ 0
 - Standard deviation of errors $\sim 9.1\text{e-}04$

Adjusted R^2 improved from 51% (iteration 1) by removing one outlier (Run # 4)



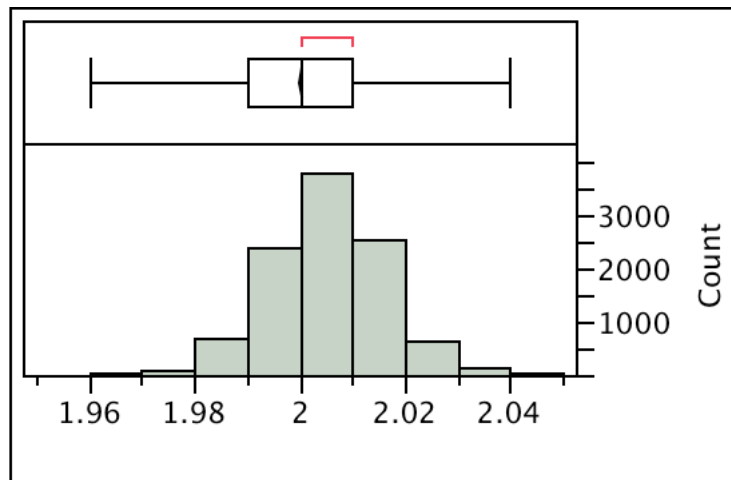
Still several outliers causing problems but we have limited number of samples so assumed the surrogate model to be adequate for the purposes of this study.

Input Uncertainty Propagation and Quantification – Non-intrusive method

- Both input parameters were assumed to be aleatory uncertainty
- Probability density functions were assigned and Monte Carlo simulation was performed by random drawings for both variables and evaluating surrogate.

(1) Inlet Flow Rate

Normal (2 kg/s , 0.01 kg/s) truncated [1.575,2.424]

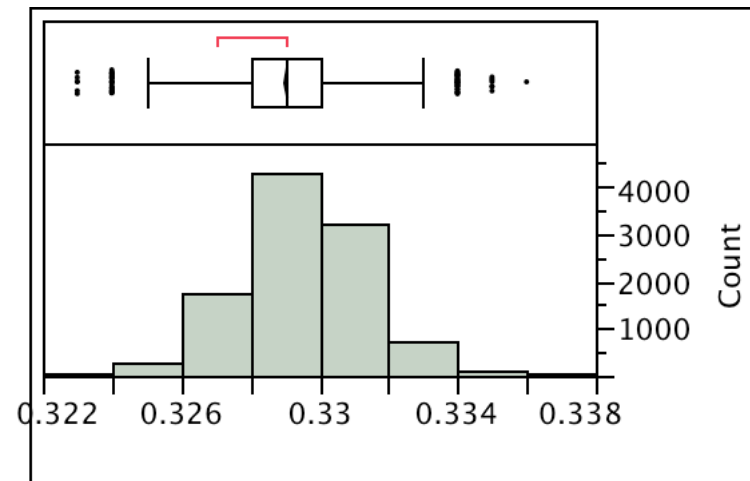


Summary Statistics

Mean	2.000115
Std Dev	0.0105938
Std Err Mean	0.0001059
Upper 95% Mean	2.0003227
Lower 95% Mean	1.9999073
N	10000

(2) O2 mass fraction

Normal (0.329 , 0.0017) truncated [0.259,0.4]

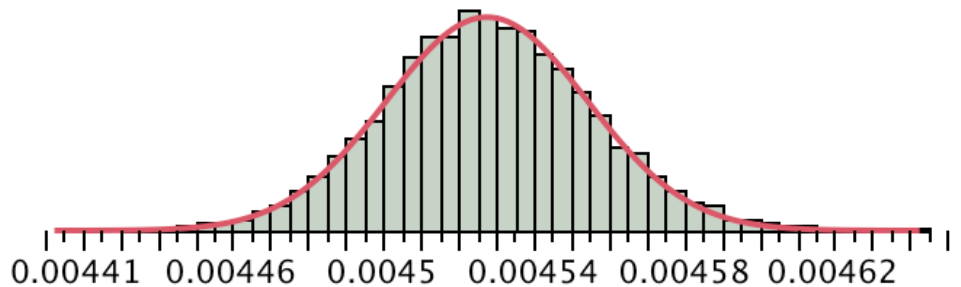


Summary Statistics

Mean	0.3290139
Std Dev	0.0017313
Std Err Mean	1.7313e-5
Upper 95% Mean	0.3290478
Lower 95% Mean	0.32898
N	10000

