

Direct Treatment of Uncertainty in Complex Models and Decision Making

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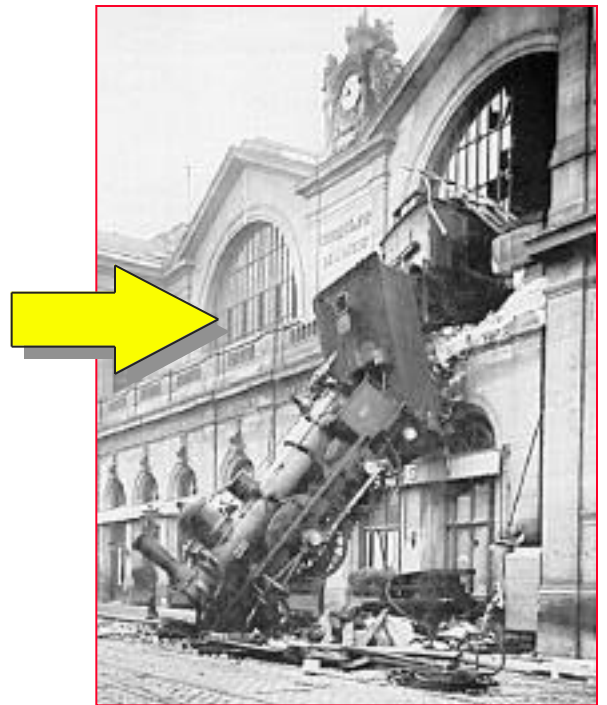
MIT
Chemical Engineering
Course 10

Cheng Wang

RD
REACTION DESIGN

Key Message – Outcomes are Important

*“ ... While there are always lots of uncertainties, the key challenge in engineering is to find those problem components that contribute most to uncertainties in **outcomes...**”*



Decision Making Under Uncertainty

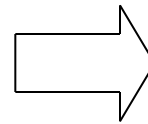
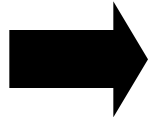


Other Dimensions of Decision Making

- Model discrimination – *Model A vs. B*
- Hypothesis testing – *Which parameter is “ best”*
- Model verification – *What are the “ stopping” rules*
- Experimental design – *Where to measure*
- Optimization objectives – *Fail-Safe vs. Safe-Fail*
- Resource allocation – *Where to spend the money*
- *etc.*

Example: Where to Allocate Resources

Physical, chemical
and decision
process models



Which
parameters
control
outcomes?

$P(k_1)$ Uncertain Inputs



k_1



$P(k_m)$



k_m



Process Model

$$y = f(k_1, k_2, \dots, k_m)$$



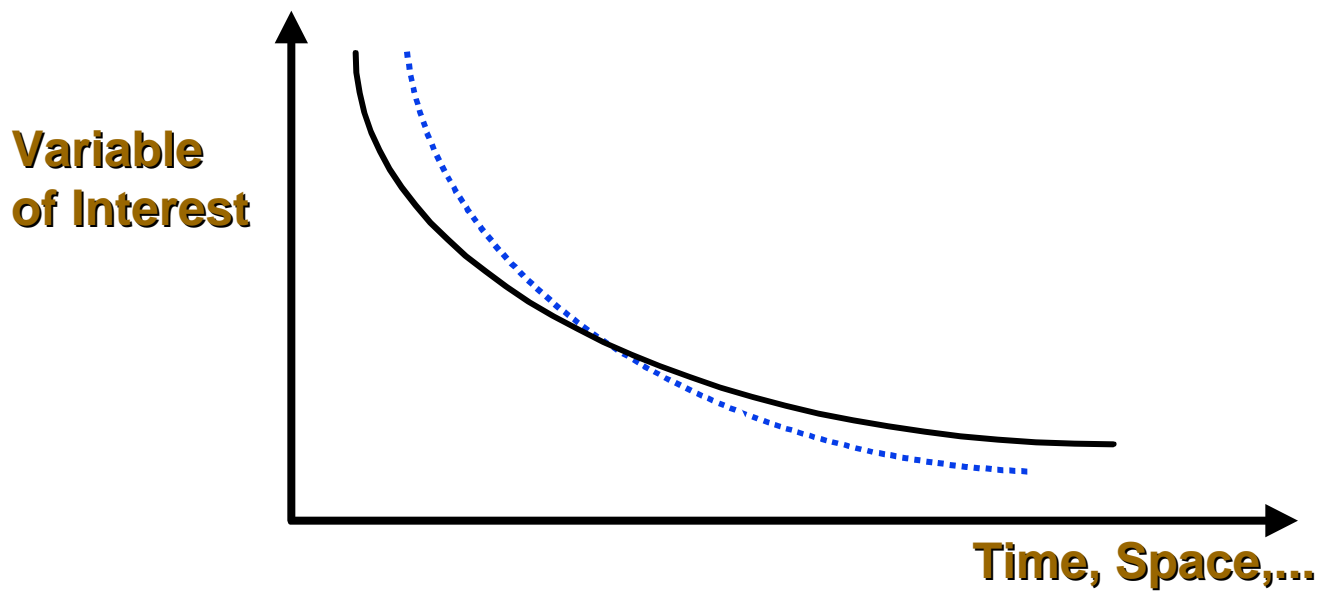
Uncertain Output

$P(y)$



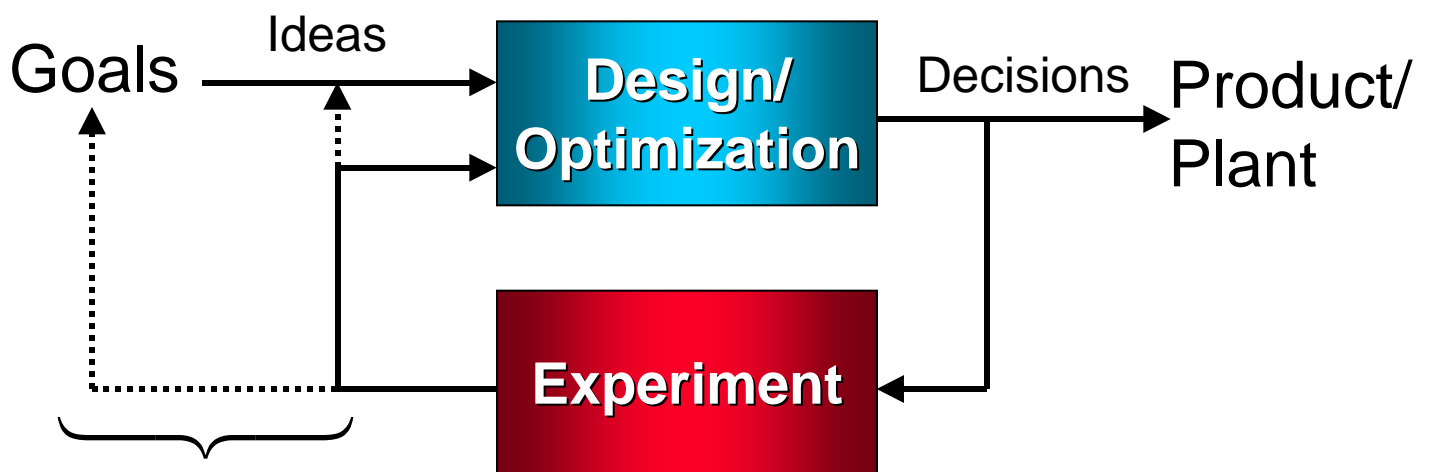
$y(k)$

Example: Model Verification / Discrimination



➔ Meaningful comparisons requires estimates of uncertainties in prediction and observations

Example: Model Based Experimental Design



Bayesian Experimental Design

- Use of prior information
- Model updating

Where should experimental resources be spent ?

Example: Risk Issues and Management

- Sales and market forecasts
- Regulatory environment
- Raw material price/availability
- Management/organizational changes
- Stakeholder patience
- Technical assumptions
- Available resource base
- Operational upsets

