Significance of NETL Supercomputer for Uncertainty Quantification Study

Impact of SBEUC on Uncertainty Quantification of Gasifier CFD Models

- The NETL Supercomputer plays a critical role in two major dimensions for our UQ applications:
  - Offers capacity computing environment where large number of sampling simulations, each running on many cores can be performed concurrently without substantial delays typically encountered in shared resource centers.
  - Offers capability computing environment where high fidelity simulations can be conducted to validate models and post-processed locally without data movement for data mining and visualization.

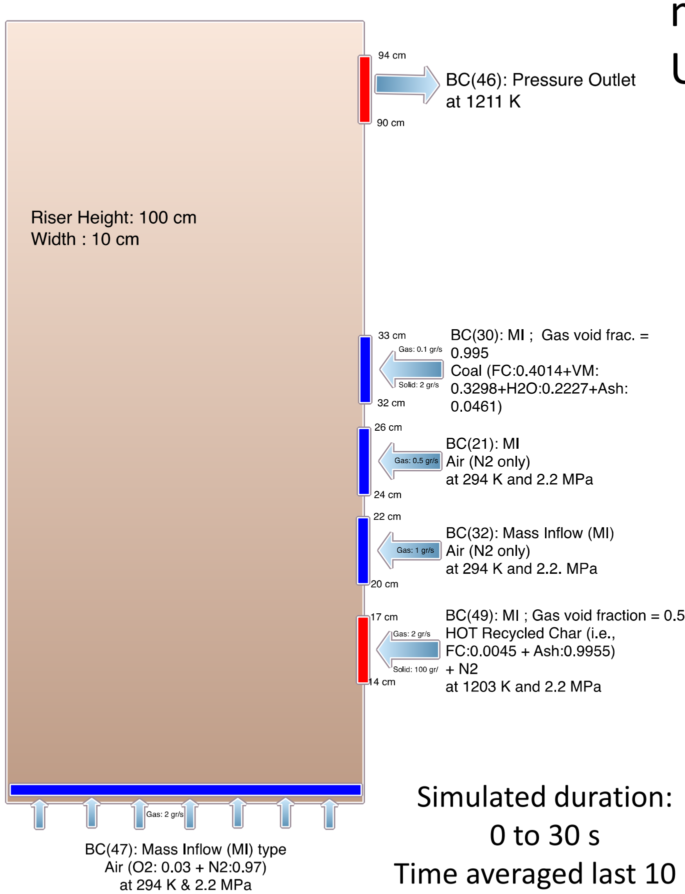
Demonstration for Capacity Computing

- We were able to perform sampling simulations with hundreds of samples of 2D MFIX runs for pyrolysis and compare MGAS kinetics versus PCCL kinetics.
- First-of-its-kind 1,000 sample Monte Carlo simulation of 2D reacting MFIX runs, each using 32 cores was only possible due to capacity computing environment available with the NETL Supercomputer.

Demonstration for Capacity Computing

- Case: 2D Gasifier

Objective: Sensitivity Analysis to compare kinetic models and Forward Propagation of Input Uncertainty with and without a surrogate model.



