Uncertainty Quantification in an IGCC Process

Using Polynomial Chaos Expansions

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The Future of Coal Power Plants

- **Coal provides half of US electricity**
- **'Clean' coal – Integrated gasification combined cycle**
- **Coal → syngas for higher efficiency, CO_2 sequestration**

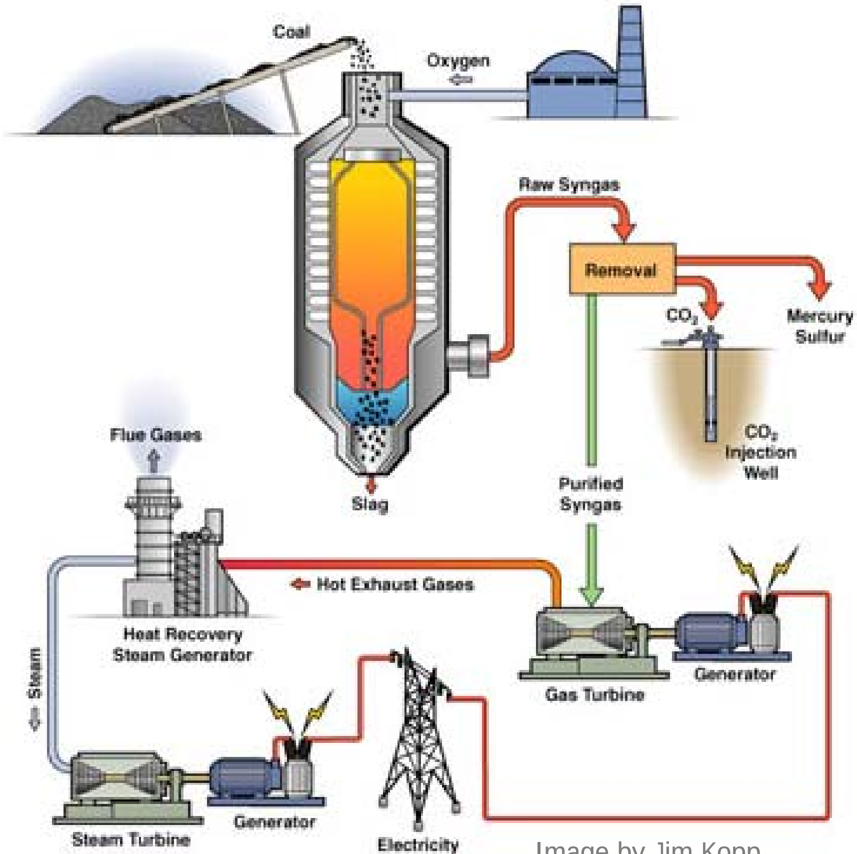


Image by Jim Kopp

Make long term policy & investment decisions

Risk = Uncertainty x consequence

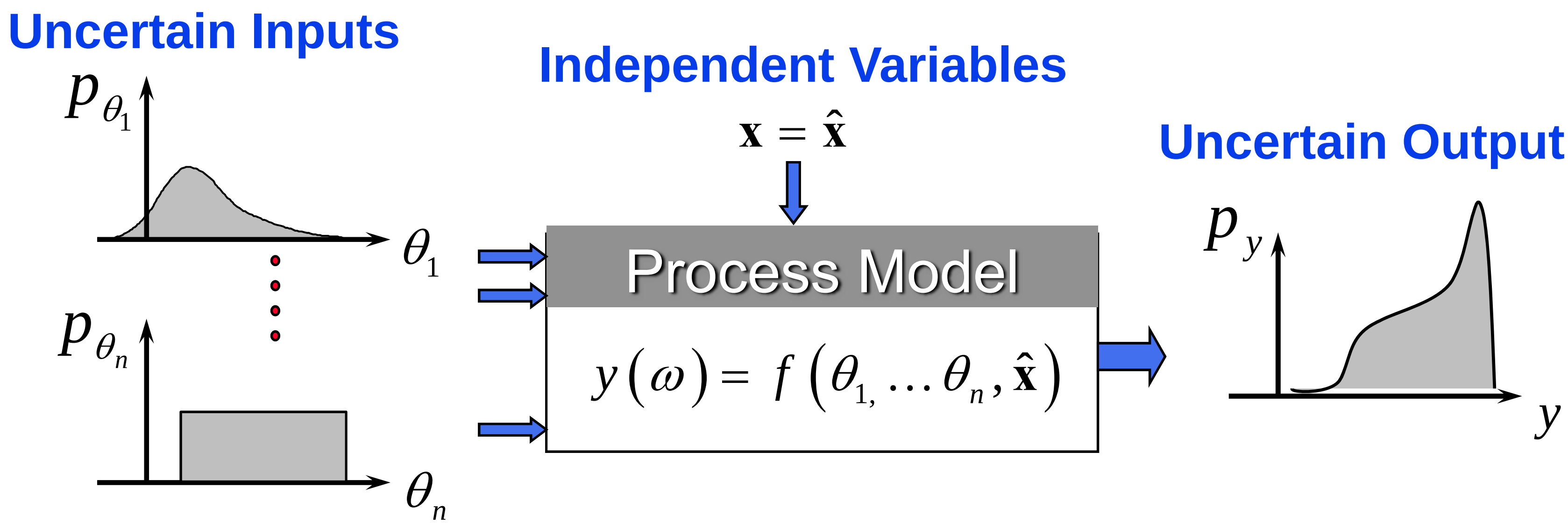
Must quantify uncertainties, especially in complex systems