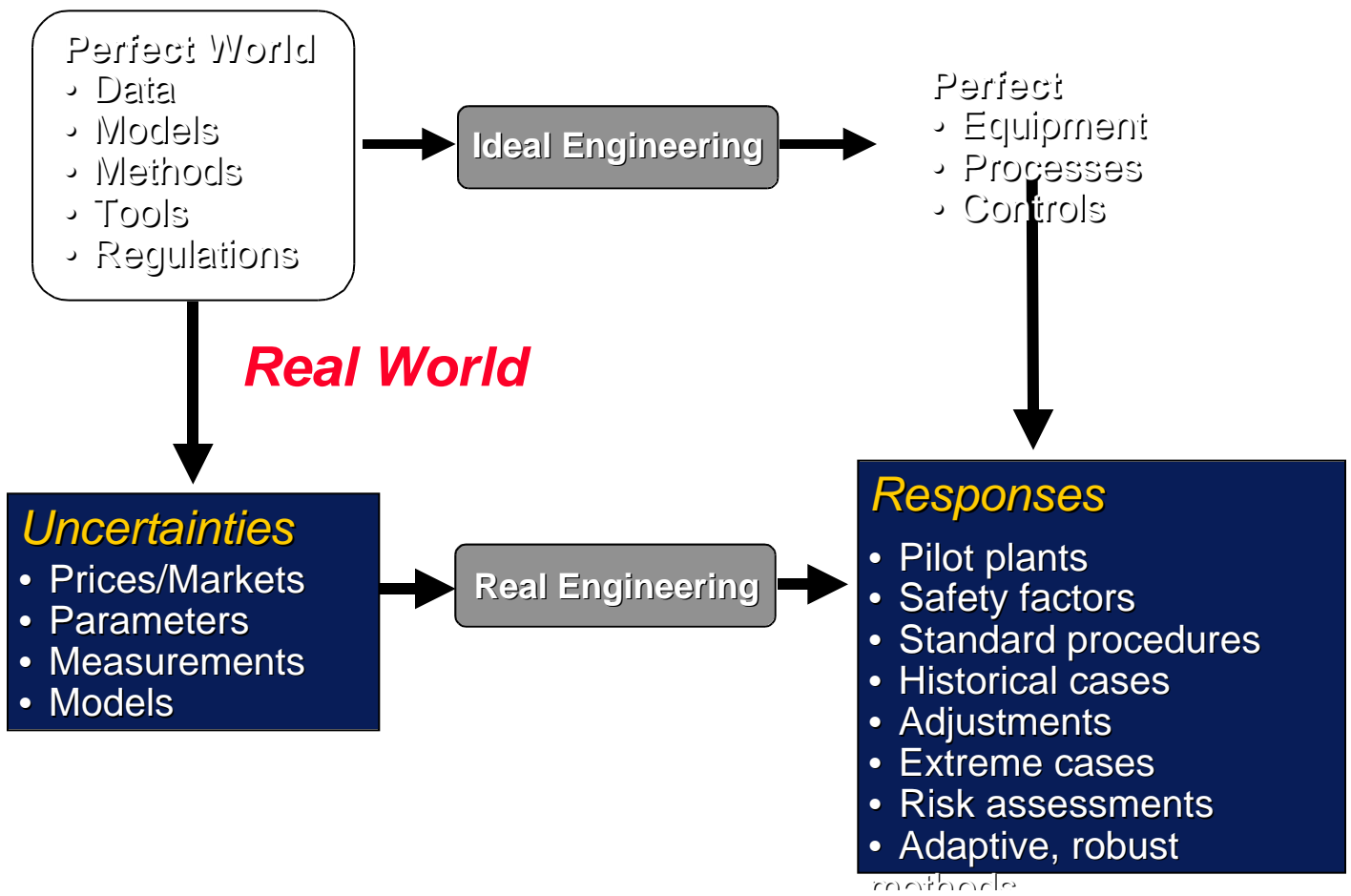
Outline of Presentation

- The nature of uncertainty in engineering
- Representation of uncertainty
- Direct treatment of parametric uncertainty
- Illustrative examples
- Recommendations and conclusions



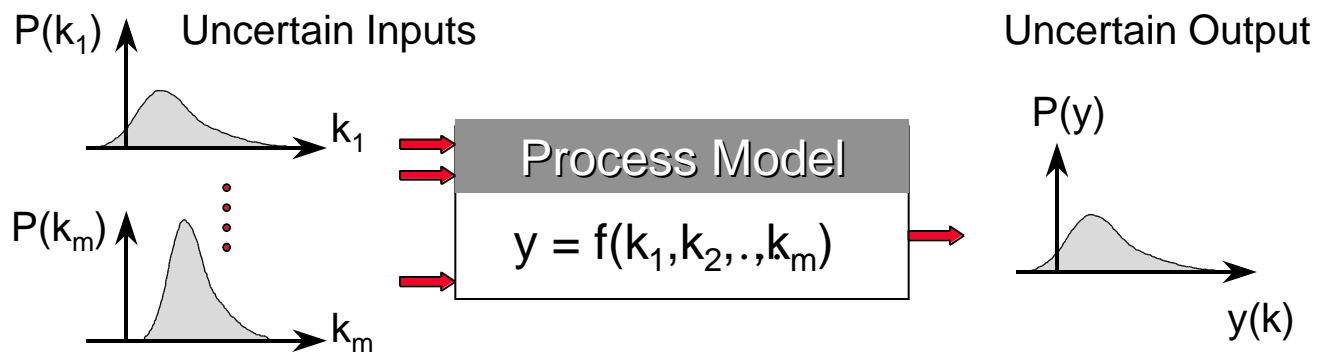
“ .How well do we need to know the answer in order to make a decision..”

Ideal” versus “ Real” Engineering

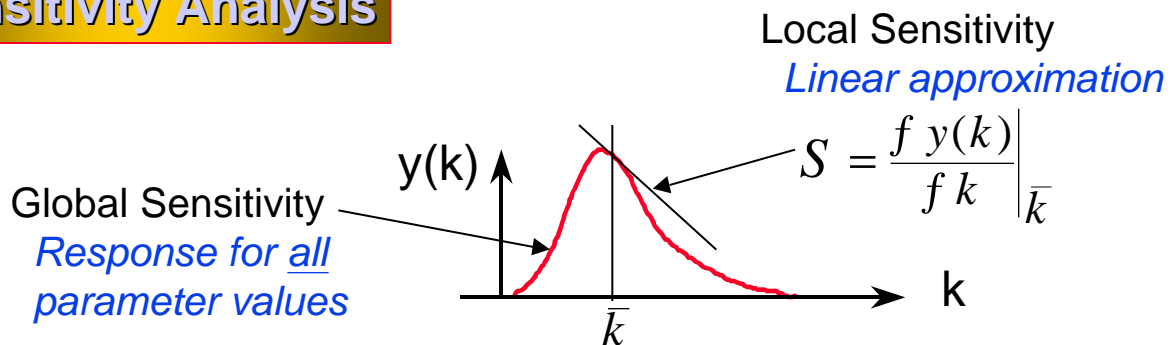


Sensitivity / Uncertainty Analysis

Uncertainty Analysis



Sensitivity Analysis



Simple Problem: Kinetics of $\text{SiH}_4 \rightarrow (\text{Si}) + 2\text{H}_2$

Model

$$\frac{dy(t)}{dt} = -k y(t) \quad ; \quad y(0) = y_0, \quad y(t) = [\text{SiH}_4(t)]$$

Solution

$$y(t) = y_0 e^{-k t}$$

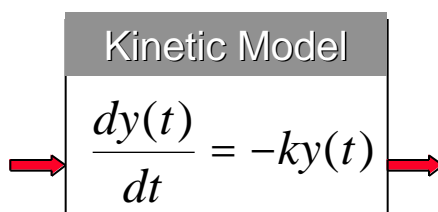
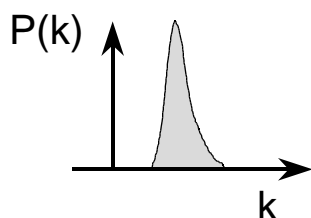
Sensitivity to parameter variations

$$S = \frac{f y(t)}{f k} \Big|_{\bar{k}} = -t y_0 e^{-\bar{k} t}$$

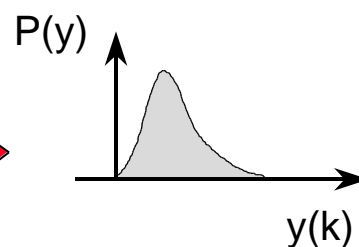
➡ But, what if k is uncertain?

Solution in Presence of Uncertainty

Uncertain Rate Constant



Uncertain Output



Normal distribution
for rate constant (k)

But

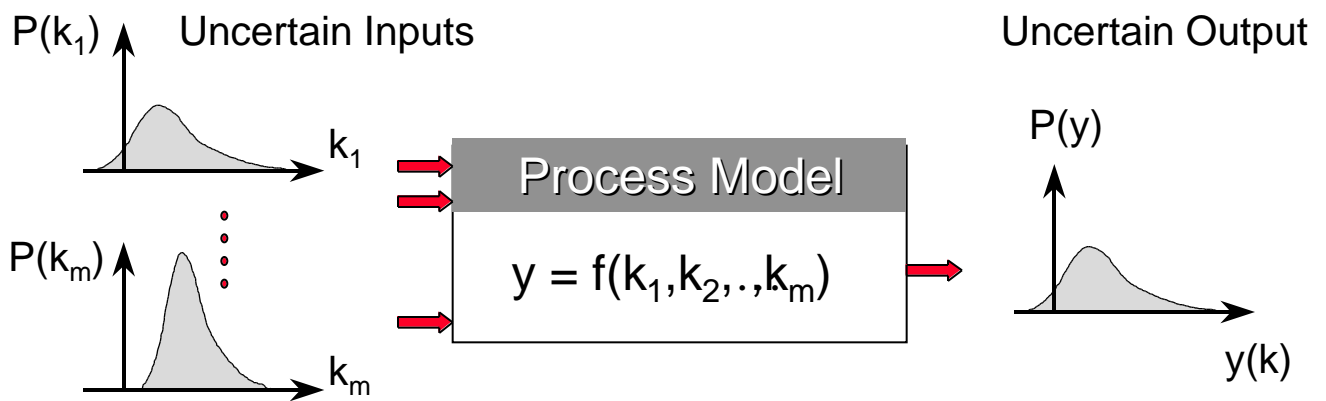


Lognormal distribution
for solution at each time

$$P(k) = \frac{1}{k_1 \sqrt{2\pi}} e^{-\frac{1}{2} \frac{(k-k_0)^2}{k_1^2}}$$

$$P(y) = \frac{1}{k_1 t y \sqrt{2\pi}} e^{-\frac{1}{2} \frac{(\ln(y/y_0) + t k_0)^2}{t k_1^2}}$$

How do Uncertain Inputs effect the Outputs?