Simulated duration:
0 to 30 s
Time averaged last 10 s

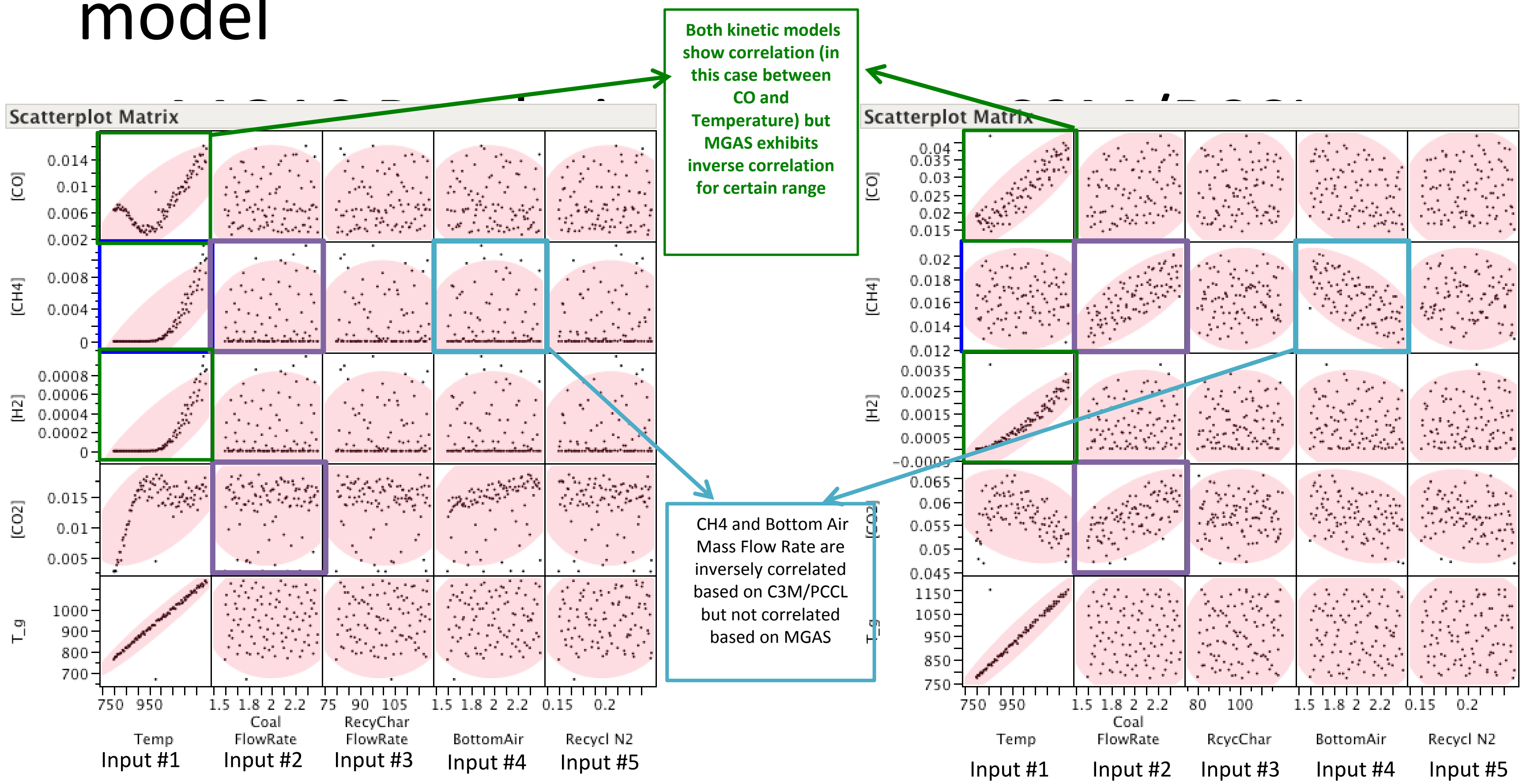
	Grid Resolution
Coarse	50 x 500
Medium	70 x 707
Fine	100 x 1000

Uncertain Input Parameters	Range (Lower – Upper)	Units
Temperature	800 – 1200	K
Coal Feed Rate (BC#30)	1.6 – 2.4	g/s
Recycled Char (BC#49)	80 – 120	g/s
Bottom Air (BC#47)	1.6 – 2.4	g/s
Side Air (BC#49)	0.16 – 0.24	g/s

(Gel, A., Li, T., Shahnam, M., Guenther, C., "Non-intrusive Parametric Uncertainty Quantification for Reacting Multiphase Flows in Coal Gasifiers", ASME V&V2013, May 22-24, Las Vegas, Nevada)

Demonstration for Capacity Computing (cont’d)