Outline

- Uncertainty Quantification in Chemical Systems
- Tools for Uncertainty Quantification
  - Polynomial Chaos Expansions
- Illustrative Examples – Batch reactor
- Coal Conversion Study – Apply to process design
- Future Applications

Key Point: The way to get orders of magnitude reduction in solution time is to change the problem representation – treat uncertainty at the beginning, not at the end.

Uncertainty Quantification in Chemical Systems



- Characterize the input uncertainty
- What impact do uncertain inputs have on the outputs?

PDF = probability density function

Not all inputs are Gaussian!

Gaussian inputs $\not\Rightarrow$ Gaussian output

What is the Goal of Uncertainty Quantification?

- **Current Methods – limitations**
  - Perturbation Method – local approximation
  - Moment Methods – linearized systems
  - Monte Carlo – expensive
- **Desired properties of uncertainty methods**
  - Accurate
  - Computationally efficient
  - Decompose output uncertainty ~ Global Sensitivities
  - Apply to nonlinear, black box models
  - Non Gaussian inputs
  - Approximate the full output PDF

Approximation Functions with Expansions

- **Fourier Series approximation of functions**

Basis functions

$$y(x) \approx \hat{y}(x) = a_0 + \sum_{n=1}^{N} a_n \sin(nx) + b_n \cos(nx)$$

Coefficients

- **Replace an unknown complex function w/ combination of simple known functions and unknown coefficients**

Approximating a Random Variable

- **Direct Representation of Random Variables (RV)**

Basis RVs

$$Y(\omega) \approx \hat{Y}(\omega) = \sum_{j=0}^{J} y_j \Psi_j(\xi)$$

Coefficients

Functionals of the Basis RVs

- **How to choose the best Basis Random Variables and functionals?**

Choosing the Basis and Functionals

Recall desired goals:

1. Decompose output uncertainties

   How – ensure inputs are independent

   Representation – Orthogonal Basis Random Variables

2. Efficient computation of PDF/ statistics

   How – Solve multidimensional integrals

ex: $$E\left[Y(\xi_1 \ldots \xi_n)\right] = \int_{\xi_1} \ldots \int_{\xi_n} Y(\xi_1 \ldots \xi_n)\, f_{\xi_1 \ldots \xi_n} d\xi_1 \ldots \xi_n$$

Representation – Orthogonal polynomial functionals

ex: $$E\left[Y(\xi_1 \ldots \xi_n)\right] = \prod_{i=1}^{n} \left[\int_{\xi_i} Y_i(\xi_1)\, f_{\xi_i} d\xi_i \right]$$

Expansion of a Known Random Variable

$$X \sim \text{logn}\left(1, \tfrac{1}{2}\right) \quad \rightarrow \quad X(\omega) \approx \hat{X}(\omega) = \sum_{k=0}^{K} x_k \Psi_k(\xi)$$

