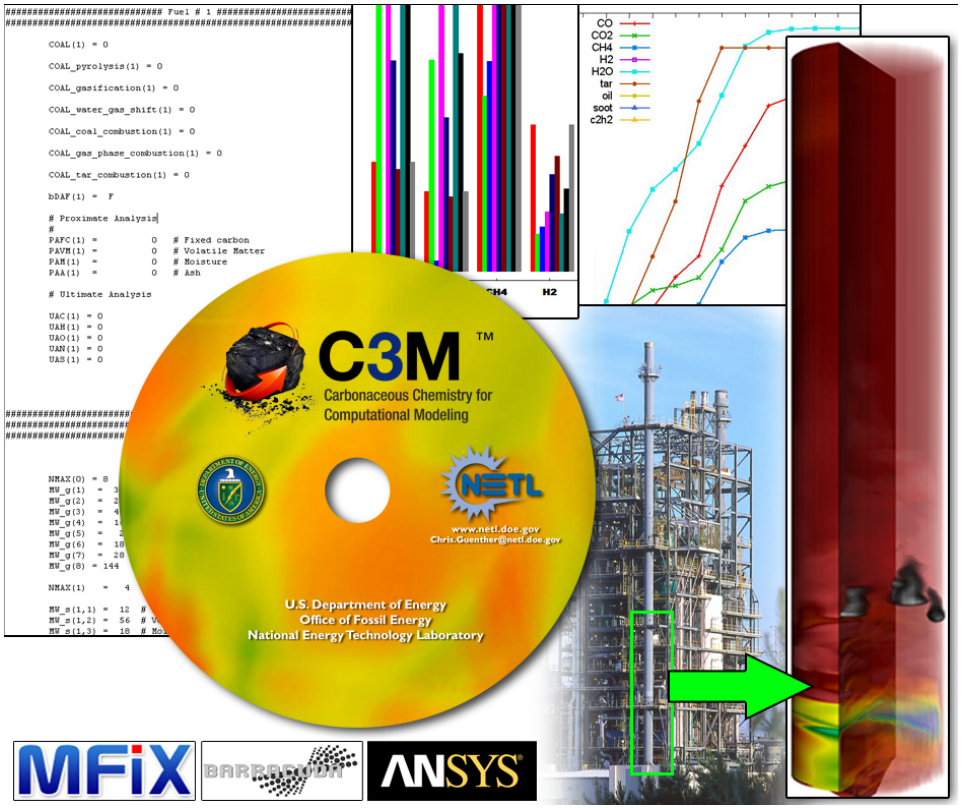
Recent Developments in Carbonaceous Chemistry for Computational Modeling (C3M) with Uncertainty Quantifications(UQ)



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Outline

- Introduction
- C3M Structure
- C3M Use For Process Models
- Uncertainty Quantifications (UQ) Analysis
  - Effect of Operating Conditions
  - Effect of Variations in Proximate and Ultimate Analysis
- Summary
- Future Work
- Acknowledgement

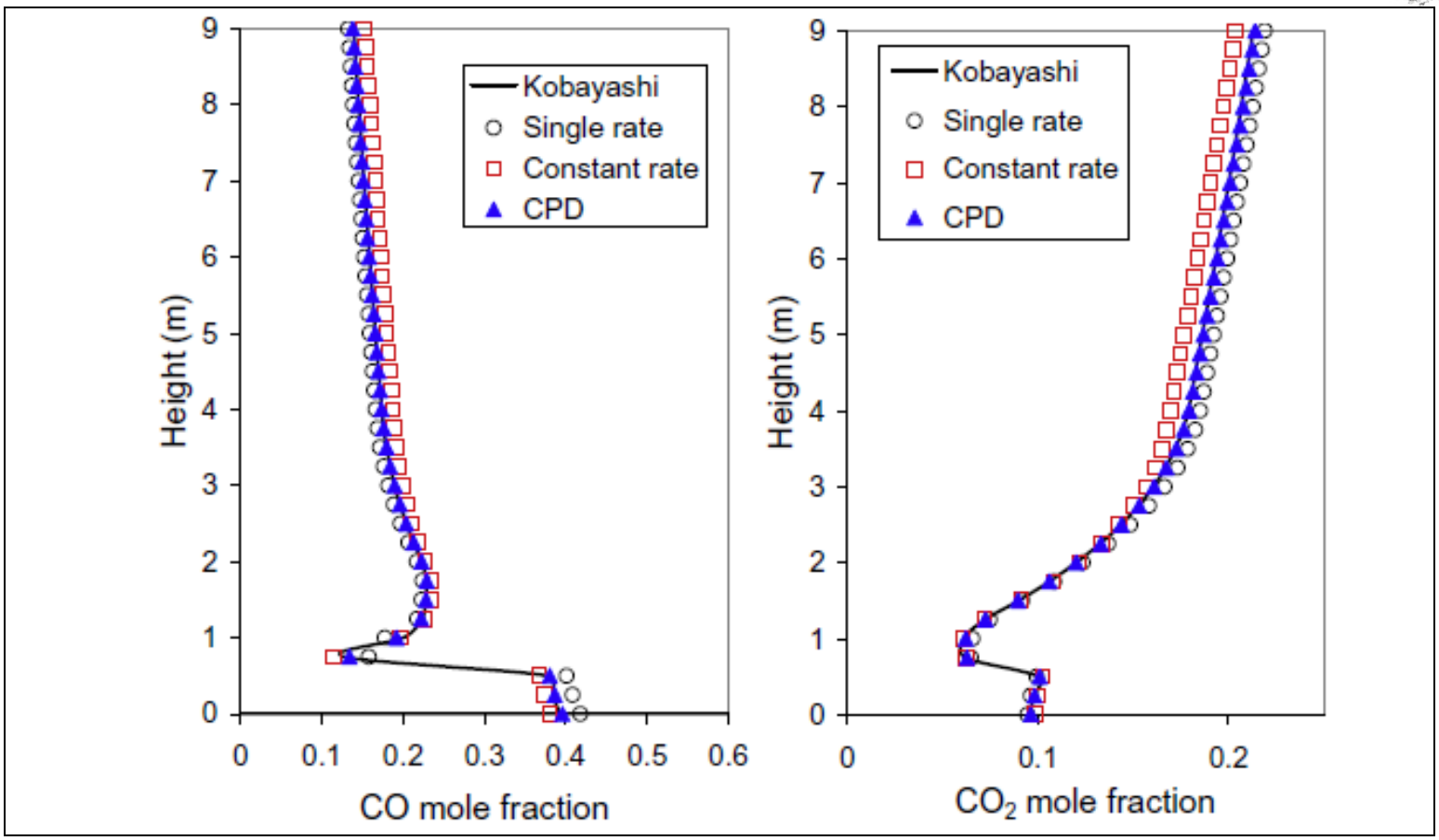
Introduction

- New gasifiers coming on-line in the 21st century will require greater fuel flexibility, reliability, availability, maintainability, and higher throughput and conversion

- Computational Fluid Dynamics (CFD) Modeling
  - Better understanding of the process
  - Scale up and Optimization
  - Experimental data for verification

- Coal gasification Process
  - Multiphase reactive system
  - Reaction kinetics is key element
  - Kinetic packages are useful