Measures of Uncertainty (Expected value, variance, pdf, etc.)

e.g. $E[y(k)] = \int y(k) P[y(k)] dy(k)$

$\dots \int \dots \int y(k) P[k] dk_1 \dots dk_m$

↑ Multi-dimensional integrals are computationally very expensive

Solution in Presence of Uncertainty

Deterministic Solution

$$y(t) = y_0 e^{-k t}$$

Density Function and Expected Value for $k \sim N[k_0, k_1]$

$$P(y) = \frac{1}{k_1 t y \sqrt{2\pi}} e^{-\frac{1}{2} \frac{\ln(y/y_0) + t k_0}{t k_1}^2}$$

$$E[y(t)] = \int_{-\infty}^{+\infty} y(t) P(k) dk = y_0 e^{-\frac{t^2 k_1^2}{2} - t k_0}$$

Solution in Presence of Uncertainty

Key points from simple example

1. Even for simple systems with normal distributions as inputs the outputs are typically not normal.
2. Simple measures, such as means do not reflect the complexity of outcomes.
3. Beware of the use of normal distributions as a way to characterize uncertainty (e.g. exponential increase in $E[y(t)]$ as $t \geq 2k_0/k_1^2$ because of finite probability of $k < 0$)

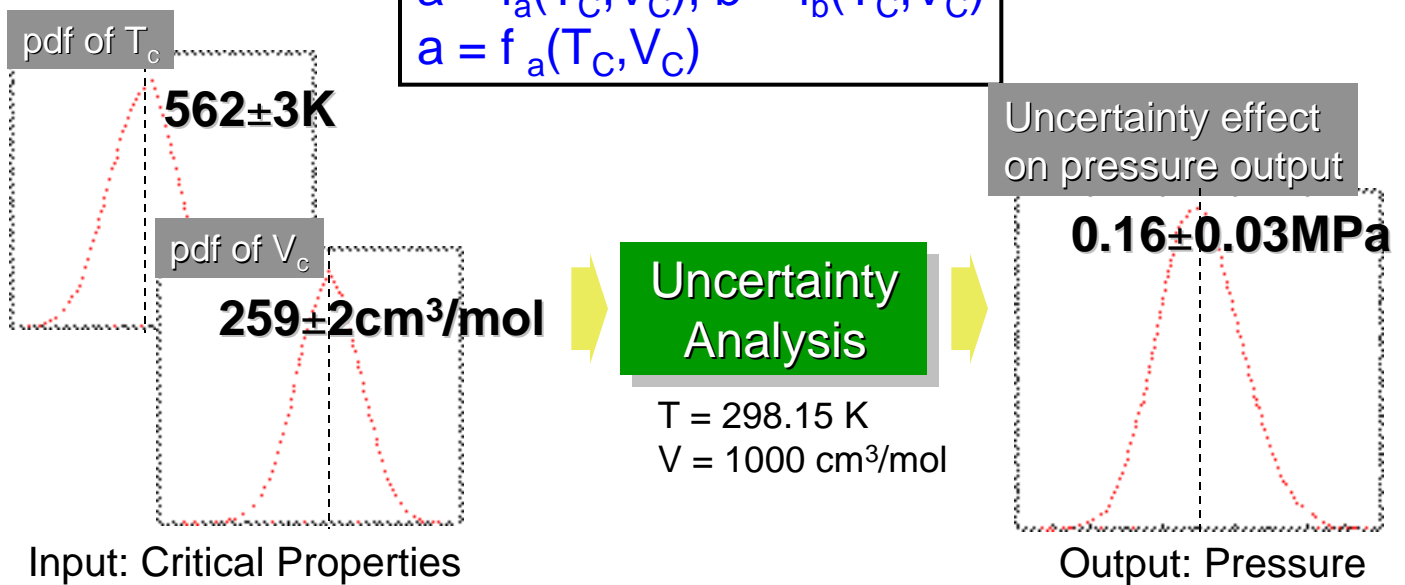
$$E[y(t)] = \int_{-\infty}^{+\infty} y(t) P(k) dk = y_0 e^{\frac{t^2 k_1^2}{2} - tk_0}$$

What if the uncertainties are small?

$$f(T_C, V_C, T_B) = \frac{RT}{V_m - b} - \frac{a\alpha}{V_m(V_m + b) + b(V_m - b)} = P$$

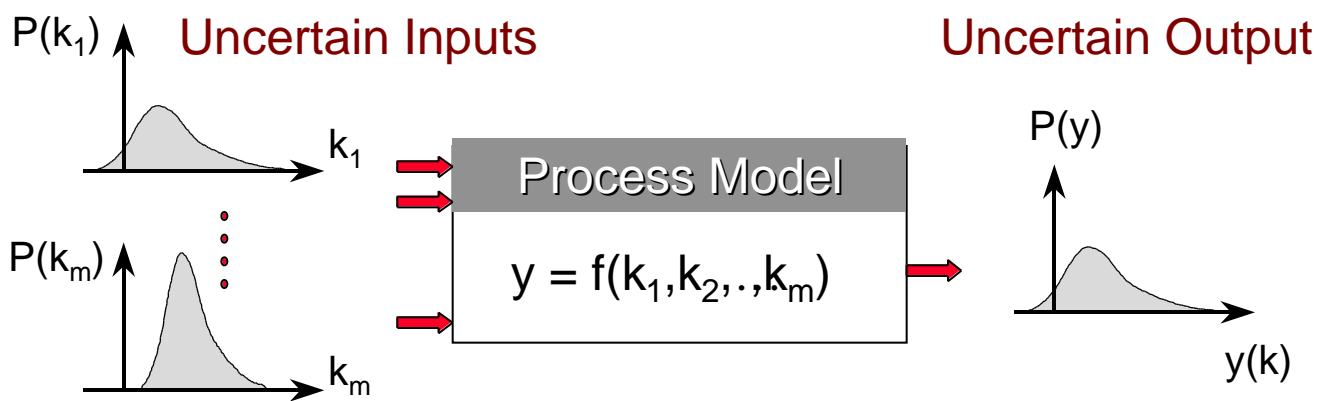
$$a = f_a(T_C, V_C), \quad b = f_b(T_C, V_C)$$

$$a = f_a(T_C, V_C)$$



➡ Model outcome can be very sensitive to input uncertainty

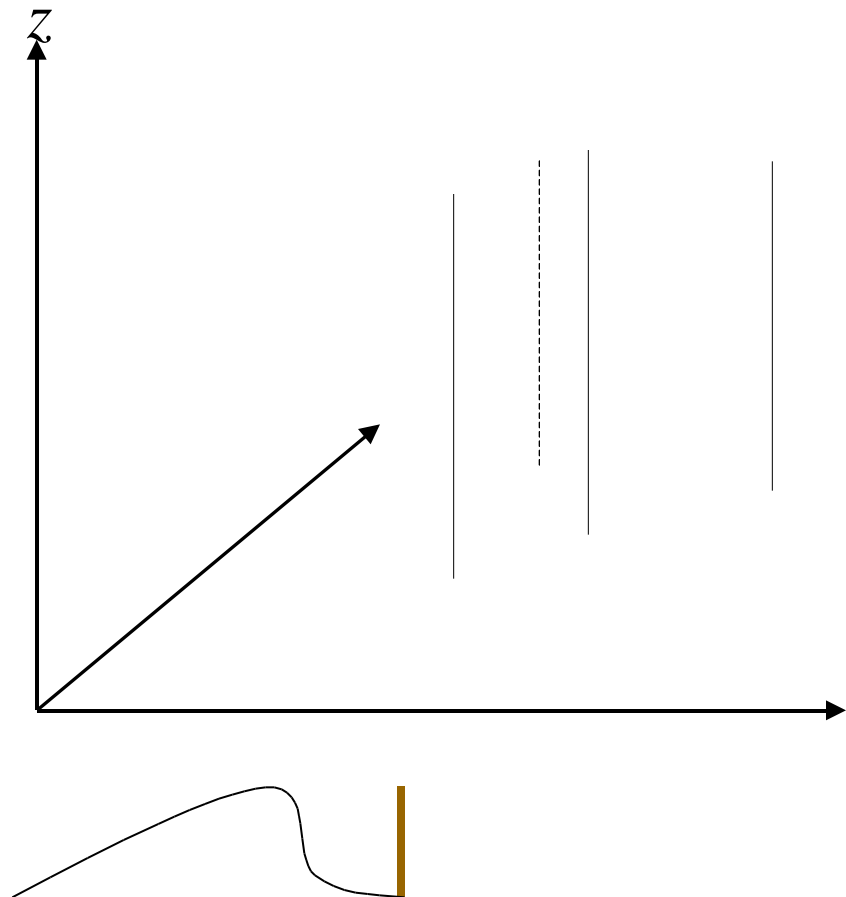
Uncertainty Analysis Problem



- Perturbation
- Monte-Carlo
- Pattern searches
- Number Theoretic Methods
- Semigroup Methods
- etc.