Choose a Basis RV

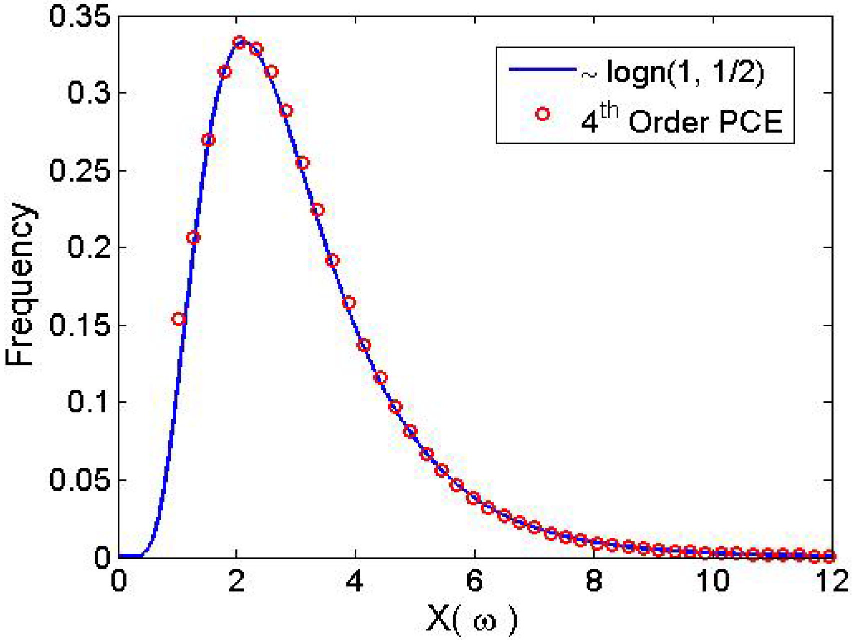
$$\xi \sim N(0,1)$$

Gaussian Basis RV →
Hermite orthogonal polynomials

$$X(\omega) \approx x_0 + x_1\xi + x_2\left(\xi^2 - 1\right) + x_3\left(\xi^3 - 3\xi\right) + x_4\left(\xi^4 - 6\xi^2 + 3\right)$$

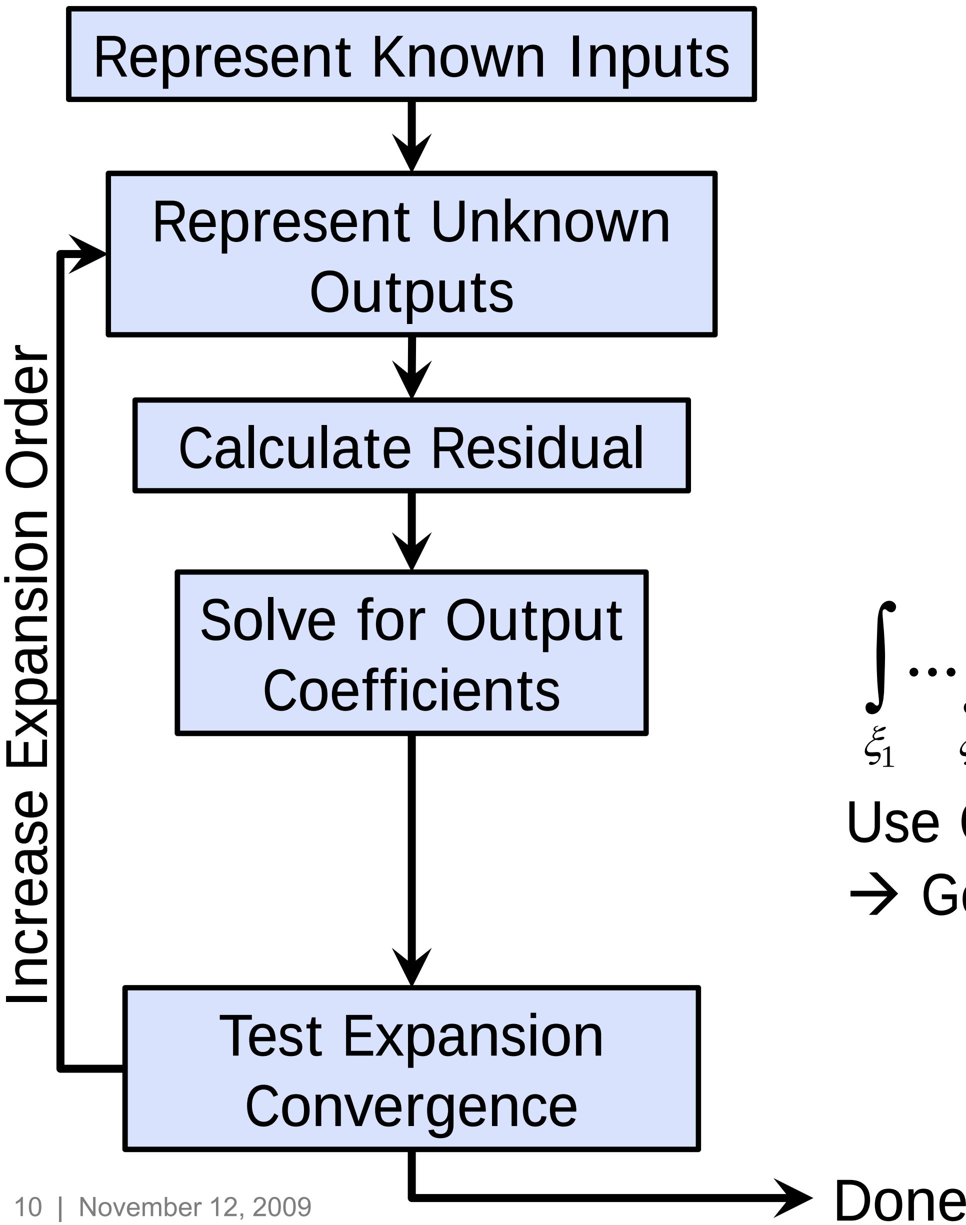
Specify

$$\mathbf{x} = \begin{bmatrix} 3.080 \\ -1.527 \\ 0.392 \\ -0.0597 \\ 0.0117 \end{bmatrix}$$