Introduction



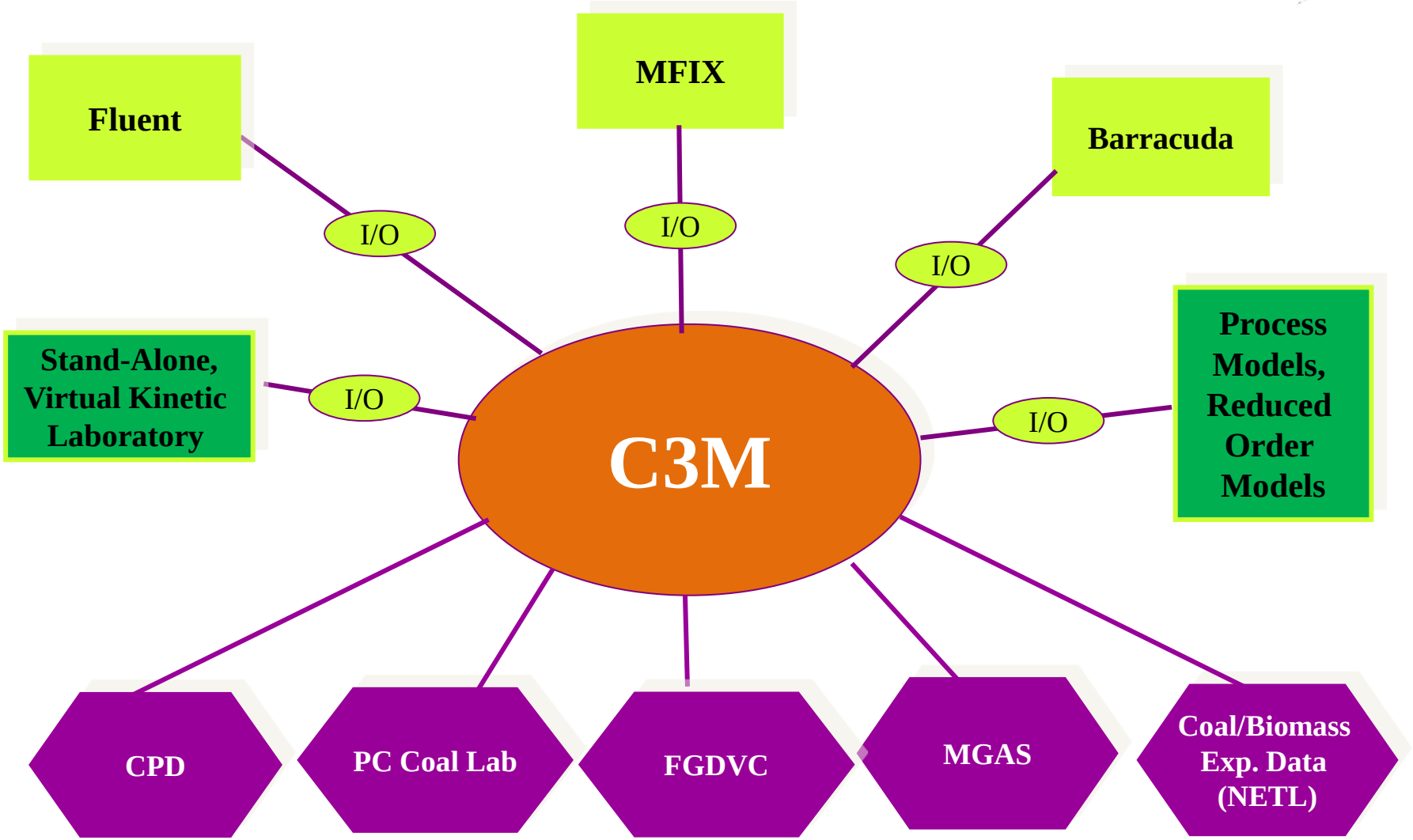
CO and CO_2 yield along the reactor based on the devolaitlizaiton model used to simulate entrained flow gasifier

Armin Silaen, Ting Wang, "Effect of turbulence and devolatilization models on coal gasification simulation in an entrained-flow gasifier", International Journal of Heat and Mass Transfer 53 (2010) 2074–2091.

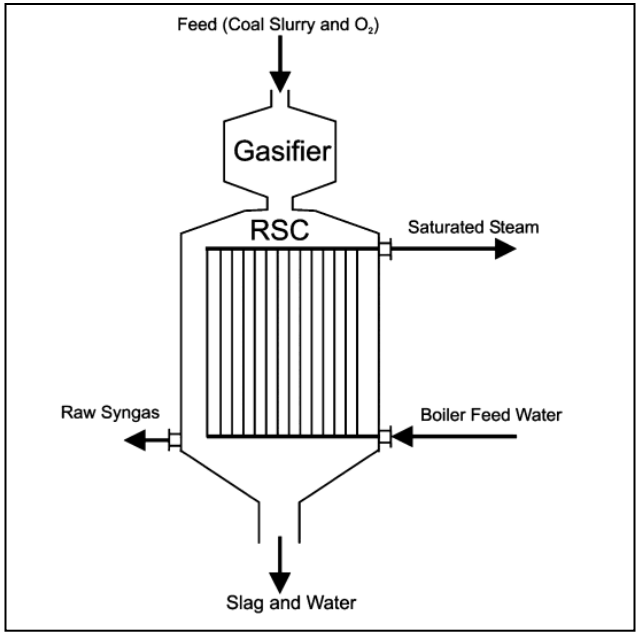
Introduction

- Lack of software platform
  - To access PC Coal Lab, CPD, FGDVC, MGAS, Experimental data
  - Do graphical comparison
  - To convert kinetic output format to CFD input
  - To link kinetic packages to CFD codes and process models

C3M Structure



C3M Use For Process Models

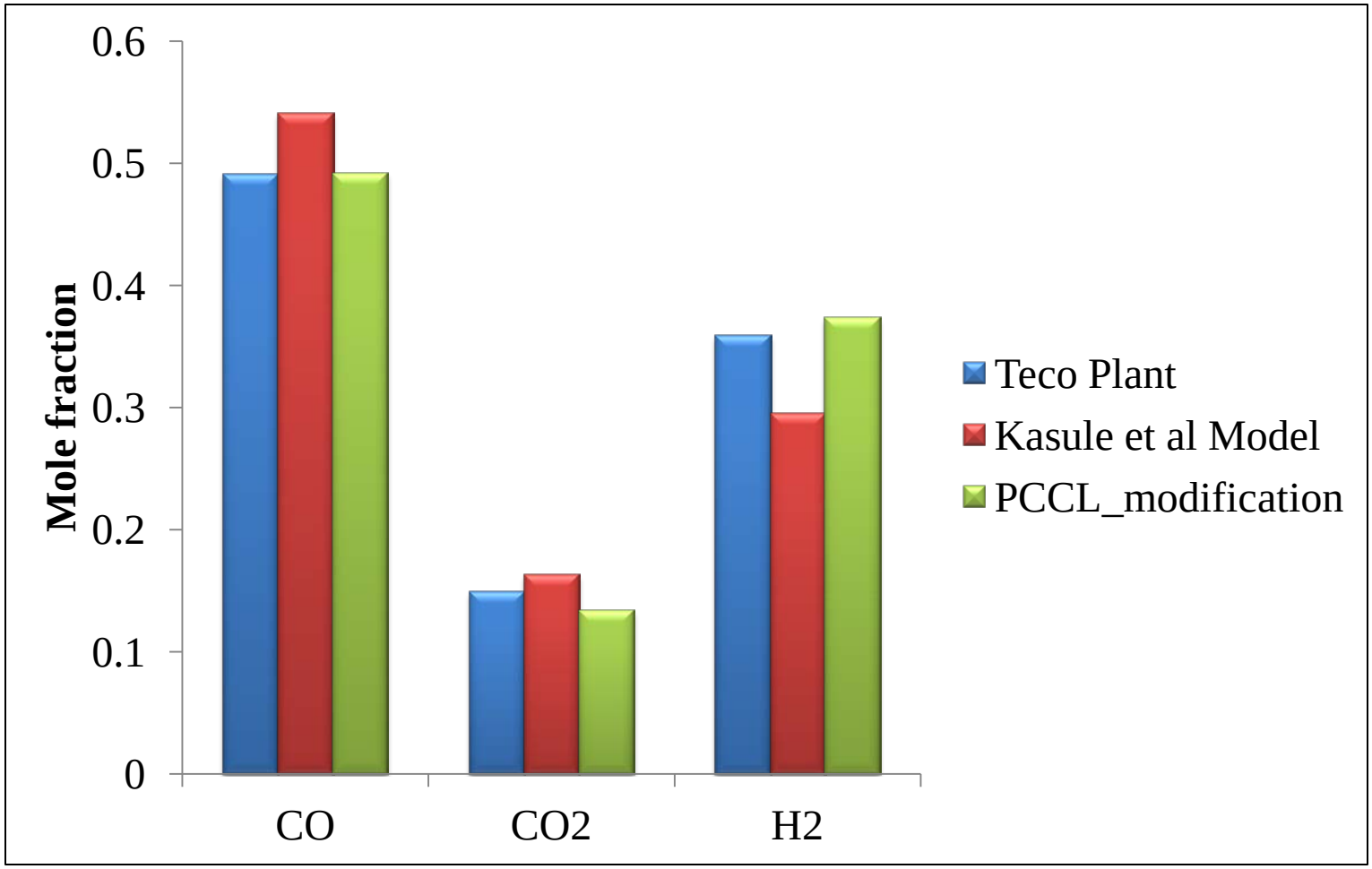


Schematic of the GEE-Texaco gasifier with RSC considered in the study.