Input Uncertainty Forward Propagation with 10000 sample Monte Carlo Simulation using the Surrogate:

Response # 3 CO



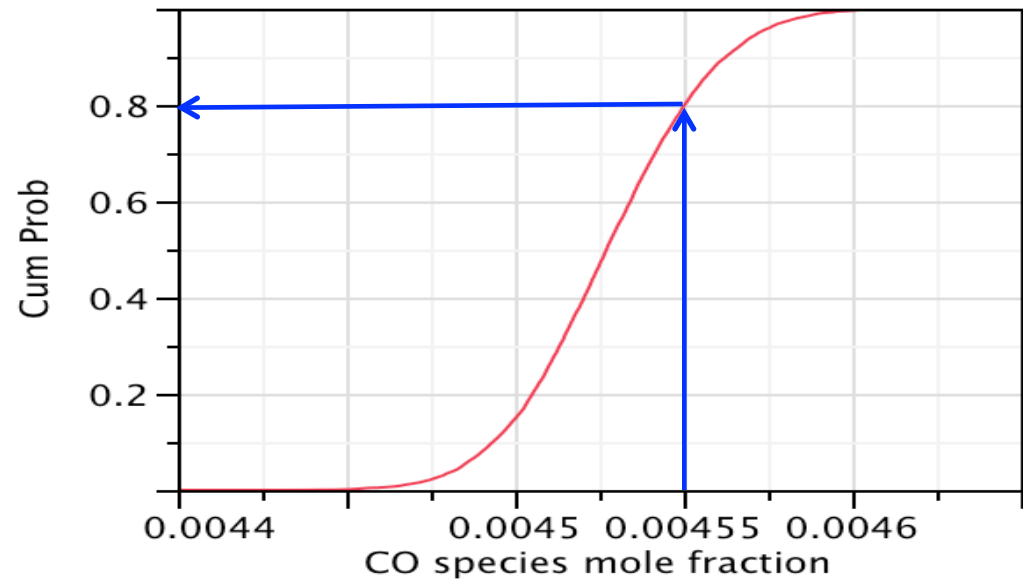
Summary Statistics	
Mean	0.0045277
Std Dev	2.678e-5
Std Err Mean	2.678e-7
Upper 95% Mean	0.0045282
Lower 95% Mean	0.0045272
N	10000

CO species mole fraction

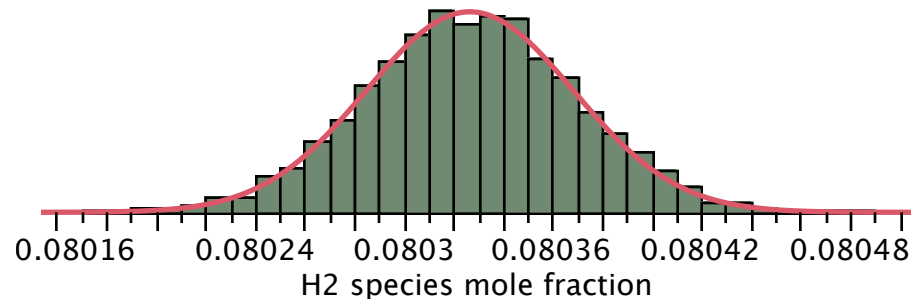
Quantiles

100.0%	maximum	0.00464
99.5%		0.0046
97.5%		0.00458
90.0%		0.00456
75.0%	quartile	0.00455
50.0%	median	0.00453
25.0%	quartile	0.00451
10.0%		0.00449
2.5%		0.00448
0.5%		0.00446
0.0%	minimum	0.00442

Empirical Cumulative Distribution Function



Input Uncertainty Forward Propagation with 10000 sample Monte Carlo Simulation using the Surrogate: Response # 4 H2