Algorithm

$$Y(\omega) = \mathcal{A}\left[X(\omega)\right]$$



$$X(\omega) \approx \hat{X}(\omega) = \sum_{k=0}^{K} x_k \Psi_k(\boldsymbol{\xi})$$

SAME Basis RV!

$$Y(\omega) \approx \hat{Y}(\mathbf{y}, \omega) = \sum_{j=0}^{J} y_j \Psi_j(\boldsymbol{\xi})$$

$$R(\mathbf{y}, \boldsymbol{\xi}) = \mathcal{A}\left[\hat{X}(\boldsymbol{\xi})\right] - \hat{Y}(\mathbf{y}, \boldsymbol{\xi})$$

$$\int_{\xi_1} \cdots \int_{\xi_n} \left[R(\mathbf{y}, \boldsymbol{\xi}) w_l(\boldsymbol{\xi})\right] d\xi_1 \ldots d\xi_n = 0 \quad l \in 1 \ldots J$$

Use Galerkin Projection or **Collocation**

→ Get output PDF

Compare to lower order expansion

UQ Example – Batch Reactor

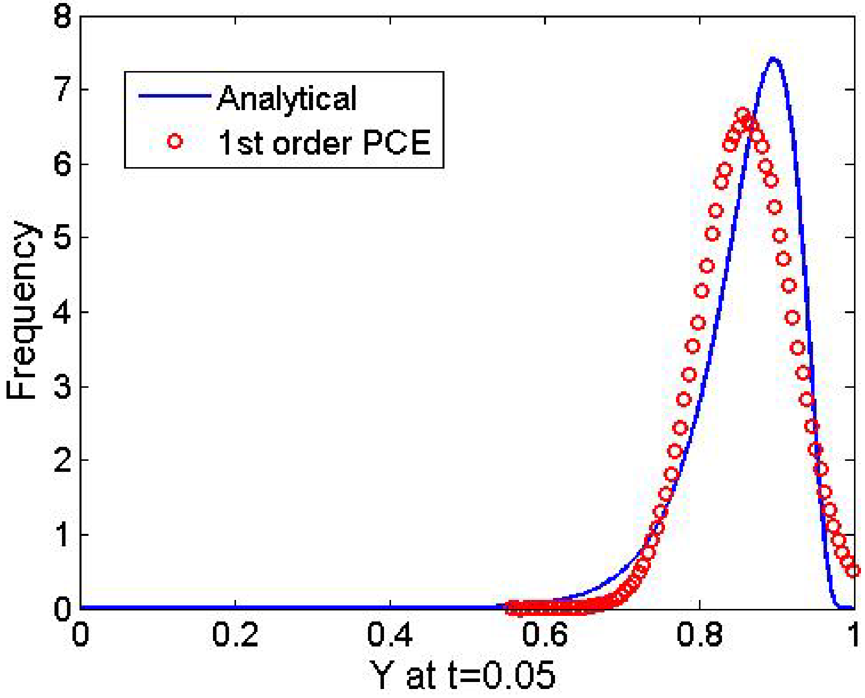
$$\frac{dY}{dt} = -X(\omega)Y \qquad Y(t=0)=1$$

Uncertain kinetic parameter

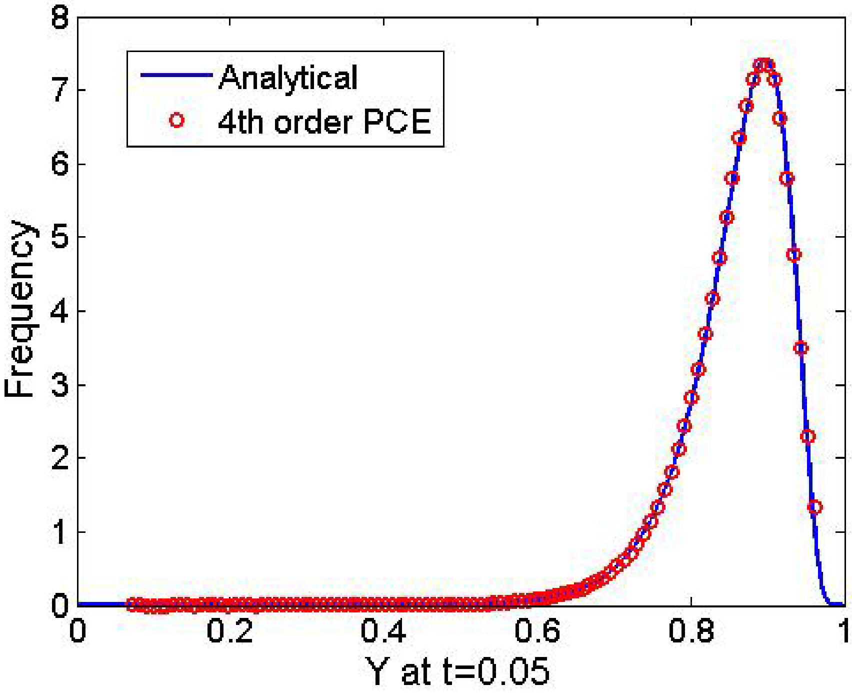
$$X \sim \operatorname{logn}(1, 1/2)$$

$$Y(t,\omega) = \mathcal{A}\left[X(\omega)\right] = \exp\left(-X(\omega)t\right) \qquad \text{fix } t = 1/20$$