- Detailed 1D model GEE-Texaco type gasifier *
- Aspen Custom Modeler
- Illinois no. 6 coal
- Coal gasification reactions
- Steady state model
- Plant data from Tampa Electric Company (TECO) gasifier

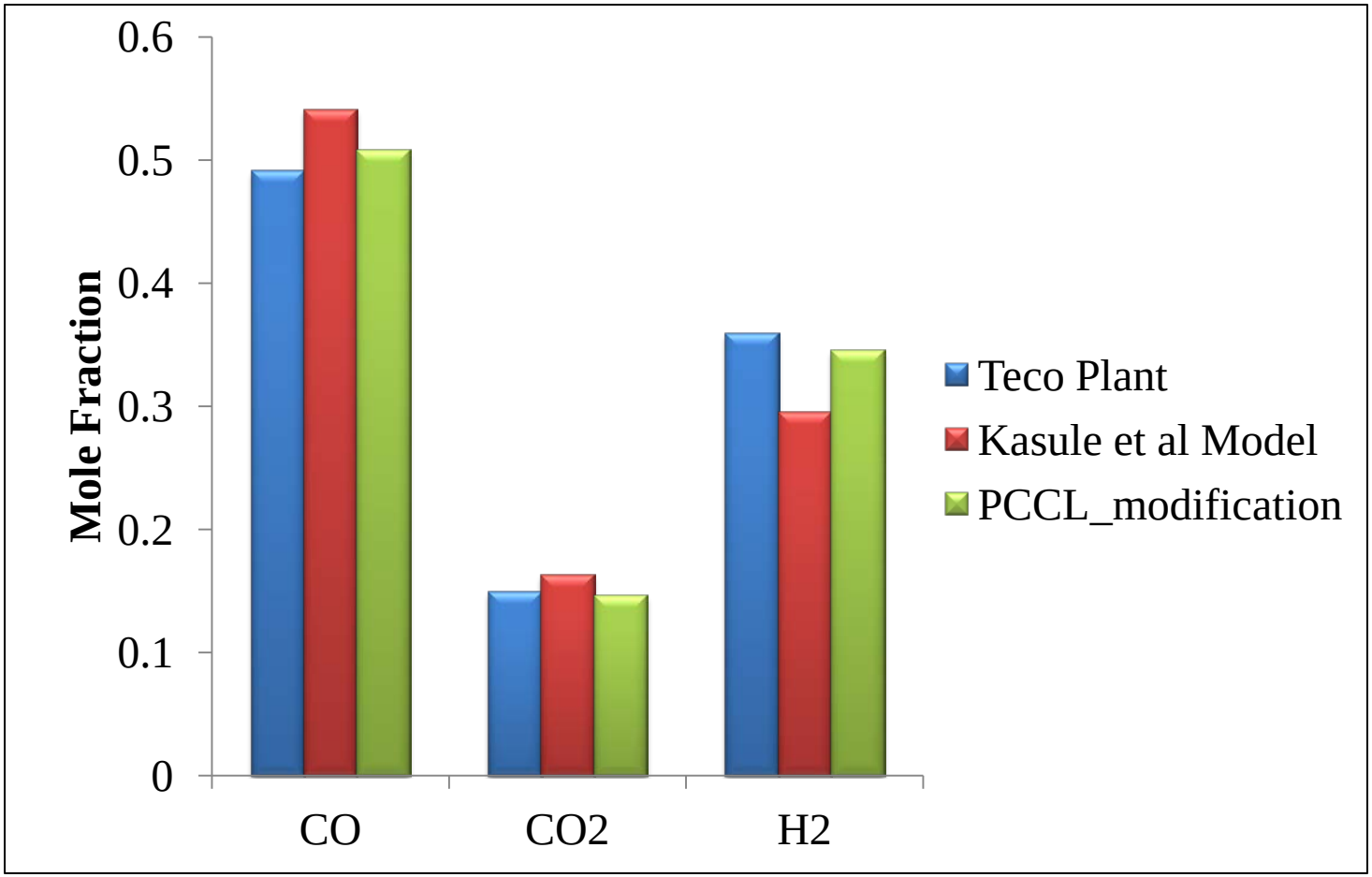
* Job S. Kasule, Richard Turton, Debangsu Bhattacharyya,and Stephen E. Zitney, "Mathematical Modeling of a Single-Stage, Downward-Firing, Entrained-Flow Gasifier", Ind. Eng. Chem. Res. 2012, 51, 6429−6440.

C3M Use For Process Models



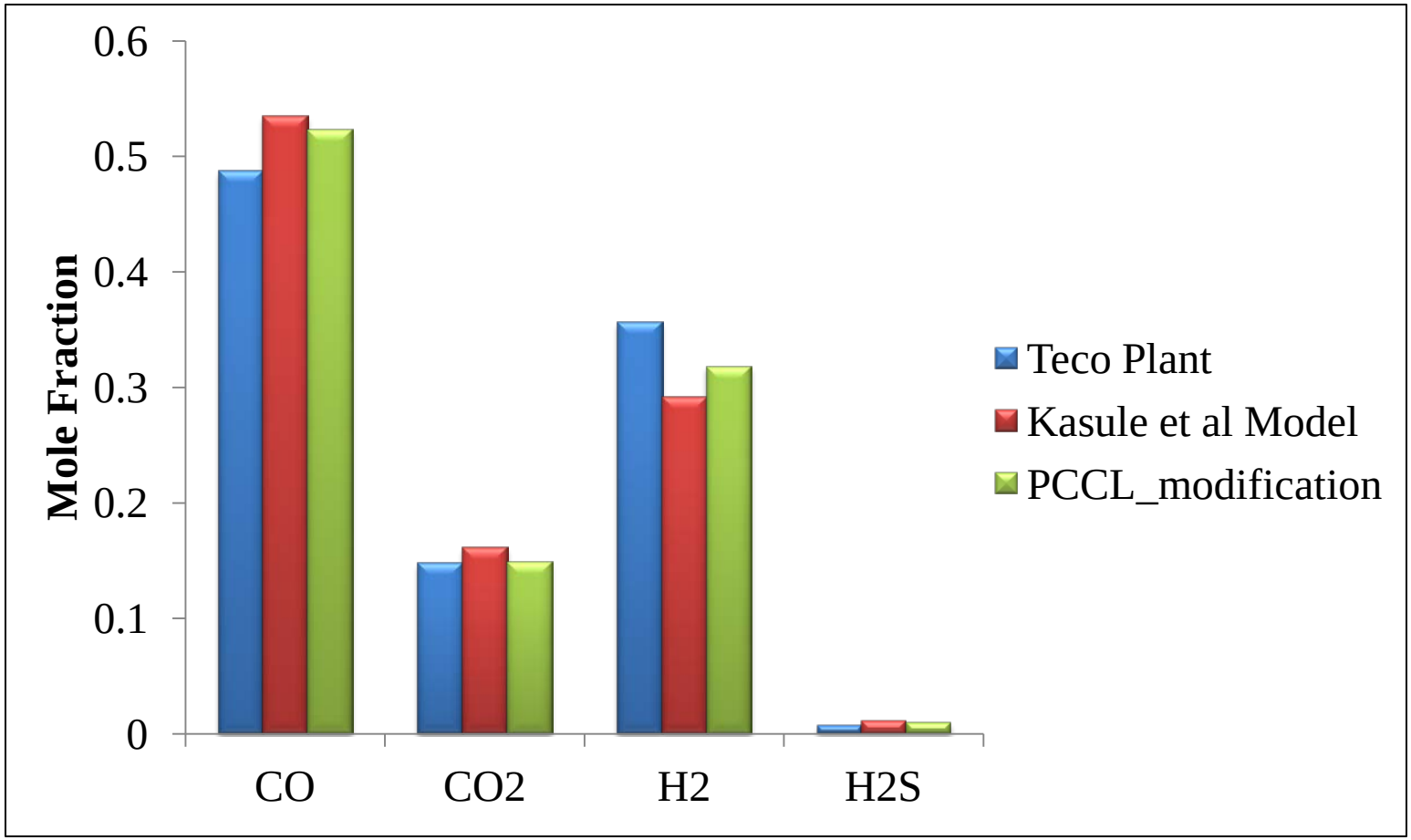
Exit composition CH_4 free, H_2S free and dry basis