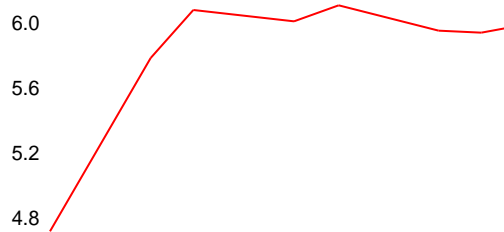
All too expensive
for “ real”
problems

Monte Carlo Sampling Method



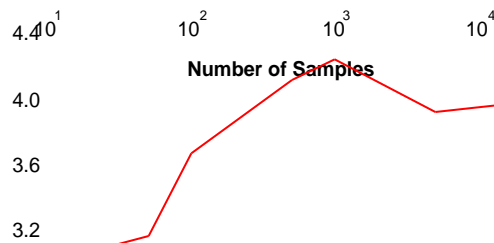
Convergence of Monte-Carlo Methods

Mean



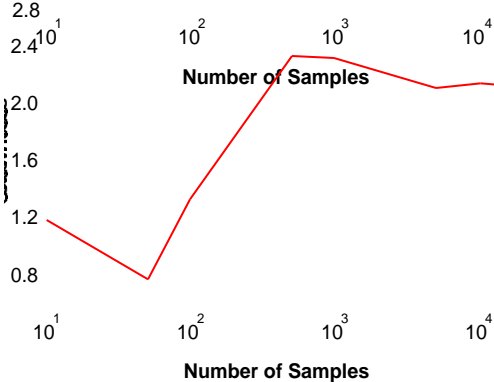
$$E[y(k)] = \int_{-\infty}^{+\infty} y(k)P(k)dk = \frac{1}{n_s} \sum_{i=1}^{n_s} y(k_i)$$

Standard Deviation



$$S_k^2 = \int_{-\infty}^{+\infty} [y(k) - E[y(k)]]^2 P(k)dk = \frac{1}{n_s} \sum_{i=1}^{n_s} [y(k_i) - E[y(k)]]^2 P(k)dk$$

Skewness



$$S_k^3 = \int_{-\infty}^{+\infty} [y(k) - E[y(k)]]^3 P(k)dk = \frac{1}{n_s} \sum_{i=1}^{n_s} [y(k_i) - E[y(k)]]^3 P(k)dk$$

Attributes of an Uncertainty Analysis System

- Compatible with existing modeling systems
- At least four orders of magnitude faster than Monte Carlo
- An ability to get the probability density function of outputs
- Be able to identify the key contributions to uncertainties in outcomes



“ ...By rethinking conventional methods and directly embedding uncertainty into the modeling process itself...”

Incorporating Uncertainty at the Beginning

Fourier Series Representation of $f(x)$

$$f(x) = a_0 + \sum_{i=1}^{\infty} a_i \sin(\omega_i x) + b_i \cos(\omega_i x)$$



What happens if x is a random variable?

Polynomial Chaos Representation of $f(\cdot)$ (Wiener, 1947)

$$f(\omega) = \sum_{i=1}^{\infty} a_i H_i[\xi_1(\omega), \dots, \xi_m(\omega)]$$

Coefficients of expansion \nearrow

Functional (e.g. Hermite Polynomial) \uparrow

Known probability distributions (e.g. unit Normal $N[0,1]$) \longleftarrow

Example of Polynomial Chaos Expansion

Known PDF of x

$$f_x(x) = \frac{1}{0.5x\sqrt{2\pi}} \exp -\frac{(\ln(x) - 1.0)^2}{2 \cdot 0.5^2} ; \quad 0 < x < \infty$$

Moments of $f_x(x)$

$$\mu = 3.08022 \quad (\text{mean})$$

$$\sigma^2 = 2.69476 \quad (\text{variance})$$

$$\gamma_1 = 1.75018 \quad (\text{skewness})$$

$$\gamma_2 = 8.89841 \quad (\text{kurtosis})$$

Expansion of x

$$x = x_0 + x_1\xi + x_2(\xi^2 - 1) + x_3(\xi^3 - \xi)$$

$$\mu_x = x_0$$

$$\sigma_x^2 = x_1^2 + 2x_2^2 + 6x_3^2$$

$$\gamma_{1x} = \frac{6x_1^2x_2 + 8x_2^3 + 36x_1x_2x_3 + 108x_2x_3^2}{\sigma_x^3}$$

$$\gamma_{2x} = \frac{1}{\sigma_x^4} (60x_2^4 + 2232x_2^2x_3^2 + 576x_1x_2^2x_3 + 60x_1^2x_2^2 + 3348x_3^4 + 1296x_1x_3^3 + 252x_1^2x_3^2 + 24x_1^3x_3 + 3x_1^4)$$

Characteristic Information Obtained from Expansion of x



Polynomial Chaos Expansion

Formulate Least-square
Criteria to Calculate
the Expansion Coefficients

Solve NLP to
Obtain Expansion
Coefficients

Polynomial Chaos
Expansion of x

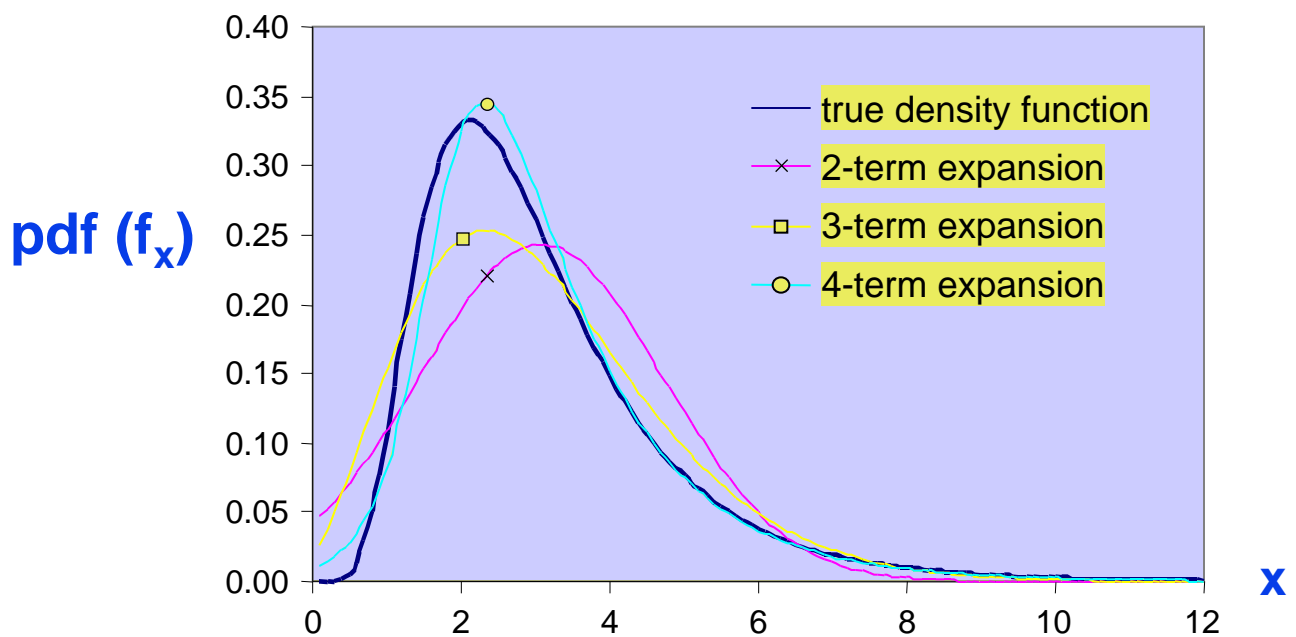
$$\begin{aligned} \min \quad & \sum_{i=1}^2 f_i^2 \\ \text{s.t.} \quad & \mu_x - \mu = 0 \\ & \sigma_x^2 - \sigma^2 = f_1 \\ & \gamma_{1x} - \gamma_1 = f_2 \\ & \gamma_{2x} - \gamma_2 = f_3 \end{aligned}$$

$$\begin{aligned} x_0 &= 3.08, x_1 = 1.54 \\ x_2 &= 0.36, x_3 = 0.09 \end{aligned}$$

$$x = 3.08 + 1.54\xi + 0.36(\xi^2 - 1) + 0.09(\xi^3 - \xi)$$

Polynomial Chaos Expansion

$$f_x(x) = \frac{1}{0.5x\sqrt{2\pi}} \exp -\frac{(\ln(x) - 1.0)^2}{2 \cdot 0.5^2} ; 0 < x < \infty$$



Curse of Dimensionality

Measures of Uncertainty (expected value, variance, etc.)