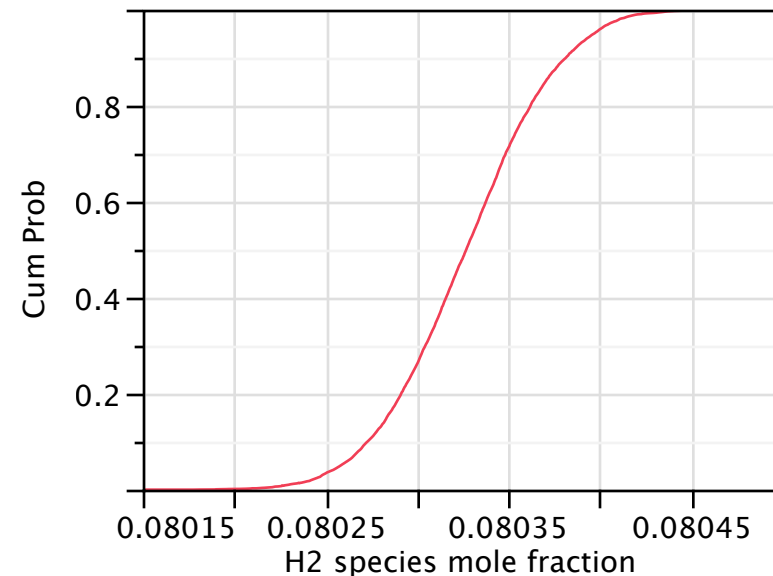
Summary Statistics

Mean	0.0803268
Std Dev	0.0000418
Std Err Mean	4.1805e-7
Upper 95% Mean	0.0803276
Lower 95% Mean	0.080326
N	10000

Quantiles

100.0%	maximum	0.08048
99.5%		0.08043
97.5%		0.08041
90.0%		0.08038
75.0%	quartile	0.08035
50.0%	median	0.08033
25.0%	quartile	0.0803
10.0%		0.08027
2.5%		0.08025
0.5%		0.08022
0.0%	minimum	0.08018

Empirical Cumulative Distribution Function



Sample Problem # 2 for Parametric Non-Intrusive UQ Study: 2D Gasification (Mixed Epistemic & Aleatory Uncertainty)

Uncertainty Quantification Study Properties:

Input parameters with Uncertainty (min-max range):

(1) Inlet mass flow rate (kg/s)

[1.575 – 2.424]

← **Epistemic
Uncertainty**

(2) O₂ species mass fraction

[0.259 – 0.4]

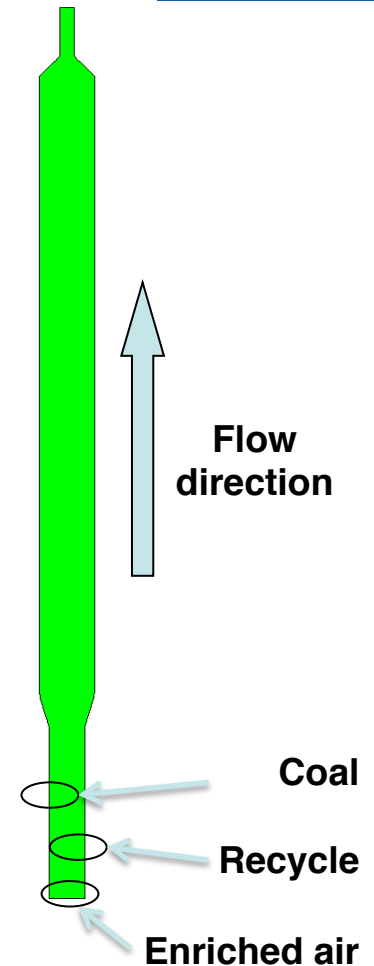
System Response Variables:

Time averaged mole fraction at the exit plane for species

(1) CH₄ (2) CO (3) H₂

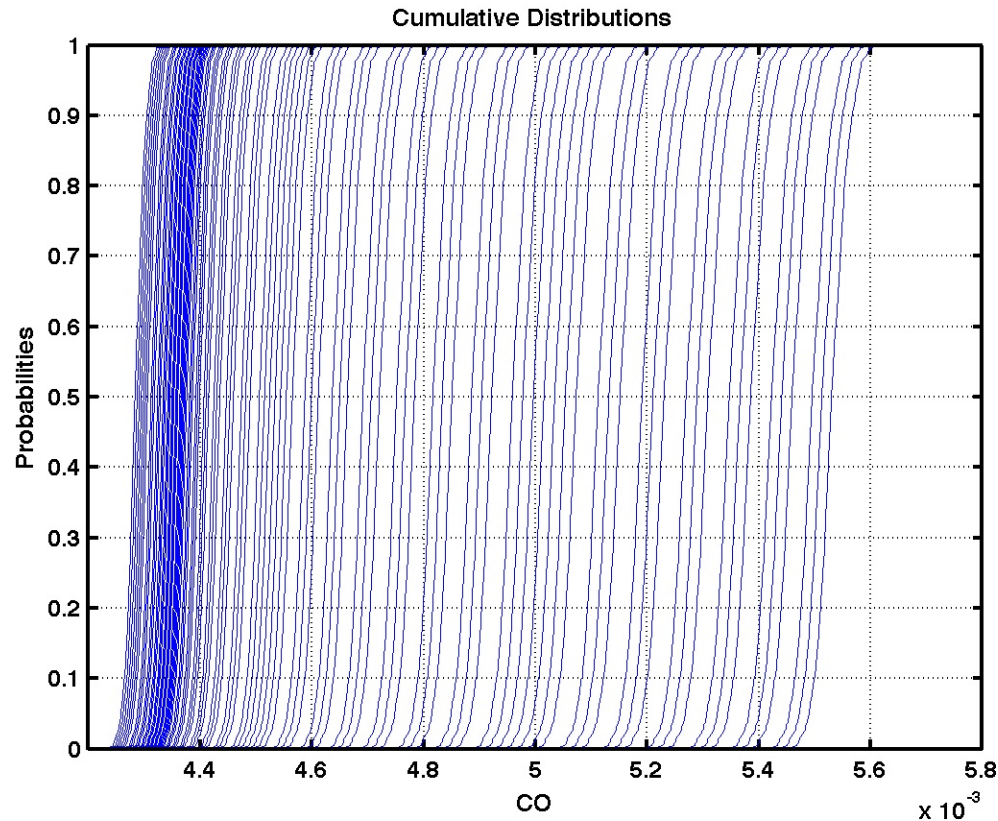
Sampling Method: CCD, SparseGrid

Sample Size = 17 (CCD), 13 (SparseGrid)



Input Uncertainty Forward Propagation for Mixed Epistemic & Aleatory Uncertainty using the Surrogate:

Response # 3 CO



- Gaussian Process Model based surrogate model employed.
- There are many CDFs
 - Each corresponds to aleatoric parameters with the epistemic fixed.
- Epistemic uncertainties are dominating.

Sample Problem # 3 for Parametric Non-Intrusive UQ Study: C3M - PC Coal Lab (Aleatory Uncertainty)

(in collaboration with K. Chaudhari and Prof. R. Turton of WVU, P. Nicoletti of URS Corp.)

Objective: Determine the effect of uncertainty in heating rate, temperature and pressure on species mass fractions

Uncertainty Quantification Study Properties:

Input parameters with Uncertainty [min-max range]:

- | | |
|-------------------------|--------------|
| (1) Heating rate (°C/s) | [200 – 9727] |
| (2) Temperature (°C) | [500 – 1010] |
| (3) Pressure (kPa) | [861 – 3447] |

System Response Variables:

Species mass fractions computed by C3M – PCCL

- (1) CO (2) CO₂ (3) tar (4) H₂ (5) H₂O (6) CH₄

Sampling Method: LPTAU, Direct Monte Carlo,
SparseGrid

Sample Size = 250 (LPTAU), 10,000 (Direct Monte Carlo)

Sample Problem # 3 for Parametric Non-Intrusive UQ Study: C3M PC Coal Lab (Aleatory Uncertainty)

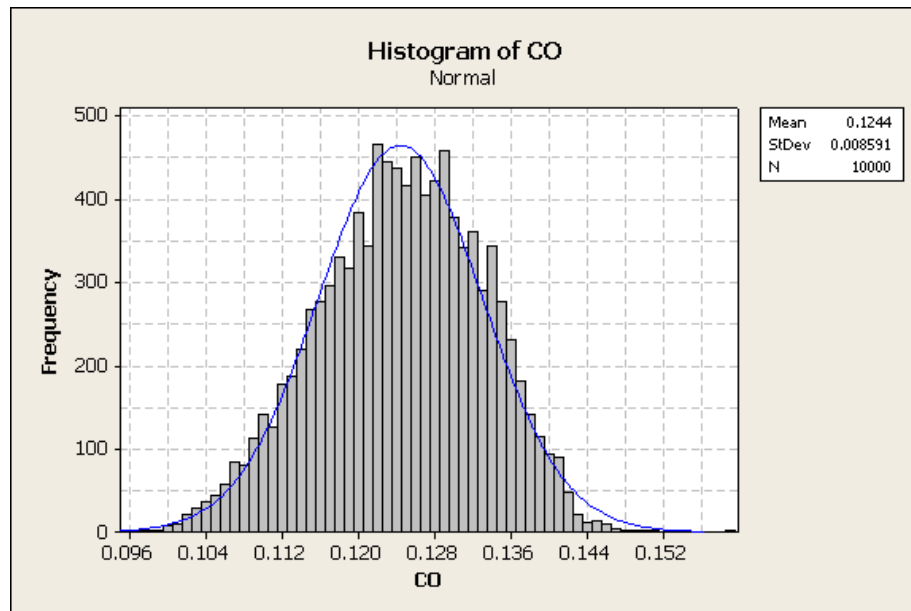
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- The input parameters were assumed as aleatory uncertainty and assigned with the following PDFs for Monte Carlo simulations:
 - Heating Rate: Normal ($\mu=3000$, $\sigma=1000$)
 - Temperature: Normal ($\mu=800$, $\sigma=100$)
 - Pressure: Normal ($\mu=2000$, $\sigma=500$)
- PSUADE UQ toolbox was used to generate truncated PDFs from the above prescribed distributions for random drawings to be used in the Monte Carlo simulations.
- Two approaches employed:
 1. Monte Carlo(MC) Simulation through a surrogate model
 - C3M-PCCL runs at 250 sample points performed to create MARS based non-parametric response surface to act as surrogate model.
 2. Direct Monte Carlo Simulation without a surrogate model
 - Instead of employing a surrogate model, C3M-PCCL was directly executed for the 10,000 sample conditions.