C3M Use For Process Models



Exit composition with modified devoltilization, H_2O and CO_2 gasification; CH_4 free, H_2S free and dry basis

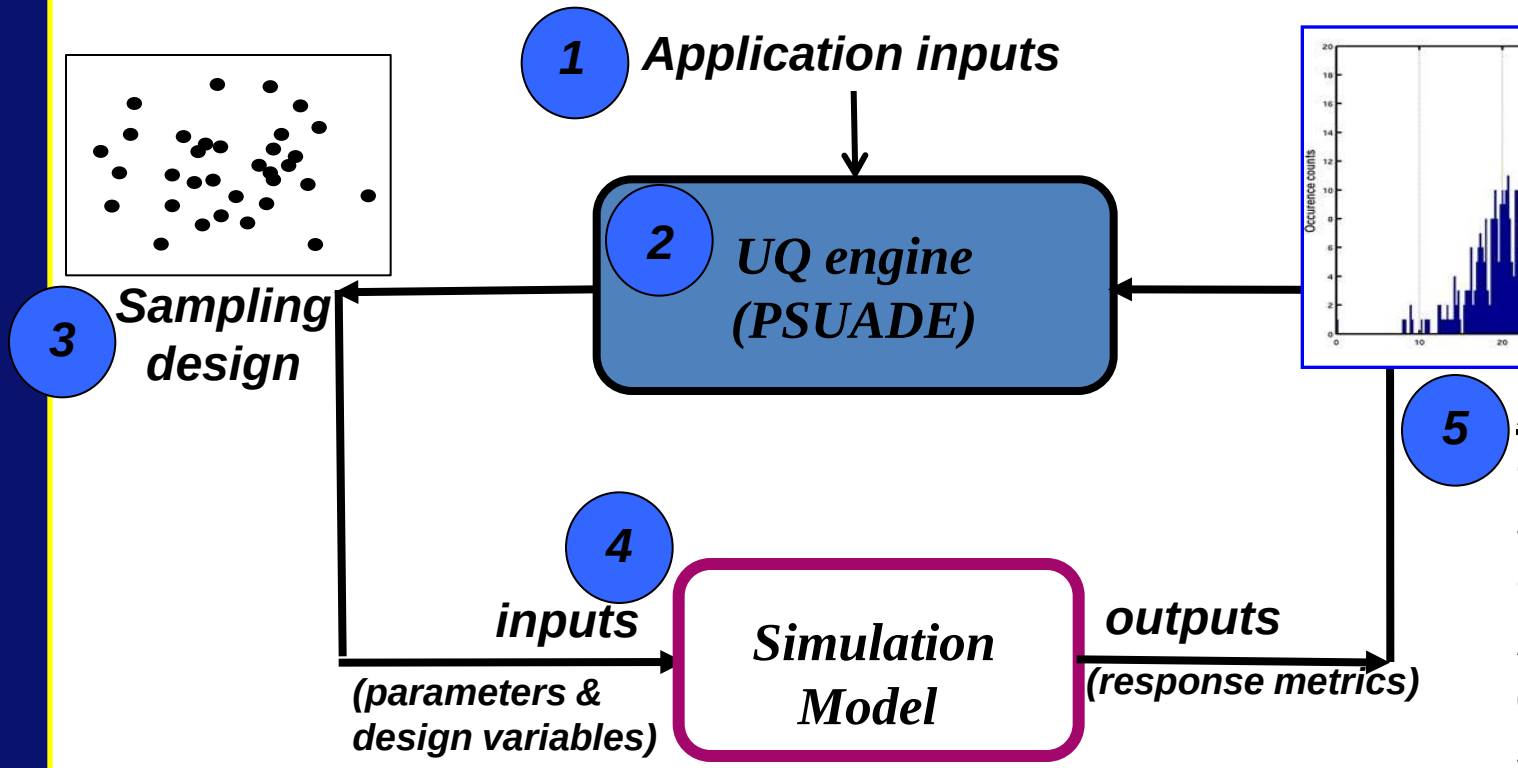
C3M Use For Process Models



Exit composition with modified devoltilization, steam and CO_2 gasification with H_2S ; CH_4 free and dry basis

Uncertainty Quantification (UQ) Analysis

Uncertainty Quantification (UQ)



Analysis:

- **Fit Response Surface (RS)**
- **Conduct UQ Analysis on RS, e.g. perform Sensitivity Study**

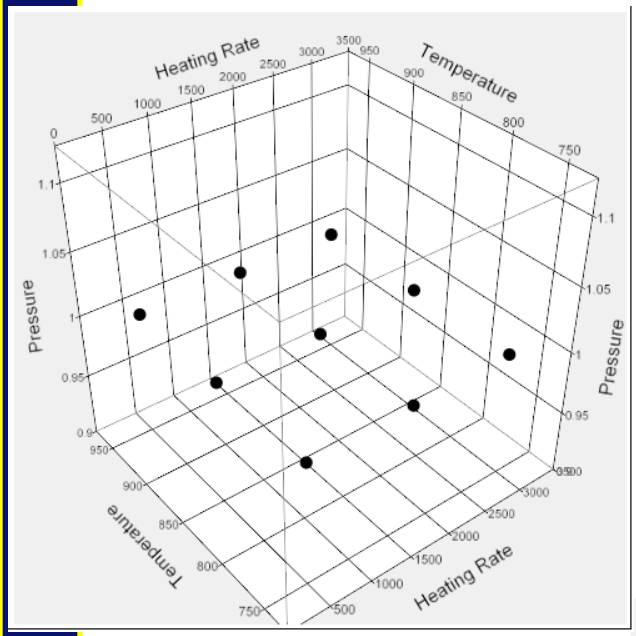
- Simulation model can be C3M or CFD codes
- May require large sample size for sufficient accuracy
- UQ analysis with respect to operating conditions and fuel characteristics

Uncertainty Analysis of Operating Conditions

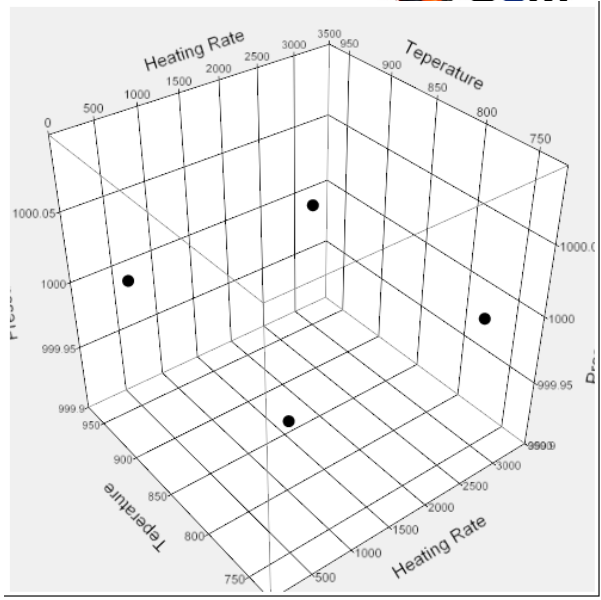
- Transport Gasifier Conditions
  - Variations in temperature and heating rate
  - Powder River Basin Coal
  - PC Coal Lab