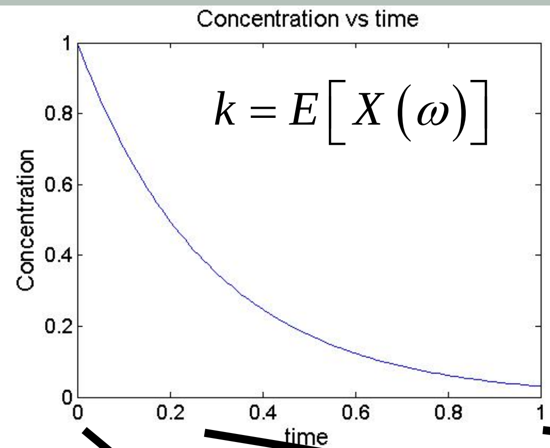
2 model evaluations



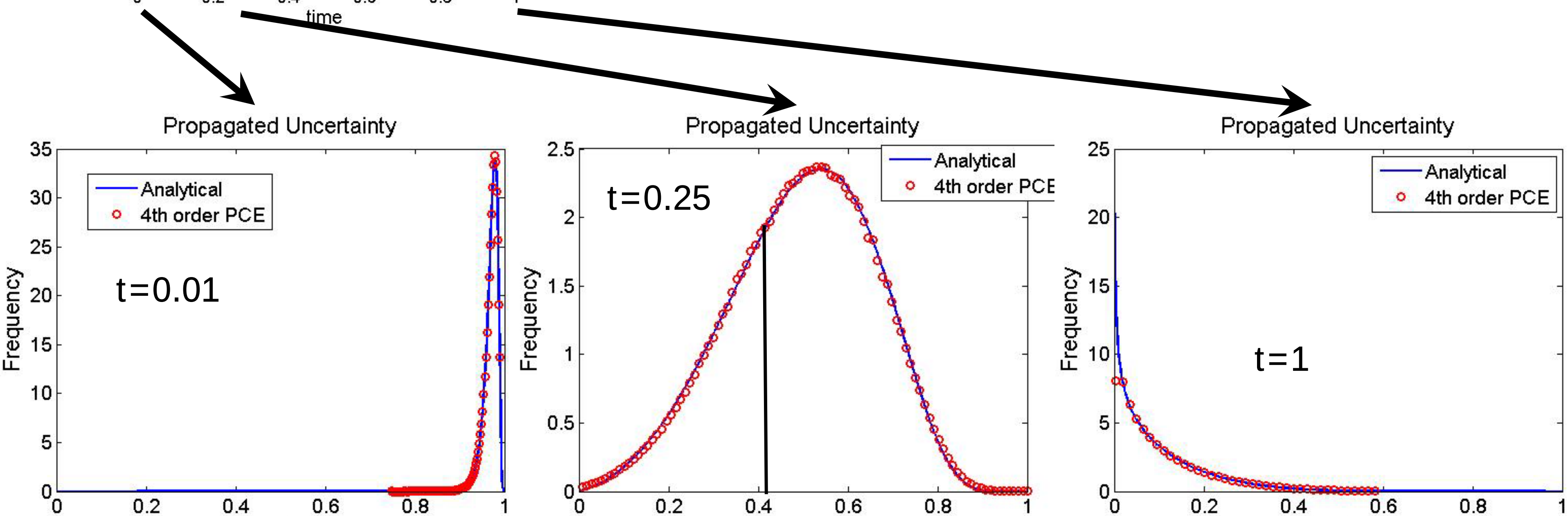
5 model evaluations



Efficient Quantification of Uncertainty



- Uncertainty quantification adds a crucial dimension to the output
- Polynomial Chaos Expansions → 'Probability response surface'