Definition

$$E\{y(\underline{\theta})\} = \int_{-\infty}^{\infty} y(\underline{\theta}) f_{y(\underline{\theta})}(y(\underline{\theta})) dy(\underline{\theta})$$

$f_{y(\underline{\theta})}(y(\underline{\theta}))$ unknown

Statistically equivalent integral definition

$$E\{y(\underline{\theta})\} = \int \dots \int y(\underline{\theta}) f_{\underline{\theta}}(\underline{\theta}) d\theta_1 \dots d\theta_n$$

Multi-dimensional integrals are computationally very expensive

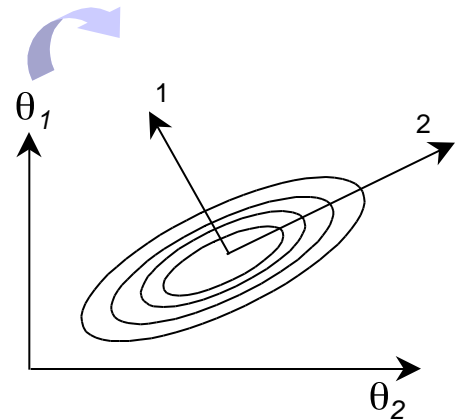
Projection into 1-D by orthogonal polynomials

$$\theta_i = \sum_j a_{ij} H_j(\underline{\xi}(\omega))$$

Polynomial chaos expansion

New definition (one-dimensional integrals)

$$E\{y(\underline{\theta})\} = \int \dots \int c_j y_j(\xi_1) f_{\xi_1}(\xi_1) d\xi_1 \dots y_j(\xi_n) f_{\xi_n}(\xi_n) d\xi_n$$



Choosing Polynomial Chaos Expansions

Requirements for $H_j(\underline{\xi}(\omega))$ and $\underline{\xi}(\omega)$

Simplify the calculation

- Pick (\cdot) as a set of independent random variables
- Choose $H_j(\cdot)$ weighting function similar to pdf of (\cdot)
- Require $H_j(\cdot)$ to be orthogonal
- Choose (\cdot) which simplifies the calculation of moments

Ensure the convergence

- Convergence everywhere, almost everywhere
- Convergence in mean-square sense
- Convergence in probability
- Convergence in distribution

Orthogonal Polynomials

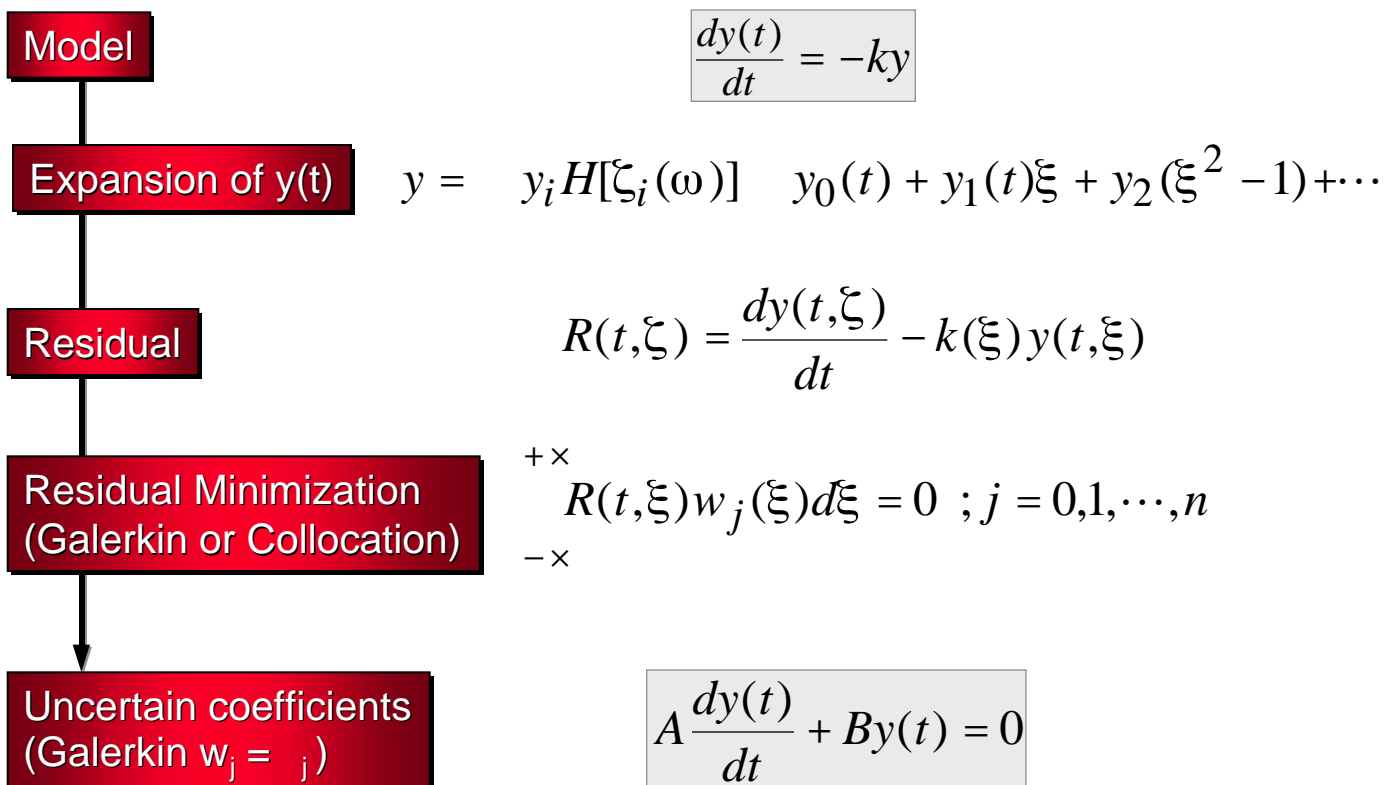
Special Orthogonal Polynomials

<i>Key Probability Density Function</i>	<i>Polynomial for Orthogonal Expansion</i>	<i>Support Range</i>
Gaussian distribution	Hermite polynomials	$(-\infty, +\infty)$
gamma distribution	Laguerre polynomials	$(0, +\infty)$
Beta or uniform distribution	Jacobi or Legendre polynomial	bounded such as $(0, 1)$

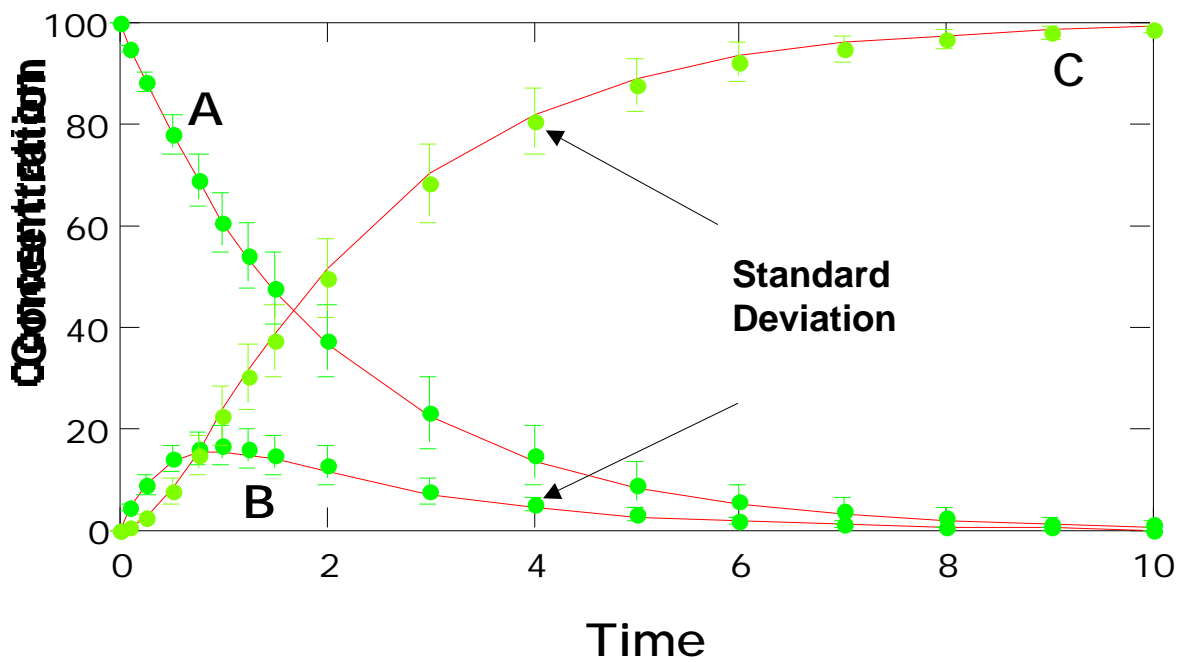
General Problem-Specific Orthogonal polynomials

$$\begin{aligned}g_{-1}(x) &= 0, \\g_0(x) &= 1, \\g_{k+1}(x) &= (x - \alpha_k)g_k(x) - \beta_k g_{k-1}(x), \\k &= 0, 1, \dots, n\end{aligned}$$