Parameter	Low	High
Temperature	750 C	950 C
Heating Rate	500 C/s	3000 C/s
Pressure	1 MPa	1 MPa

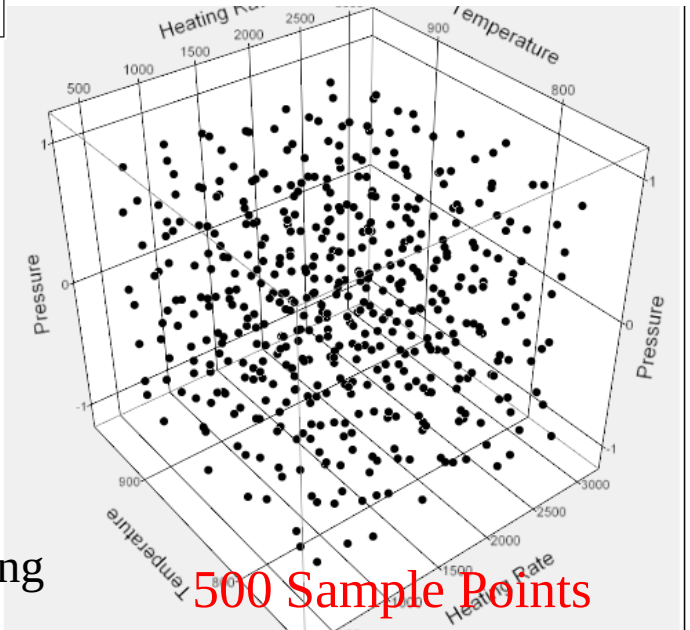
Sampling Methods



Central Composite Design



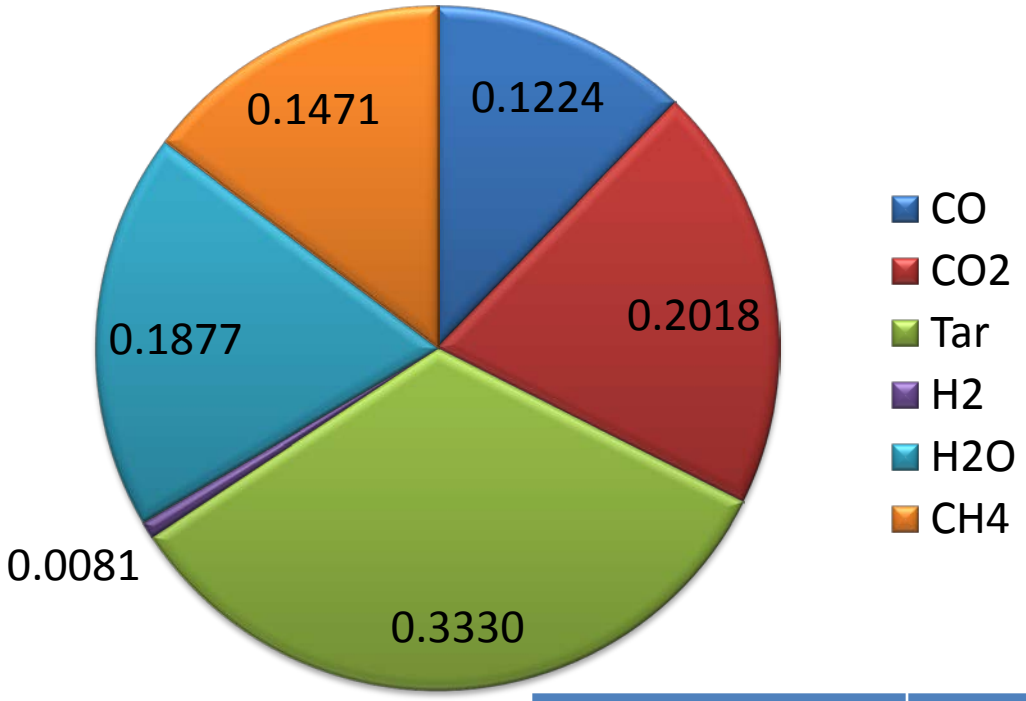
Full Factorial Design



Latin Hypercube space filling

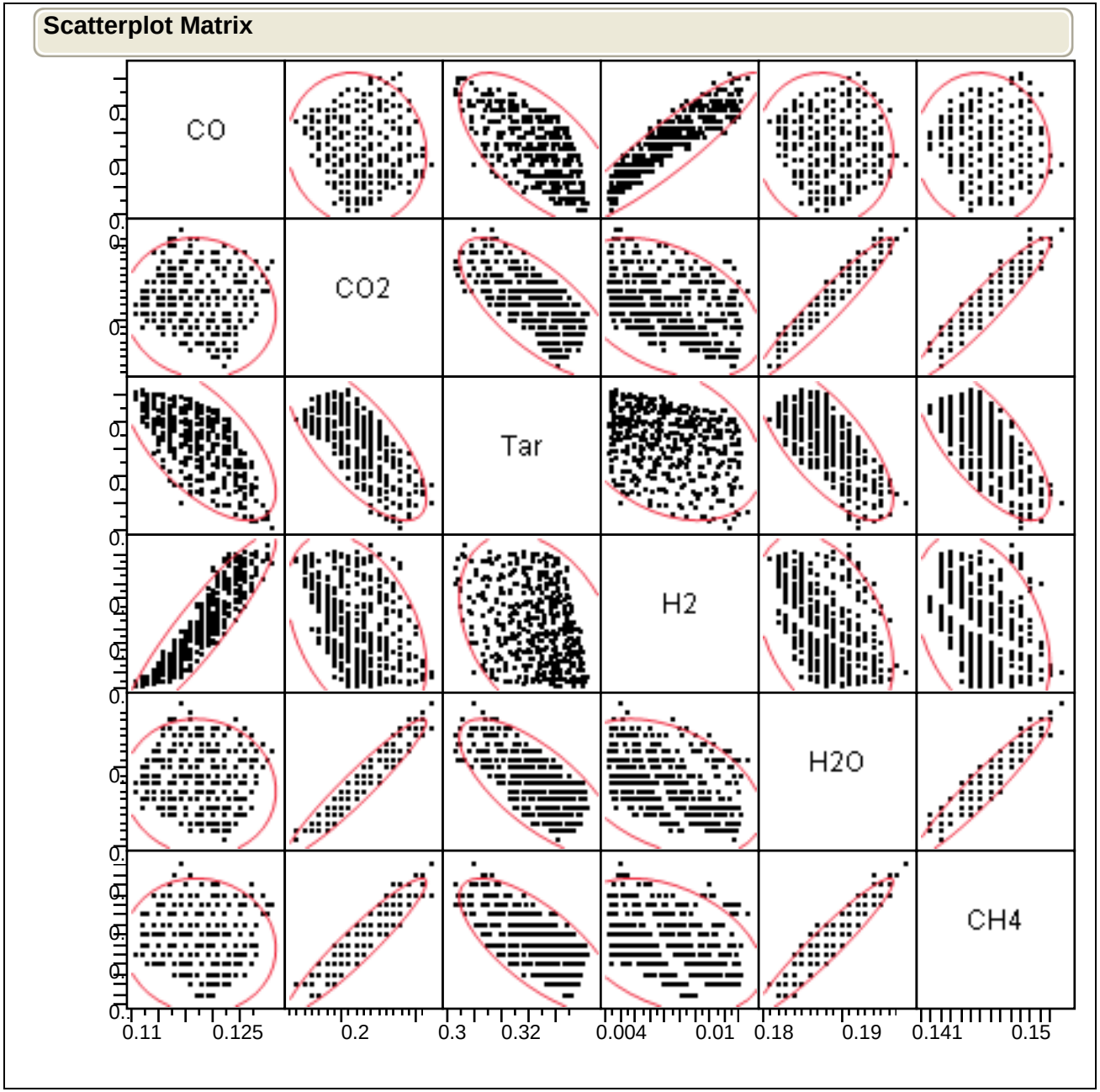
500 Sample Points

Uncertainty Analysis of Operating Conditions



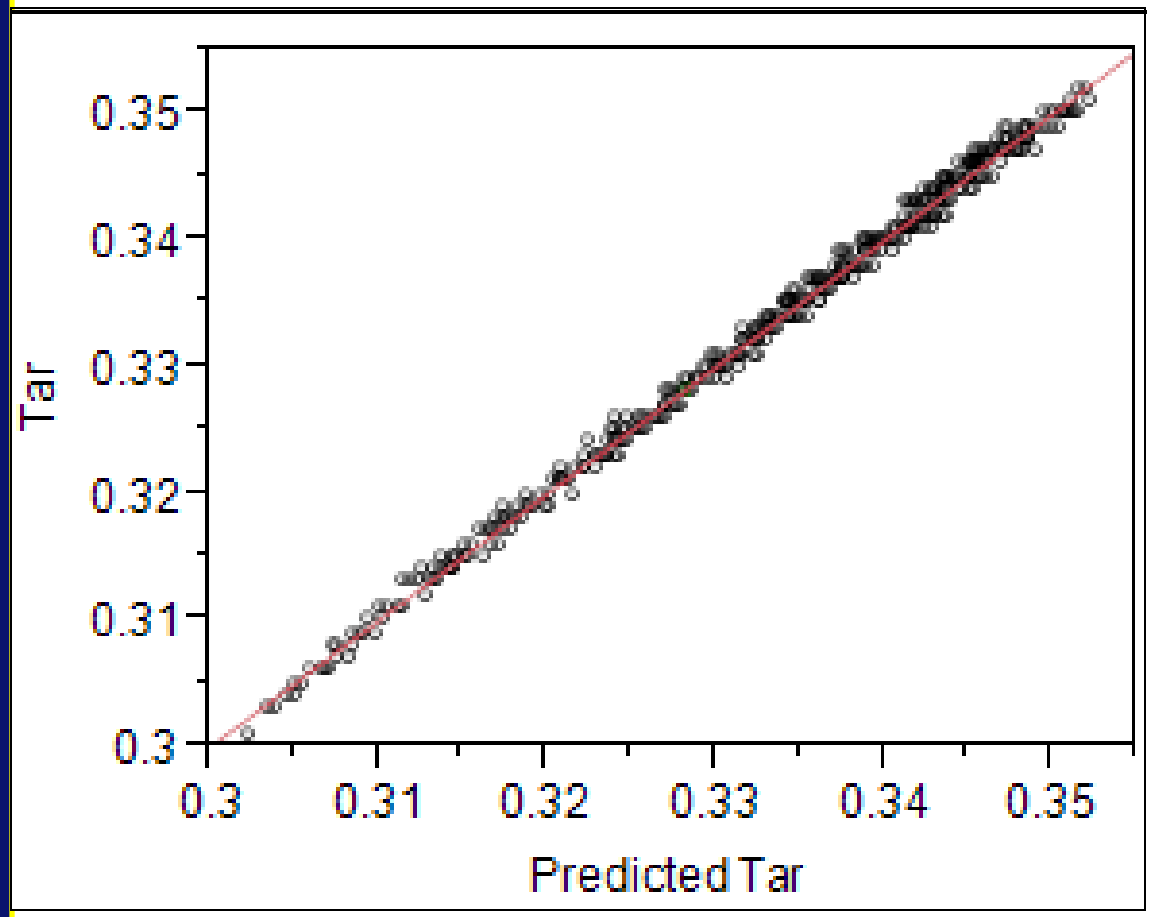