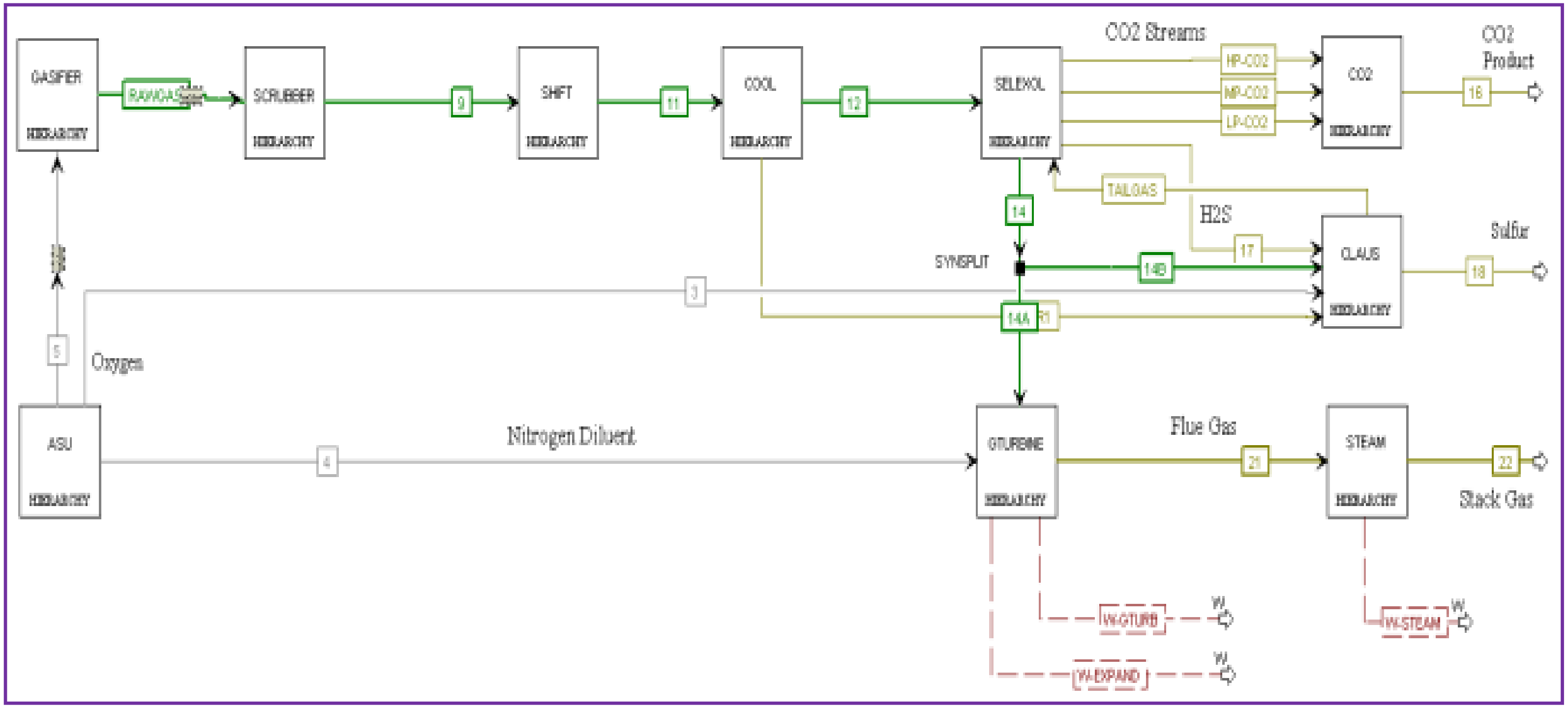
Mean parameter value cannot accurately predict the outcomes

Polynomial Chaos Expansions – Summary

- Recap
  - Widely applicable tool for uncertainty quantification
  - Orders of magnitude faster than Monte Carlo
  - Easily identify significant input uncertainties
- Assumptions/ Issues
  - Assume the approximate functional form of the output density
  - Requires well behaved models
  - Uses concepts from numerical quadrature
  - Convergence rate

Evaluating competing clean coal technologies

- Integrated gasification combined cycle modeled in ASPEN Plus
- Quantify uncertainties
  - Identify parameters that require more study
  - Assess impact on design



Characterize Uncertain Input Parameters

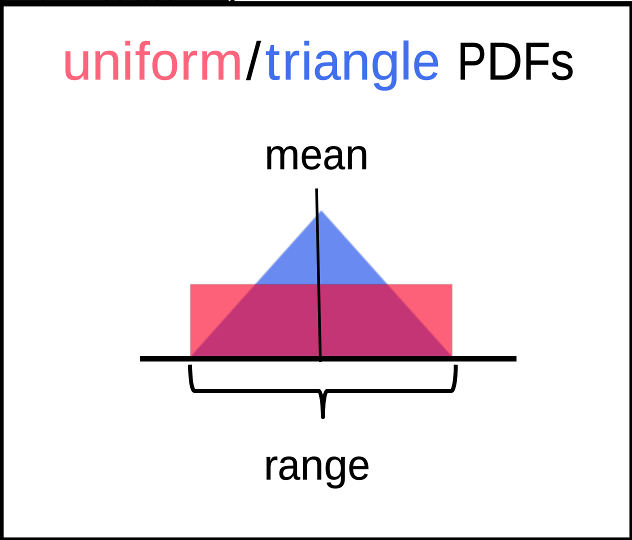
#	Unit	Parameter	Distribution	Mean	Var	Range	σ/μ
1	Feedstock	[redacted]					
2		[redacted]					
3		[redacted]					
4		[redacted]					
5		[redacted]					
6		[redacted]					
7		[redacted]					
8	Gasification	[redacted]					
9		[redacted]					
10		[redacted]					
11	Gas turbine	[redacted]					
12		[redacted]					
13		[redacted]					
14		[redacted]					
15	Steam turbine	[redacted]					
16		[redacted]					
17		[redacted]					
18		[redacted]					
19		[redacted]					
20	Air Separation	[redacted]					
21		[redacted]					
22		[redacted]					
23	CO_2 Compression	[redacted]					
24		[redacted]					
25		[redacted]					
26		[redacted]					