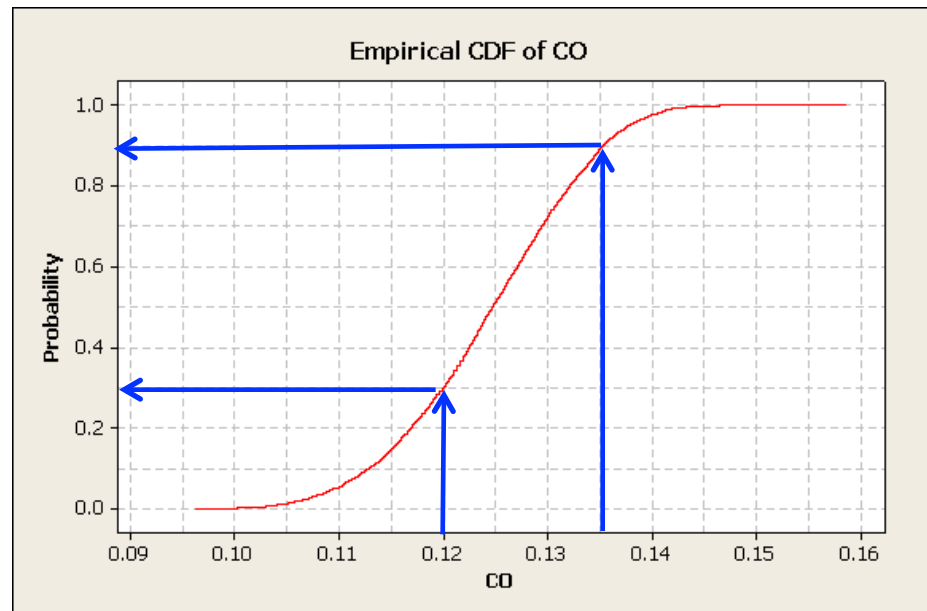
Sample Problem # 3 for Parametric Non-Intrusive UQ Study: C3M PC Coal Lab (Aleatory Uncertainty)

cont'd

Empirical CDF Plots Response 1: CO species mass fraction



Direct Monte Carlo Simulation Results for
Species Mass Fraction CO



Above plot shows Empirical Cumulative Density
Function plot from Direct Monte Carlo simulations.