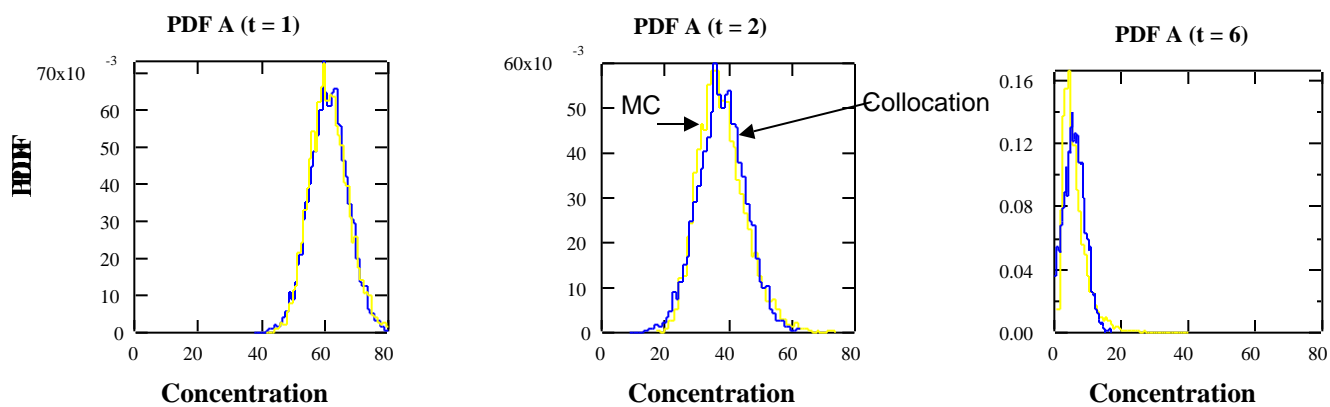
Example of Uncertainty Analysis



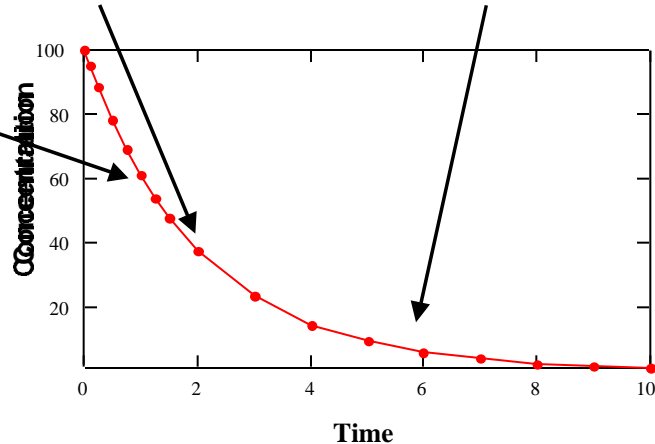
Simple Reaction Sequence A B C



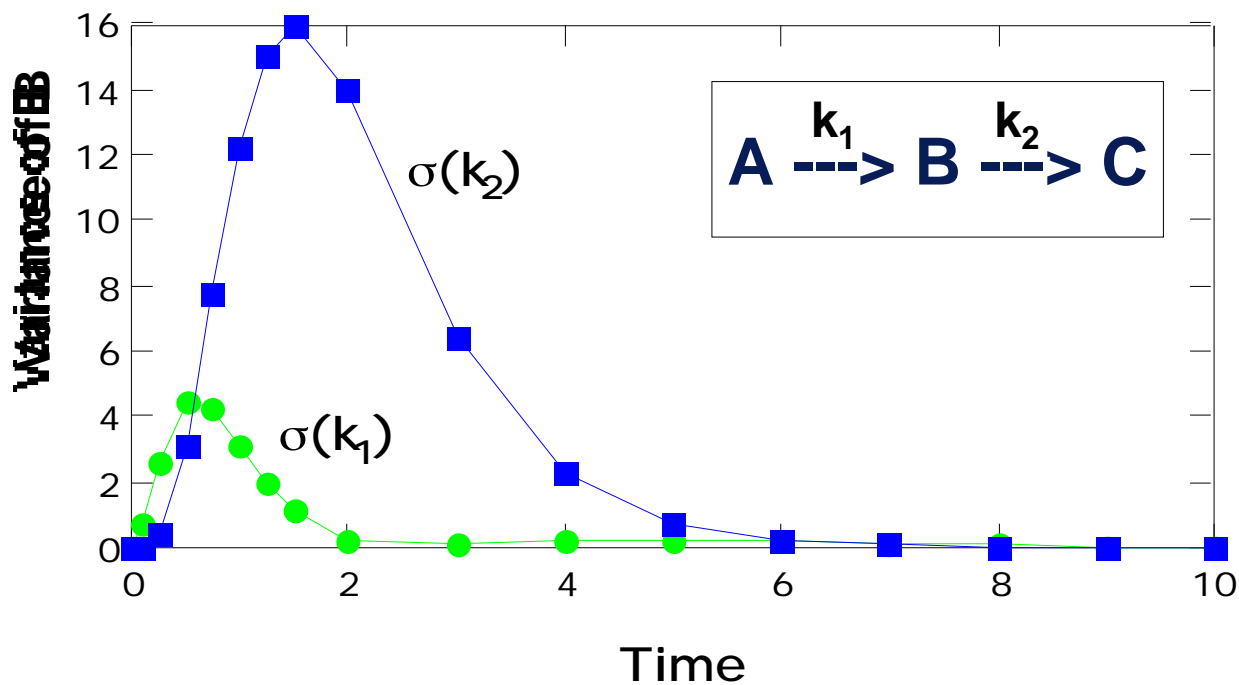
Evolution of Probability Density Functions



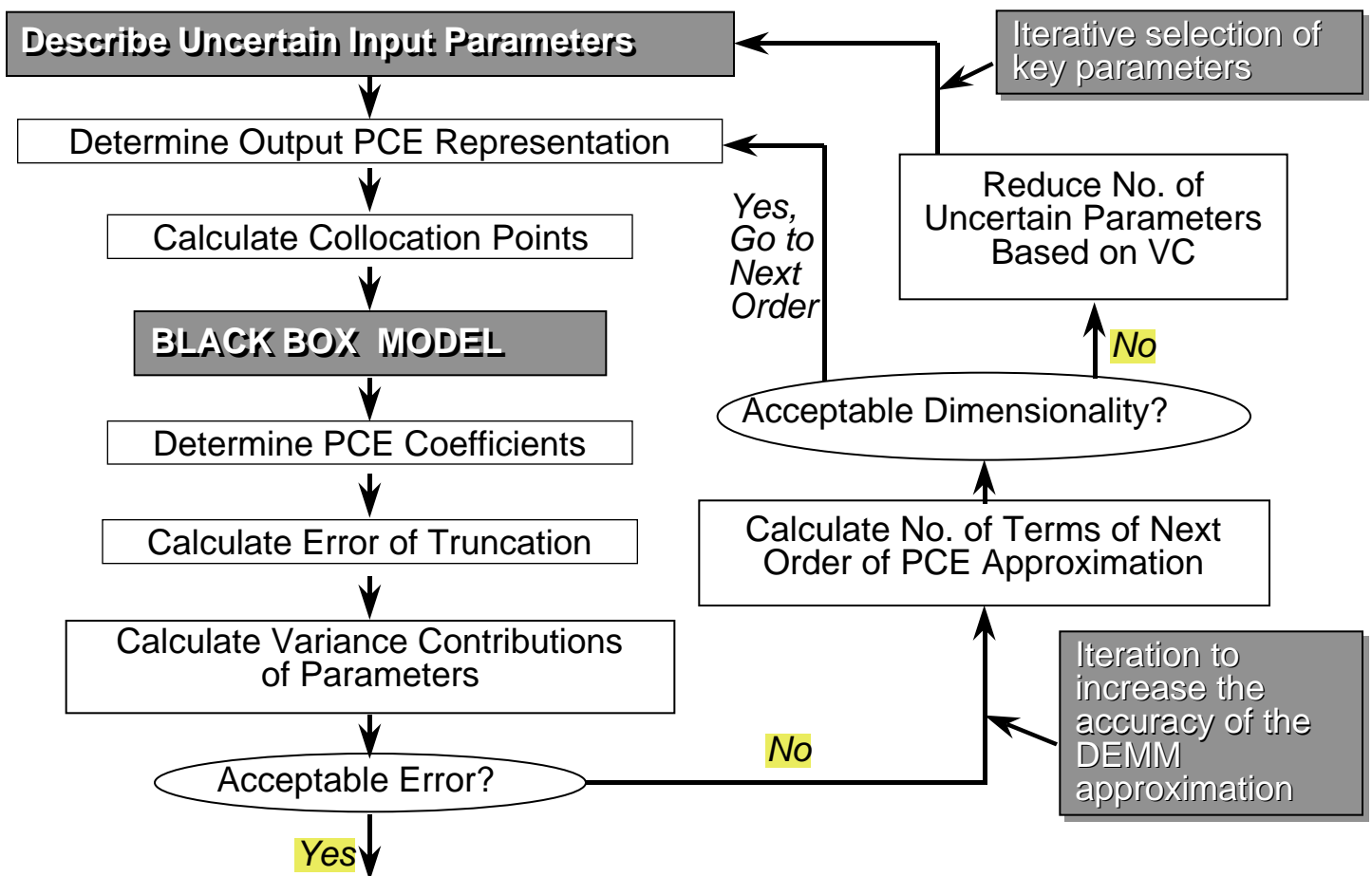
Collocation Agrees with Monte Carlo but is Orders of Magnitude Faster



Effect of Parameter Uncertainty on Variance



Steps in Application of Uncertainty Analysis



Variational Formulation (Summary)