21 Parameters

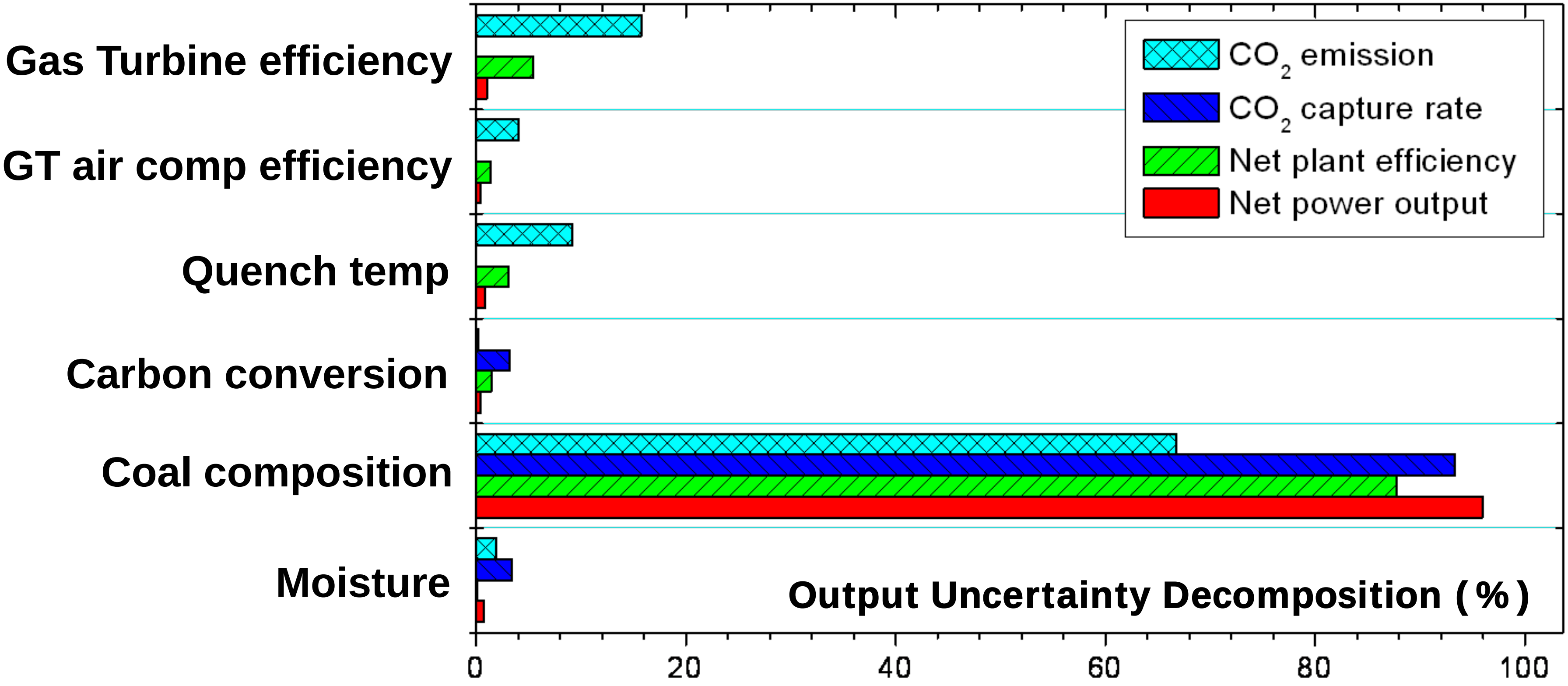
Significant uncertainties

Coal Composition Parameters

Non Gaussian Distributions

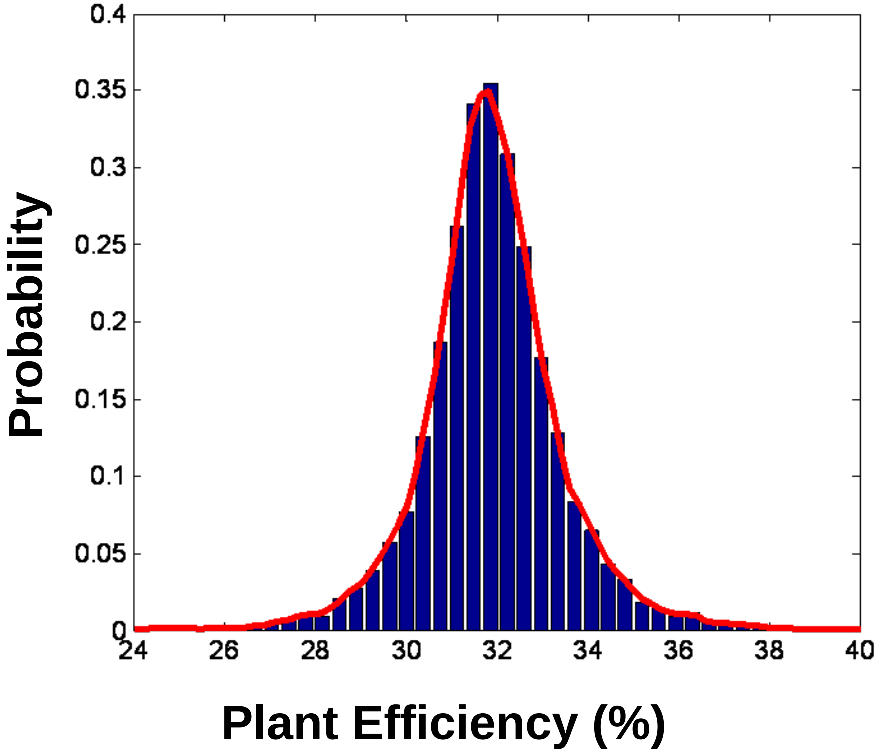


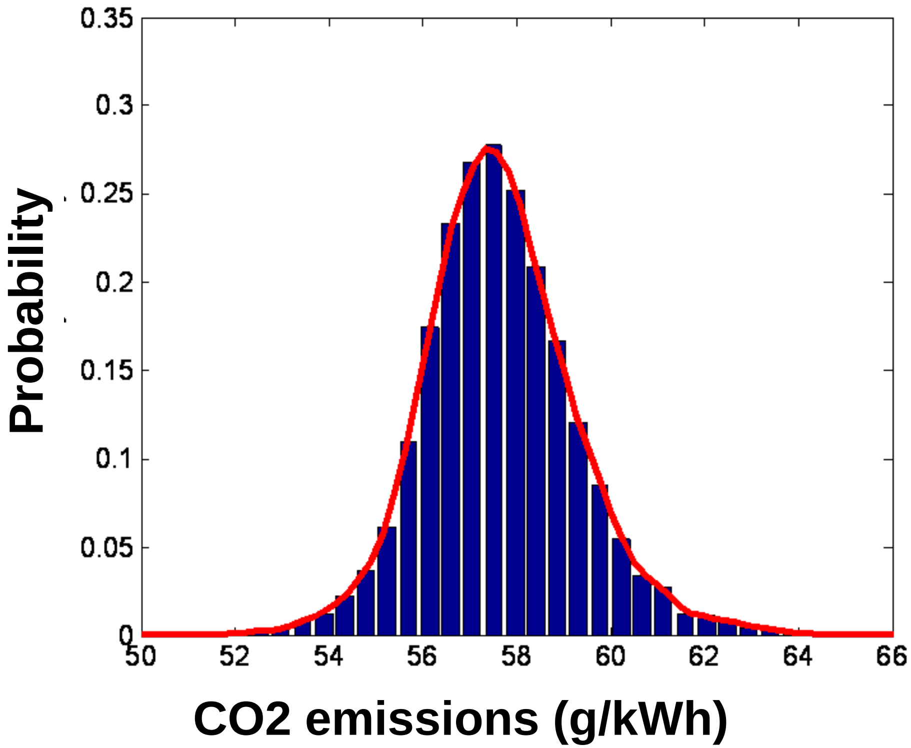
Identify Critical Process Parameters



- **Only six parameters have significant impact**
- **Feedstock is the major factor**

Plant Performance Metrics





- **Nearly Gaussian, with significant uncertainties**

Results

- **Model is roughly linear in the significant parameter (Coal composition)**
- **Significant uncertainty in the outputs warrants further study of coal composition, matching of process conditions to coal source.**

- **Efficiency – 48 model evaluations, ~O(2) fewer than Monte Carlo**

- **Future work – integrate rigorous uncertainty quantification with process design**

Application Areas

- Current uses
  - Computational Fluid Dynamics
  - Combustion
  - Subsurface flow
- Potential Chemical Engineering areas
  - Process Design
  - Experimental Design
  - Economic Analysis
  - Model Predictive Control
  - Anything related to Stochastic Optimization

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