Mean devolatilization products yield

Parameter	Low	High
Temperature	750 C	950 C
Heating Rate	500 C/s	3000 C/s
Pressure	1 MPa	1 MPa



Multivariate Plot showing correlation between devolatilization product gas species

Uncertainty Analysis of Operating Conditions



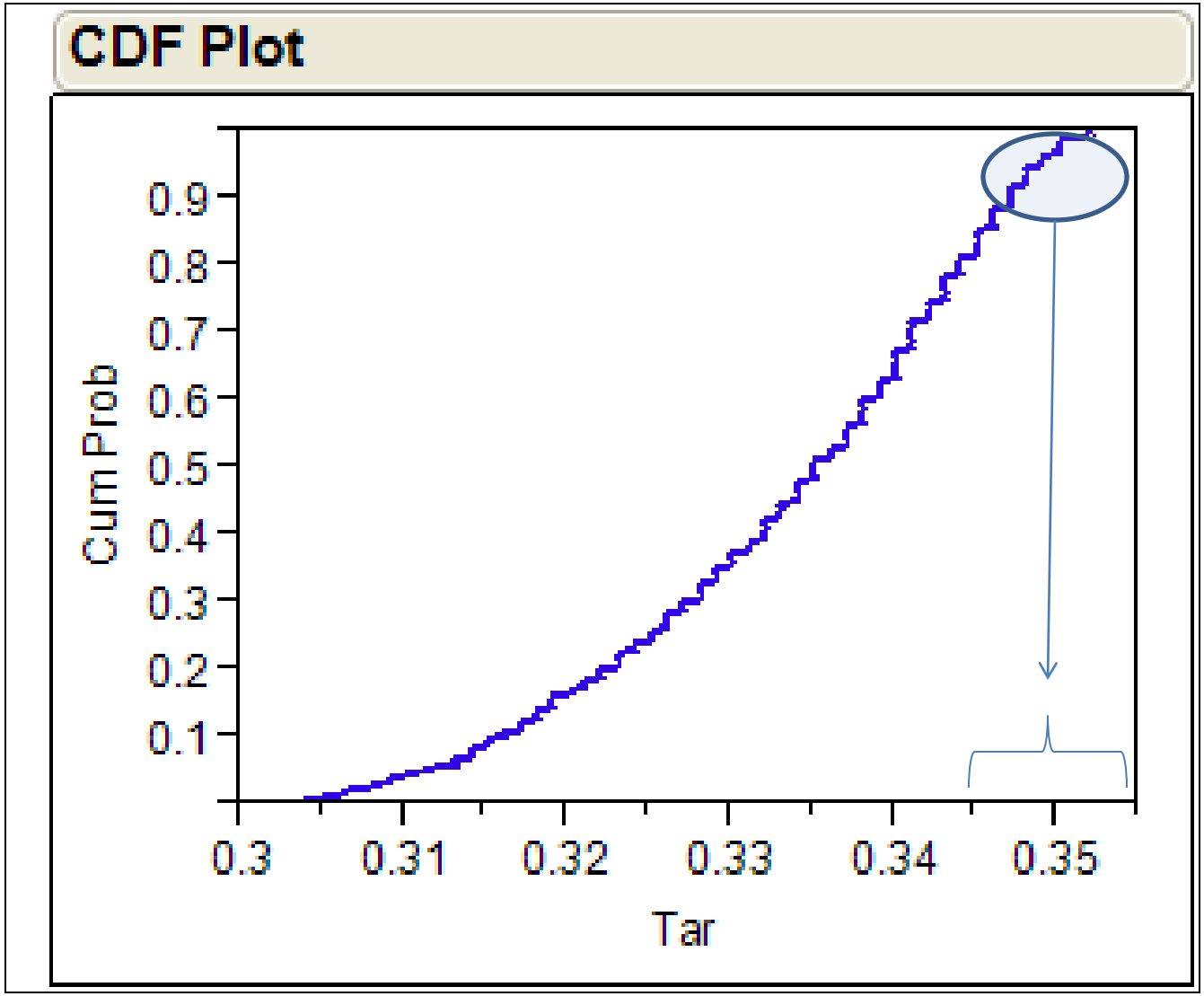
Prediction Expression

0.45368209135923
+0.0540742171180 1*Log(HR)
+-0.1002764911974*Log(Temp)