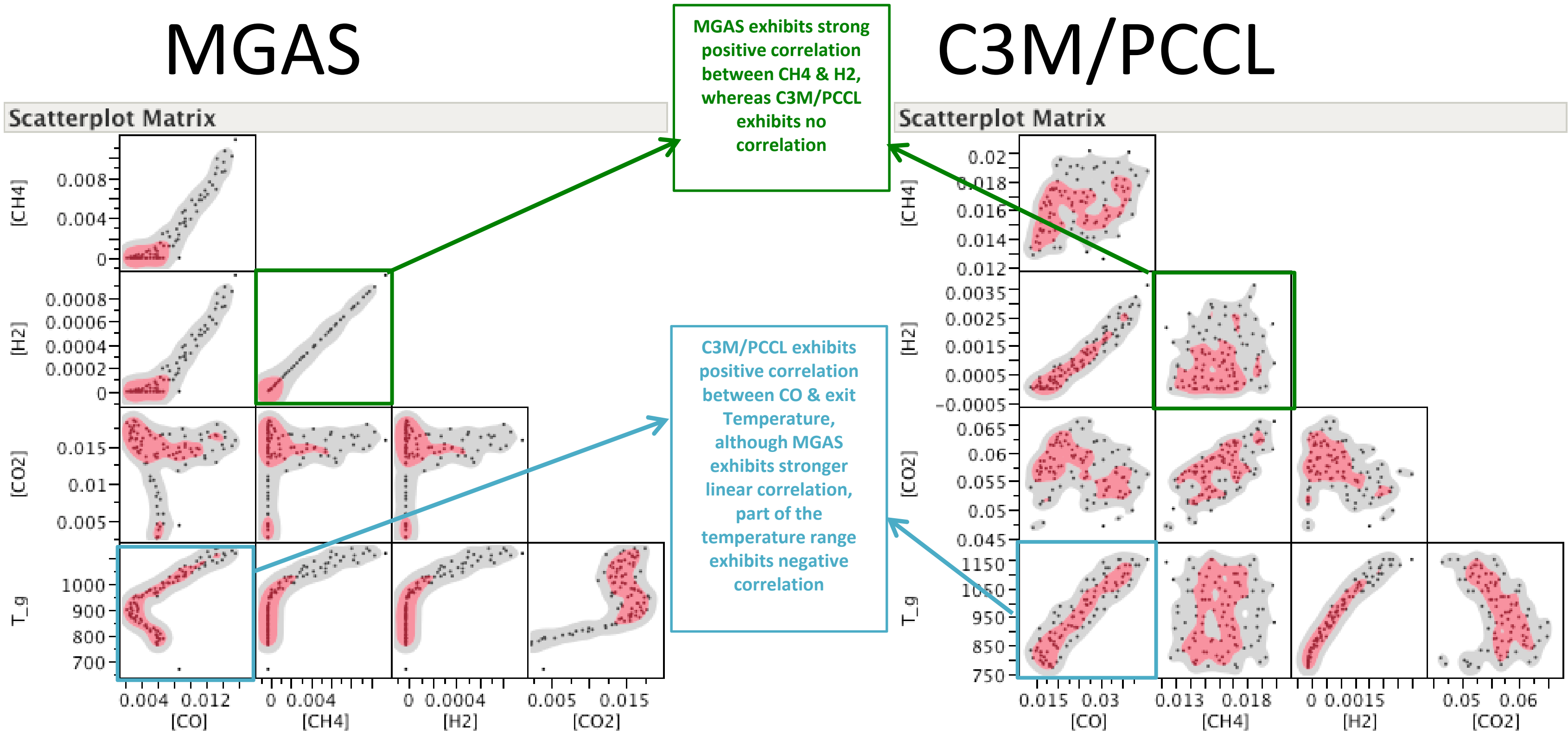
- General Overview & Comparison of Kinetics model



Scatterplot for Input versus Quantities of Interest (based on 100 samples generated at 100 x 1000 grid resolution MFIX simulations)

Demonstration for Capacity Computing (cont'd)

- Comparison of Kinetics model for pyrolysis:

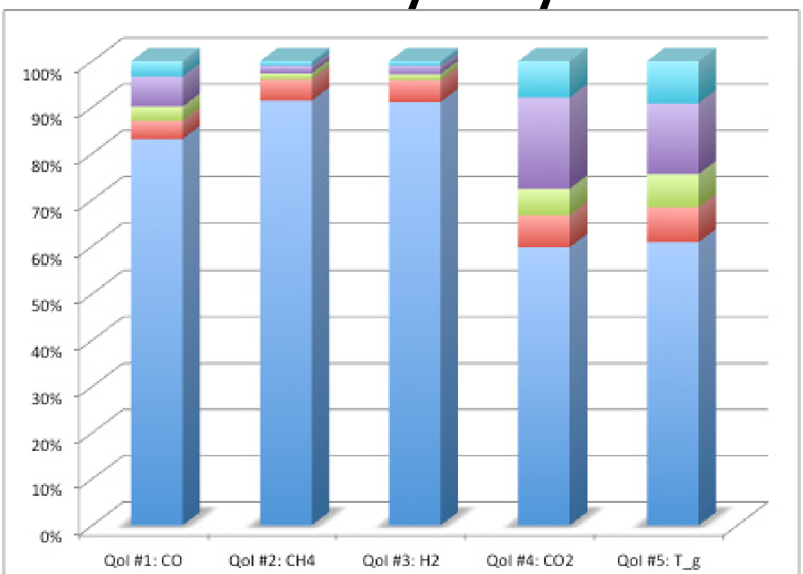


Scatterplot shown for only Quantities of Interest based on 100 samples of 100 x 1000 grid resolution MFIX simulations
(nonparametric density contours of two level colors show where most of the points are located and helps distinguish patterns in a dense structure)