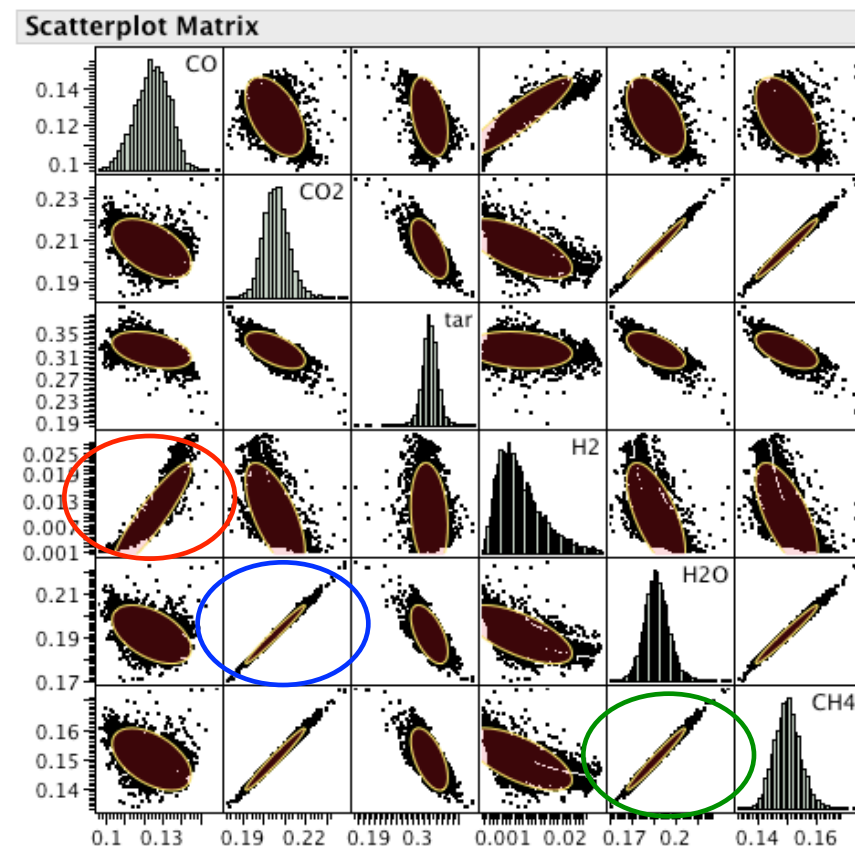
Given prescribed input uncertainties the probability of CO mass
fraction being between 0.12 and 0.135 is about 60% .

Sample Problem # 3 for Parametric Non-Intrusive UQ Study: C3M PC Coal Lab (Aleatory Uncertainty)

cont'd

Correlation Matrix and Scatterplot for Species Mass Fractions (Response Variables 1 to 6)

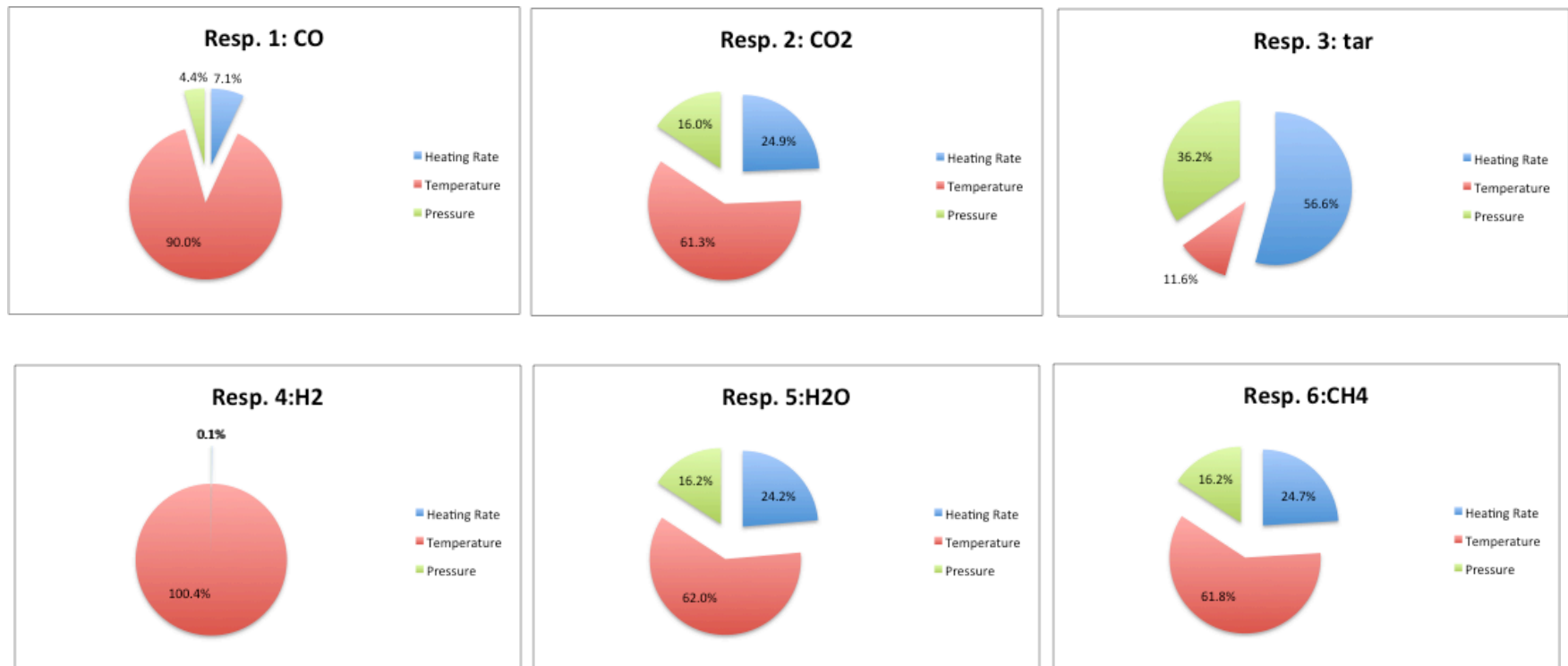
Multivariate						
Correlations						
	CO	CO2	tar	H2	H2O	CH4
CO	1.0000	-0.4990	-0.3964	0.9087	-0.4965	-0.5003
CO2	-0.4990	1.0000	-0.5844	-0.6626	0.9836	0.9802
tar	-0.3964	-0.5844	1.0000	-0.1835	-0.5870	-0.5804
H2	0.9087	-0.6626	-0.1835	1.0000	-0.6586	-0.6615
H2O	-0.4965	0.9836	-0.5870	-0.6586	1.0000	0.9802
CH4	-0.5003	0.9802	-0.5804	-0.6615	0.9802	1.0000