Summary of Fit

RSquare	0.995979
RSquare Adj	0.995962
Root Mean Square Error	0.000748
Mean of Response	0.332972
Observations (or Sum Wgts)	500

Uncertainty Analysis of Operating Conditions



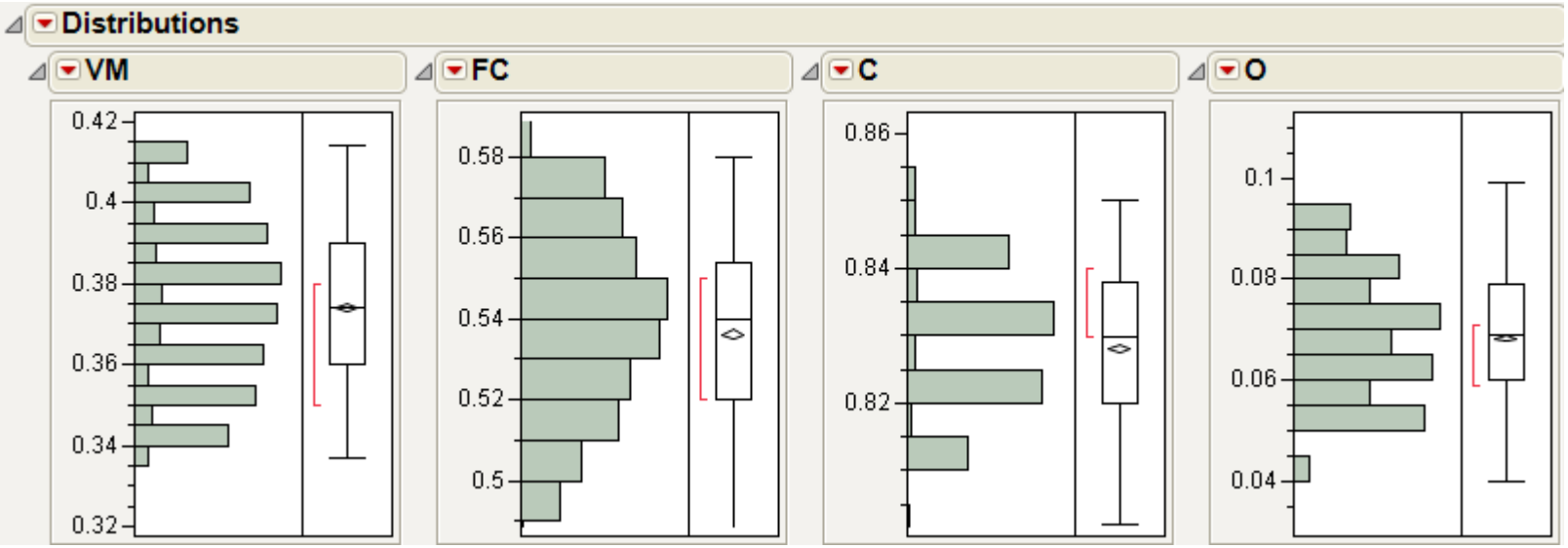
Uncertainty Analysis of Proximate and Ultimate Analysis

Coal Type: Pittsburgh 8

	Proximate Analysis:				Ultimate Analysis:				
Source:	**Volatile Matter**	**Fixed Carbon**	**Moisture**	**Ash**	**% C**	**% H**	**% O**	**% N**	**% S**
Ref #1	33.50	57.70	1.00	7.80	84.20	6.10	6.60	1.50	1.60
Ref #2	37.81	52.07	1.08	8.90	84.21	5.58	4.96	1.53	3.86
Ref #3	35.40	56.30	1.40	6.90	82.90	5.60	7.70	1.60	2.20
Ref #4	35.26	55.63	1.55	7.56	82.19	5.52	8.61	1.65	2.03
Ref #5	41.10	50.02	2.02	6.86	82.47	5.47	7.76	1.70	2.60
Ref #6	40.89	49.76	1.94	7.41	82.30	5.56	7.92	1.71	2.51
Ref #7	39.30	49.00	1.00	10.70	81.43	5.21	9.51	1.59	2.27
Ref #8	35.66	55.44	1.66	7.24	83.18	5.69	5.84	1.55	3.73
Ref #9	33.52	57.69	1.00	7.79	83.70	5.98	4.26	1.53	4.53
Ref #10	36.41	57.69	1.87	4.03	84.70	5.40	7.26	1.71	0.93
Mean	36.89	54.13	1.45	7.52	83.13	5.61	7.04	1.61	2.63
Std Dev	2.79	3.55	0.41	1.67	1.06	0.26	1.63	0.08	1.11
Max	41.10	57.70	2.02	10.70	84.70	6.10	9.51	1.71	4.53
Min	33.50	49.00	1.00	4.03	81.43	5.21	4.26	1.50	0.93

*Aytekin Gel

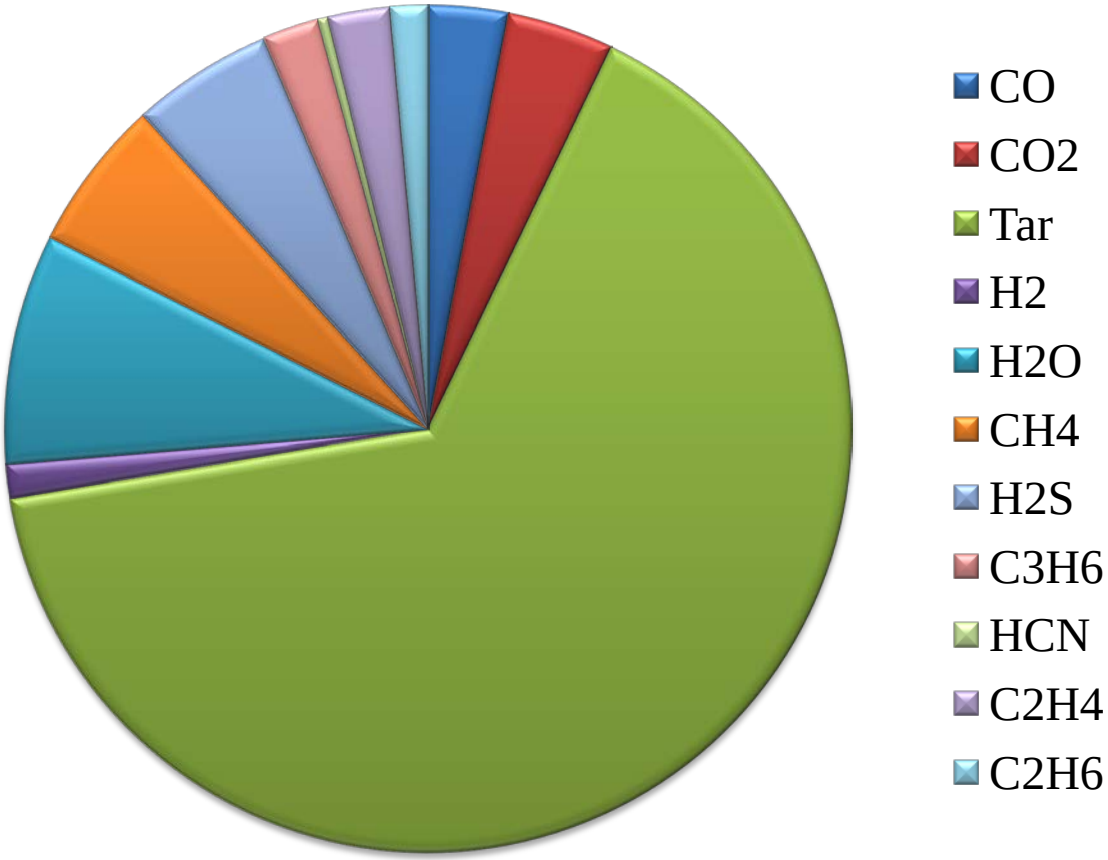
Uncertainty Analysis of Proximate and Ultimate Analysis



- Samples generated to reflect the uncertainty in PA and UA
- PA and UA adding up to 100 %
- PC Coal Lab devolatilization with 1689 sample points