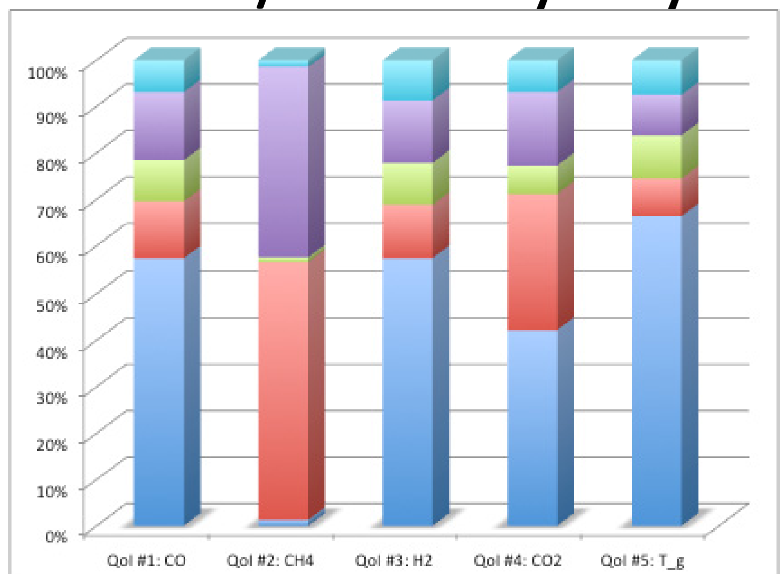
Demonstration for Capacity Computing (cont'd)

- Global Sensitivity Analysis: How much each input contribute to the observed variability in output?

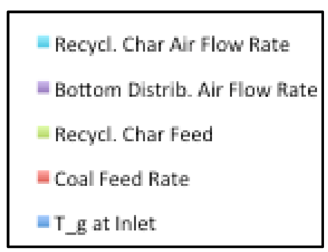
MGAS Pyrolysis



C3M/PCCL Pyrolysis



Sobol Total Sensitivity Indices Analysis Results for MGAS based pyrolysis shows temperature at the inlet to be the primary and most pronounced contributor to the variability observed in QoIs.

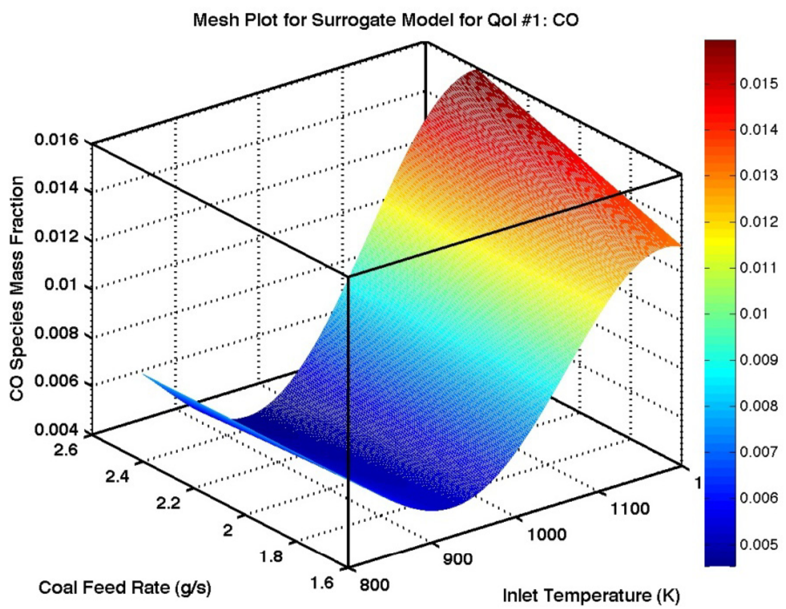


Sobol Total Sensitivity Indices Analysis Results for C3M/PCCL based pyrolysis shows temperature has significant effect but not as strong as in the MGAS results.
Methane production is mostly due to coal flow rate variability

Demonstration for Capacity Computing (cont'd)

- Input Uncertainty Forward Propagation:
  - Comparison of results between direct Monte Carlo (MC) simulation and surrogate model.
  - MC sample size = 1000 (i.e., 1000 MFIX simulations)
  - Surrogate model constructed from 50 samples generated from MFIX simulations (sampling method quasi-random MC)
  - Quantity of Interest : CO mass fraction
  - Uniform distribution employed for all input parameters when performing forward propagation.