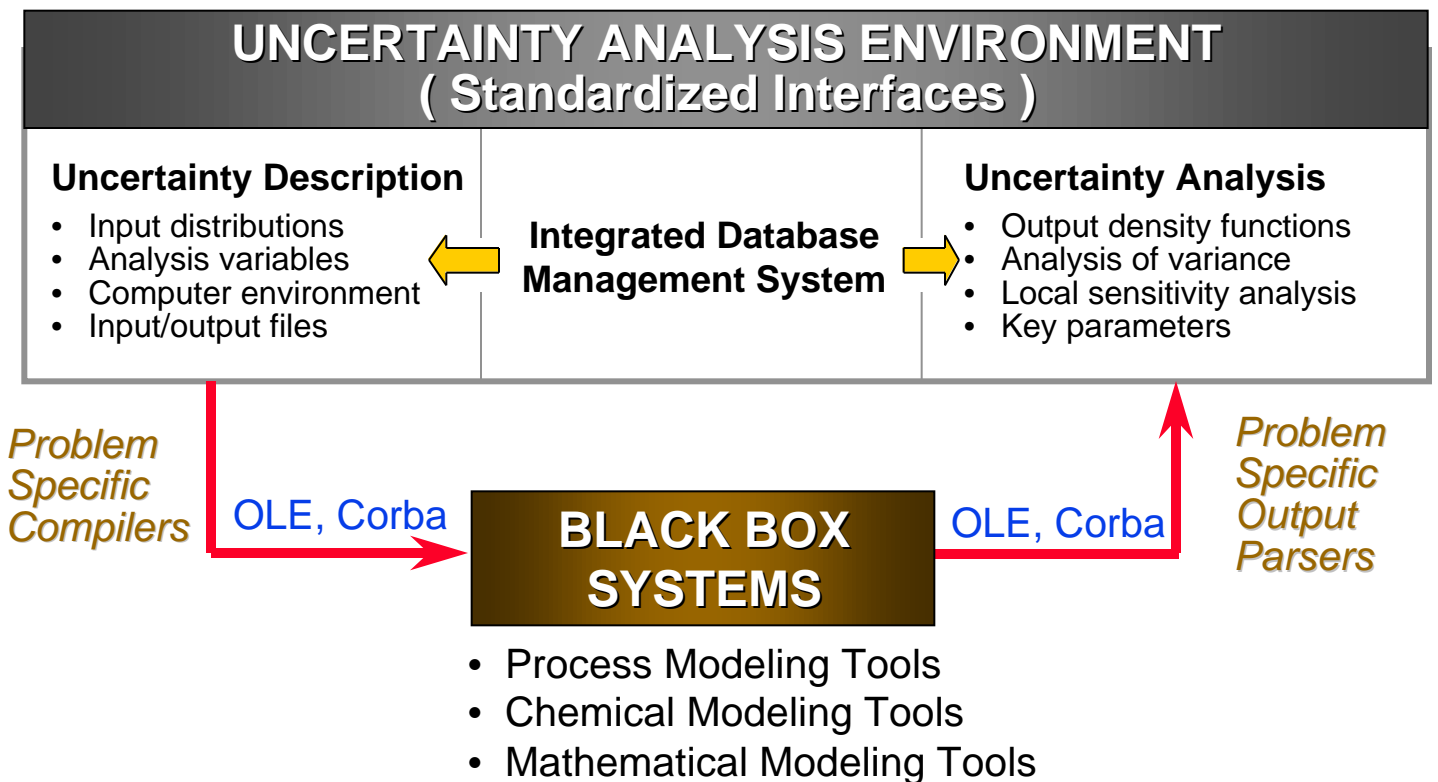
Galerkin (*Weight function same as basis function*)

- Model + Equations for coefficients in expansion
- Model and uncertainty equations have the same form
- Need access to the original equations

Collocation (*All weight at the nodal values*)

- Model solved at each of the collocation points
- Implementation is highly parallel
- Model can be treated as a “black box”
- Number of runs = $C \times \text{number of parameters} \times \text{number of terms in expansion}$ (typically 5)

Models



Example: $ax = b$ (a and b uncertain)

Model

$$a(w)x(w) = b(w)$$

1 Develop the polynomial chaos expansions for pdf of a and b

$$a = a_1 + a_2\zeta_1 + a_3\zeta_2 + a_4(\zeta_1^2 - 1) + a_5\zeta_1\zeta_2 + a_6(\zeta_2^2 - 1) + \dots$$

$$b = b_1 + b_2\zeta_1 + b_3\zeta_2 + b_4(\zeta_1^2 - 1) + b_5\zeta_1\zeta_2 + b_6(\zeta_2^2 - 1) + \dots$$

where ζ_1 and ζ_2 are independent Gaussian random variables

2 Expand x into its polynomial chaos expansion

$$x = x_1 + x_2\zeta_1 + x_3\zeta_2 + x_4(\zeta_1^2 - 1) + x_5\zeta_1\zeta_2 + x_6(\zeta_2^2 - 1) + \dots$$

3 Determine the residue (assume a and b are independent)

$$R(x, w) = a(w)x(w) - b(w) = (a_1 + a_2\zeta_1)(x_1 + x_2\zeta_1 + x_3\zeta_2 + x_4(\zeta_1^2 - 1) + x_5\zeta_1\zeta_2 + x_6(\zeta_2^2 - 1) + \dots) - (b_1 + b_2\zeta_2)$$

Example: $ax = b$ (a and b uncertain)

4 Minimize the residue to solve for coefficients x_i

Collocation method

$$\int_{-x}^x \int_{-x}^x f_{\zeta_1}(\zeta_1) f_{\zeta_2}(\zeta_2) \delta(\{\zeta_1, \zeta_2\}_j - r_j) R(x, w) d\zeta_1 d\zeta_2 = 0$$

where r_j is the j -th collocation point, constructed from zeros of the third order Hermite polynomial

$$H_3(z) = z^3 - 3z \Rightarrow z = -1.732, 0, 1.732$$

The two-dimensional collocation points are

$$\begin{aligned} r_1 &= (0, 0) & r_2 &= (1.732, 0) \\ r_3 &= (-1.732, 0) & r_4 &= (0, 1.732) \\ r_5 &= (0, -1.732) & r_6 &= (1.732, 1.732) \end{aligned}$$

For the case of $j=2$, $r_2=(1.732,0)$, the integral becomes

$$R(x, r_2) = (a_1 + 1.732a_2)(x_1 + 1.732x_2 + 2x_4 - x_6) - b_1 = 0$$

Example: $ax = b$ (a and b uncertain)

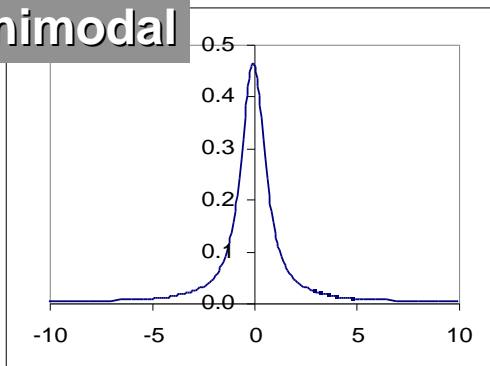
$$\begin{array}{cccccccc}
 a_1 & 0 & 0 & -a_1 & 0 & -a_1 & x_1 & b_1 \\
 a_1 + \sqrt{3}a_2 & \sqrt{3}a_1 + 3a_2 & 0 & 2a_1 + 2\sqrt{3}a_2 & 0 & -a_1 - \sqrt{3}a_2 & x_2 & b_1 \\
 a_1 - \sqrt{3}a_2 & -\sqrt{3}a_1 + 3a_2 & 0 & 2a_1 - 2\sqrt{3}a_2 & 0 & -a_1 + \sqrt{3}a_2 & x_3 & b_1 \\
 a_1 & 0 & \sqrt{3}a_1 & -a_1 & 0 & 2a_1 & x_4 & b_1 + \sqrt{3}b_2 \\
 a_1 & 0 & -\sqrt{3}a_1 & -a_1 & 0 & 2a_1 & x_5 & b_1 - \sqrt{3}b_2 \\
 a_1 + \sqrt{3}a_2 & \sqrt{3}a_1 + 3a_2 & \sqrt{3}a_1 + 3a_2 & 2a_1 + 2\sqrt{3}a_2 & 3a_1 + 3\sqrt{3}a_2 & 2a_1 + 2\sqrt{3}a_2 & x_6 & b_1 + \sqrt{3}b_2
 \end{array} =$$

Solution

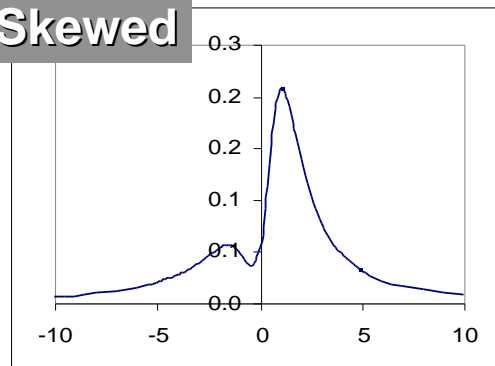
$$x_1 = \frac{b_1}{a_1} \quad \frac{2a_2^2 - a_1^2}{3a_2^2 - a_1^2} \quad x_2 = \frac{a_2 b_1}{3a_2^2 - a_1^2} \quad \dots$$

pdf's for $x = b/a = [b \pm N(0,1)] / [a \pm N(0,1)]$

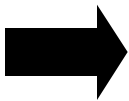
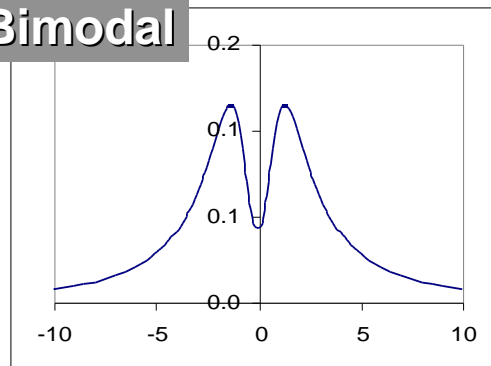
Unimodal