Input	Values
Temperature	800 C
Pressure	1 Mpa
Heating rate	1000 C/s
Particle Diameter	100 µm
Residence time	5 sec

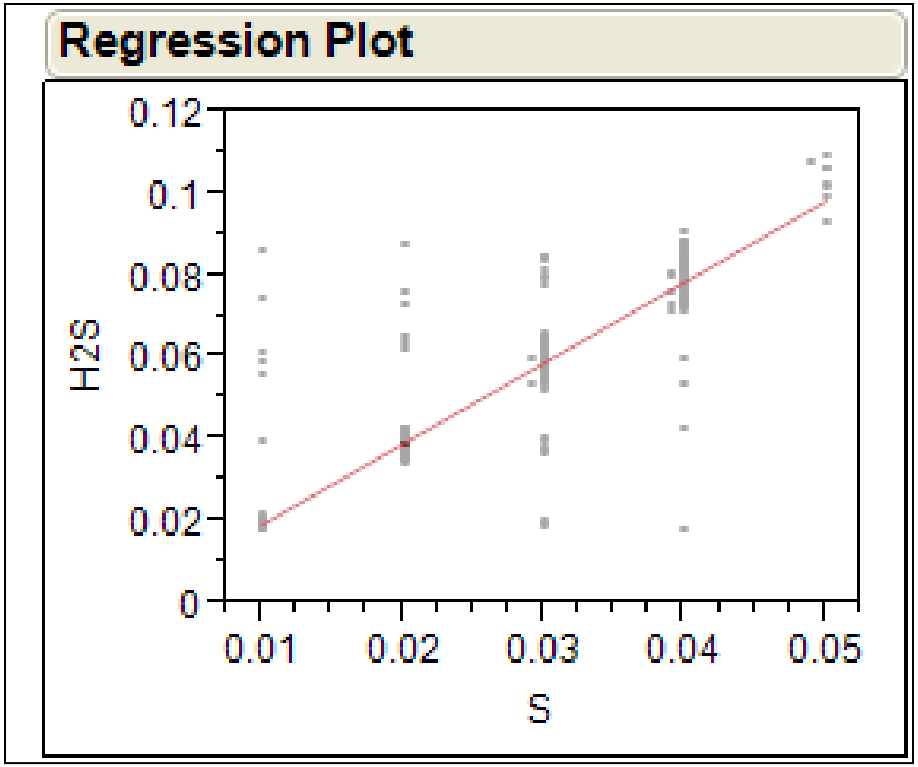
Uncertainty Analysis of Proximate and Ultimate Analysis



Devolatilization products yield

	μ	σ^2
CO	0.031	0.0091
CO_2	0.041	0.0028
Tar	0.653	0.0467
H_2	0.013	0.0011
H_2O	0.088	0.0205
CH_4	0.058	0.0254
H_2S	0.054	0.0211
C_3H_6	0.022	0.0085
HCN	0.004	0.0005
C_2H_4	0.023	0.0113
C_2H_6	0.014	0.0063

Uncertainty Analysis of Proximate and Ultimate Analysis



Summary of Fit

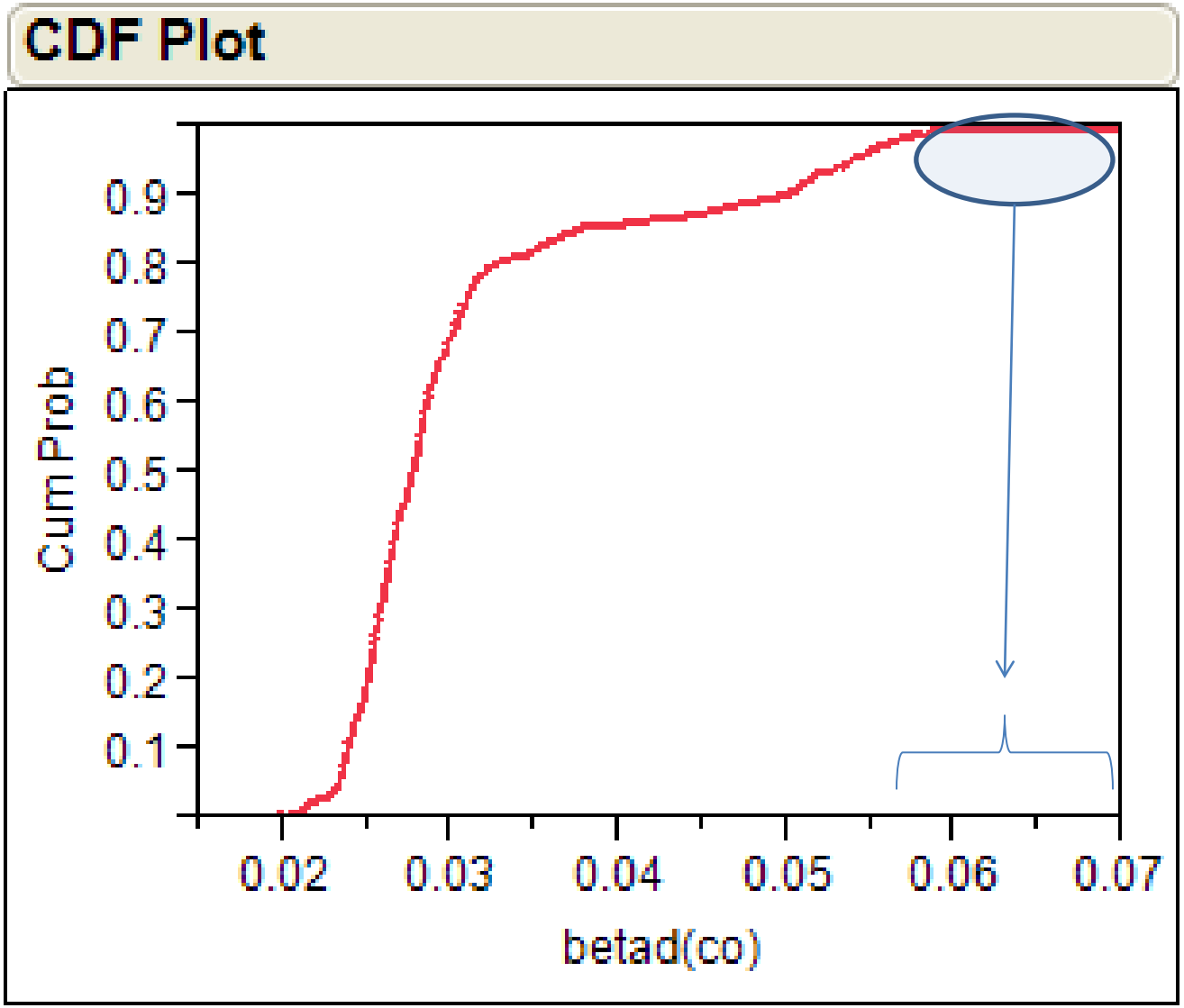
RSquare	0.921567
RSquare Adj	0.92152
Root Mean Square Error	0.005899
Mean of Response	0.053774
Observations (or Sum Wgts)	1689

Prediction Expression

-0.0003633281033 + 1.97651578761069 *S

Effect of S on H_2S production

Uncertainty Analysis of Proximate and Ultimate Analysis



Summary

- Kinetic packages → C3M → CFD models
- C3M serves as virtual kinetic laboratory
- C3M is a kinetic data bank for coal gasification process
- C3M is helpful in performing UQ analysis
- UQ analysis was performed for operating conditions and PA /UA variations

Future Work

- Develop the UQ tool.

- Experimental Kinetic Data:
  - Soot formation reaction
  - Coal and biomass gasification
  - Entrained Flow reactor gasification
  - High pressure, high temperature water gas shift reaction
  - Chemical Looping
  - CO_2 adsorbent

Contact Info For C3M

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Guenther C., VanEssendelft D., Chaudhari K., Nicoletti P., Shahnam M., Li T., Turton R., Weiland N., and Wang P., "Gasification Modeling in the 21st Century," Power Engineering, **116** (6), 2012.

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