Non-parametric surrogate model constructed from Gaussian Process Model with 50 sampling simulations of MFIX



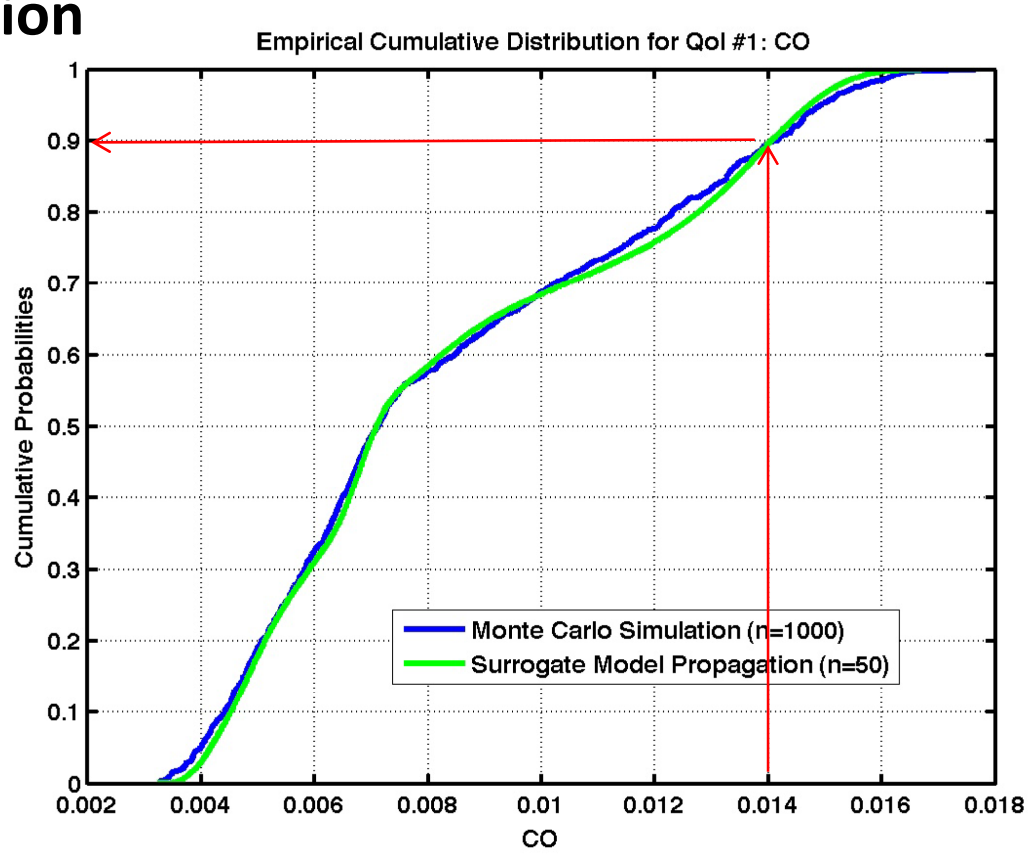
Remaining 3 input parameters set at their nominal values for Mesh Plot

Demonstration for Capacity Computing (cont'd)

- **Surrogate model can predict what Monte Carlo simulation with 1000 samples can predict for input uncertainty propagation**

Given uncertainties in the input parameters, the probability of CO mass fraction being ≤0.014 is 90 %

Note: Other sources of uncertainties such as model form uncertainties, or numerical approximation are not taken into account.



Empirical Cumulative Distribution Function plot comparing forward propagation results generated from Surrogate model (constructed with 50 sampling MFIX simulations) and MC performed with 1,000 sampling runs of MFIX

Publications & Presentations

- Gel, A., Shahnam, M., Subramaniyan, A., Musser, J., Dietiker, J.,"Non-intrusive Uncertainty Quantification for Reacting Multiphase Flows in Coal Gasifiers", ASME V&V Symposium, 2014, Las Vegas, NV
- Gel, A., Shahnam, M., Subramaniyan, A, Musser, J., "Application and Comparison of Non-intrusive Uncertainty Quantification Methods in Multiphase Flow Simulations for Coal Gasifiers" SIAM UQ Conference, 2014, Savannah, GA.
- Gel, A., Li, T., Shahnam, M., Guenther, C., "Non-intrusive Parametric Uncertainty Quantification for Reacting Multiphase Flows in Coal Gasifiers", ASME V&V Symposium, 2013, Las Vegas, NV