Sample Problem # 3 for Parametric Non-Intrusive UQ Study: C3M PC Coal Lab (Aleatory Uncertainty)

cont'd

Sensitivity Analysis with Sobol Total Indices Method (Response Variables 1 to 6 with MARS based surrogate model from 250 runs)



Summary and Conclusions

- Identification and characterization of uncertainties are as important as propagation/analysis of uncertainties
- Effective and efficient UQ requires cross fertilization between various disciplines.
- Non-intrusive UQ enables black box treatment of the application code but requires many samples to achieve the necessary accuracy by reducing sampling error.
- Typically 80% of effort spent goes into constructing an adequate surrogate model.
- The surrogate model adequacy check points out to the need for better convergence criteria in CFD
- The surrogate model is able to capture when pyrolysis is dominant and when gasification is dominant.

Survey To Identify Various Parametric Sources of Uncertainties and Their Mathematical Characterization

Columns: A B C D E F G H I J K L M N

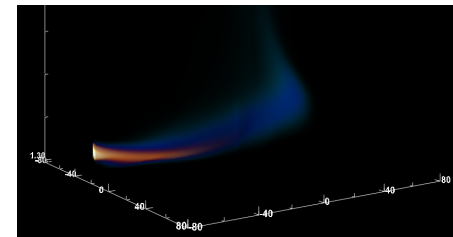
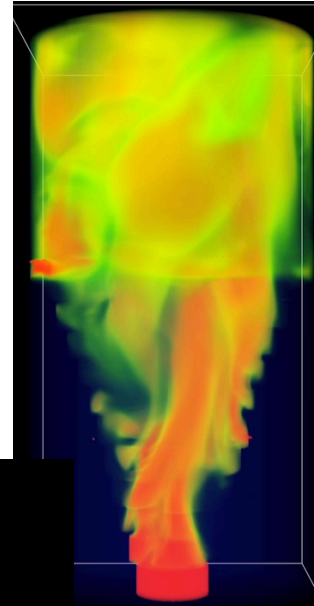
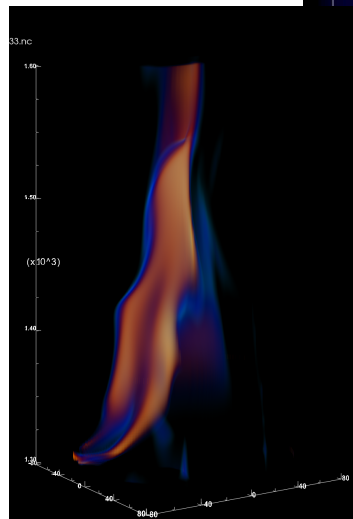
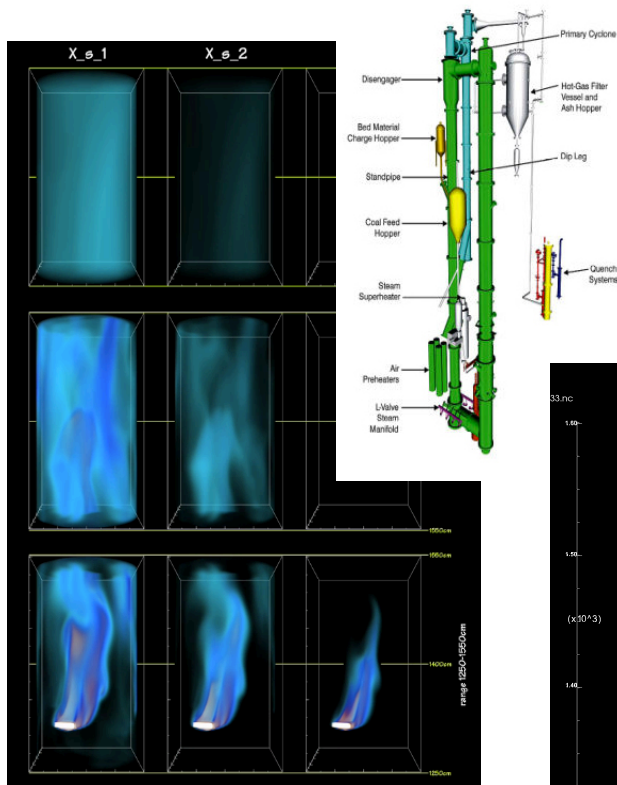
Importance Rank (Select)	Sources of Uncertainty in Model Input or Uncertain Input Parameters	Symbol or Variable Name	Units	Enter either Nominal value ΔN (Min/Max values OR Min/Max %)					Justification for the provided "most likely value" and lower/upper bounds (Please provide reference citations)	Classification of Uncertainty (Select from list)	Characterize Uncertainty (Select from list)	if Aleatory, set Probability distribution & parameters	Is it correlated with any other source of uncertainty?	If correlated then specify input parameter & why
				The most likely value (n) or the Nominal value	Minimum value: (a) { (a) < (n) }	Maximum value: (b) { (n) < (b) }	Minimum value (% of n)	Maximum value (% of n)						
1	Mean solids circulation rate	Gs	kg/s	14			90	110.00%	Experimental data [1,2]	Aleatory (A)	PDF	N(13.97,0.34)	Y	Fsl
2	Mean superficial gas velocity at bottom	Ug	m/s	7.58			95	105.00%	Experimental data [1,3]	Aleatory (A)	PDF	N(7.57,0.04)	Y	Fsl
5	Gas flow rate from standpipe and L-valve	Fsl	SCMs	0.029			99.955	100.05%	Experimental data [1,3]	Aleatory (A)			N	
11	Temperature	T	K	293	287	299			Experimental data [1,3]	Aleatory (A)			N	
10	Pressure at top exit	P	kPa	105			99.996	100.00%	Experimental data [1,3]	Aleatory (A)			N	
6	Particle diameter	dp	um	802	784	820			Experimental data [1]	Aleatory (A)			N	
7	Particle density	rho	kg/m3	863			99.99	100.01%	Experimental data [1]	Aleatory (A)			N	
8	restitution coefficient	e	-	0.8					Literature [4]	Epistemic (E)			N	
9	sphericity (*)	phi	-	0.95					Experimental data [1]	Aleatory (A)			N	
3	wall boundary for solids phase (\$))	BC	-	partial-slip					Expert opinion [5]	Epistemic (E)			N	
4	Interphase drag (&)	beta	-							Epistemic (E)				

Justification for the provided "most likely value" and lower/upper bounds (Please provide reference citations)	Classification of Uncertainty (Select from list)	Characterize Uncertainty (Select from list)	if Aleatory, set Probability distribution & parameters	Is it correlated with any other source of uncertainty?	If correlated then specify input parameter & why
Experimental data [1,2]	Aleatory (A)	PDF	N(13.97,0.34)	Y	Fsl
Experimental data [1,3]	Aleatory (A)	PDF	N(7.57,0.04)	Y	Fsl
Experimental data [1,3]	Aleatory (A)			N	
Experimental data [1,3]	Aleatory (A)			N	
Experimental data [1,3]	Aleatory (A)			N	
Experimental data [1]	Aleatory (A)			N	
Experimental data [1]	Aleatory (A)			N	
Literature [4]	Epistemic (E)			N	
Experimental data [1]	Aleatory (A)			N	
Expert opinion [5]	Epistemic (E)			N	
	Epistemic (E)				

Future Work

- Improve identification and characterization of uncertainties for application domain.
- Expand the work on mixed aleatory and epistemic uncertainty cases.
- Explore Bayesian techniques
 - GPM/SA toolbox from Los Alamos Lab.
- Better quantification of sampling error and surrogate model errors
- Extend stochastic collocation and polynomial chaos based surrogate model using sparse grids.

Questions?



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