Skewed



Bimodal



Even a simple function can have a complex pdf

Illustrations of Uncertainty Analysis

- **Gas Phase Photochemistry**
 - Illustration of uncertainty analysis method
 - Comparison against Monte Carlo methods
- **Production of Semiconductors**
 - Illustration of uncertainty gas and surface reactions
- **Process Development**
 - Stages in development
 - Resource allocation for uncertainty reduction

Sources of Uncertainties in Photochemistry

- Photolysis Rates (j) $NO_2 + h\nu \xrightarrow{j} NO + O^3P$
- Reaction Rates (k) $O^3P + O_2 \xrightarrow{k_2} O_3$
- Lumping $RH + HO \xrightarrow{k_3} RO_2$
- Product Coefficients $RO_2 + NO \xrightarrow{k_4} p_1(NO_2 + RO) + p_2RNO$
 $RO \xrightarrow{k_5} p_3RCHO + p_4KET + \dots$
- Inventory (IC, Source) $IC(RH) = RH_0$
 $IC(NO) = NO_0$



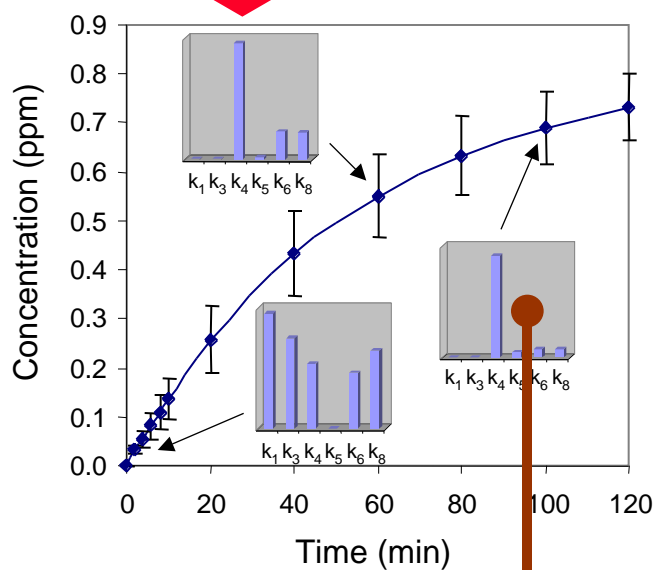
Parametric and Structural Uncertainties Lead to Uncertain Predictions of Photo-Oxidation Products

Uncertainty Analysis -- Reaction Mechanism

Photochemical Reaction Mechanism

1	$\text{NO}_2 + h\nu$	$\text{NO} + \text{O}$
2	$\text{O} + \text{O}_2 + M$	$\text{O}_3 + M$
3	$\text{O}_3 + \text{NO}$	$\text{NO}_2 + \text{O}_2$
4	$\text{HCHO} + h\nu$	$2\text{HO}_2 + \text{CO}$
5	$\text{HCHO} + h\nu$	$\text{H}_2 + \text{CO}$
6	$\text{HCHO} + \text{OH}$	$\text{HO}_2 + \text{CO} + \text{H}_2\text{O}$
7	$\text{HO}_2 + \text{NO}$	$\text{NO}_2 + \text{OH}$
8	$\text{OH} + \text{NO}_2$	HNO_3

Predicted Ozone (O_3) \pm 1 std



Variance Contributions from different parameters to uncertainty in predicted ozone concentrations

Implications of Uncertainty Results Rates

$$k_j = \int_0^{\infty} \phi(\lambda)_j \sigma(\lambda)_j I[\lambda, z] d\lambda$$

✓ Quantum yield (Lab.)

Absorption cross section

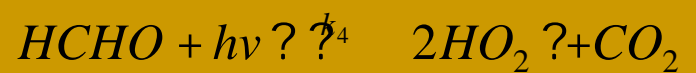
✓ Actinic flux (Field)

Experimental Implications



, Well Known

Better Values for I



Not Well Known

Measurement of I and ϕ

Three Phases in Process Development

1. Technical Feasibility

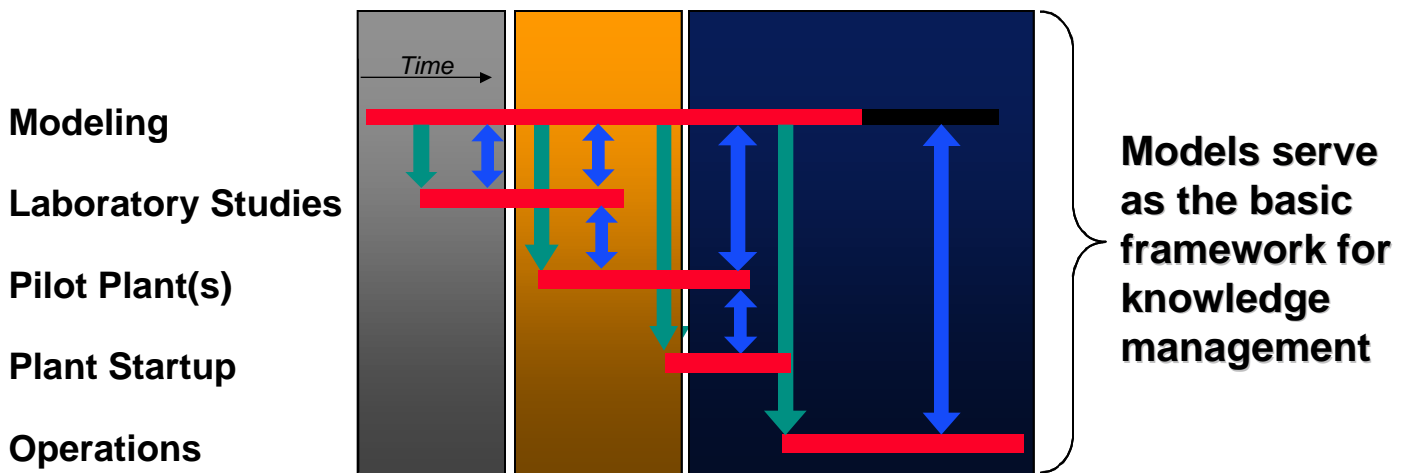
- *Synthesis routes*
- *By-products*
- *Separation issues*

2. Operational Feasibility

- *Safety*
- *Robustness*
- *Consistency*

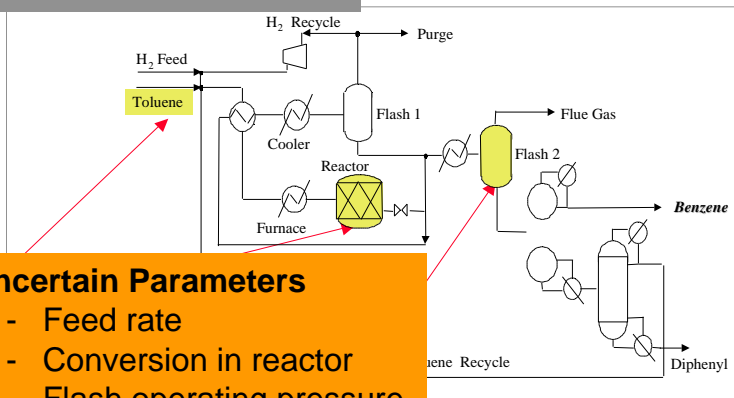
3. Performance Improvements

- *Yield*
- *Throughput*
- *Quality*



Example -- Aspen Process Simulation

Process Flow Sheet

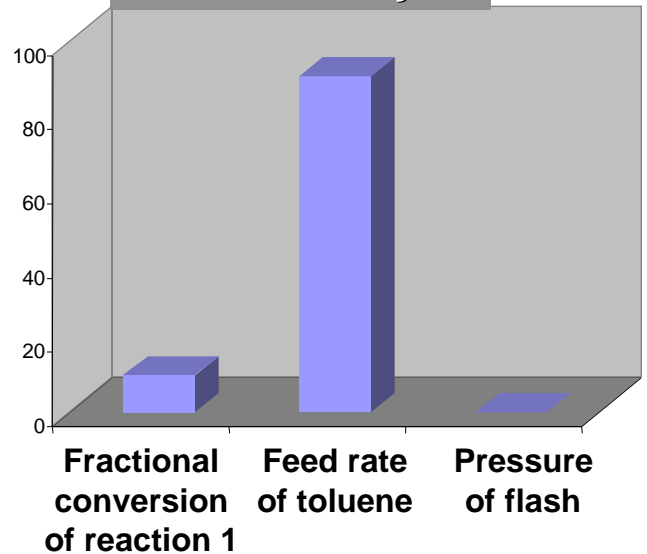


Uncertain Parameters

- Feed rate
- Conversion in reactor
- Flash operating pressure

Uncertainty Analysis

Variance Analysis



➔ Identification of key parameters for further work

Uncertainty is Endemic in an Organization

● Board of Directors

- How should capital be allocated to maximize long term profitability?
- What is the appropriate funding level for new products?
- How should resources be deployed on a global basis?

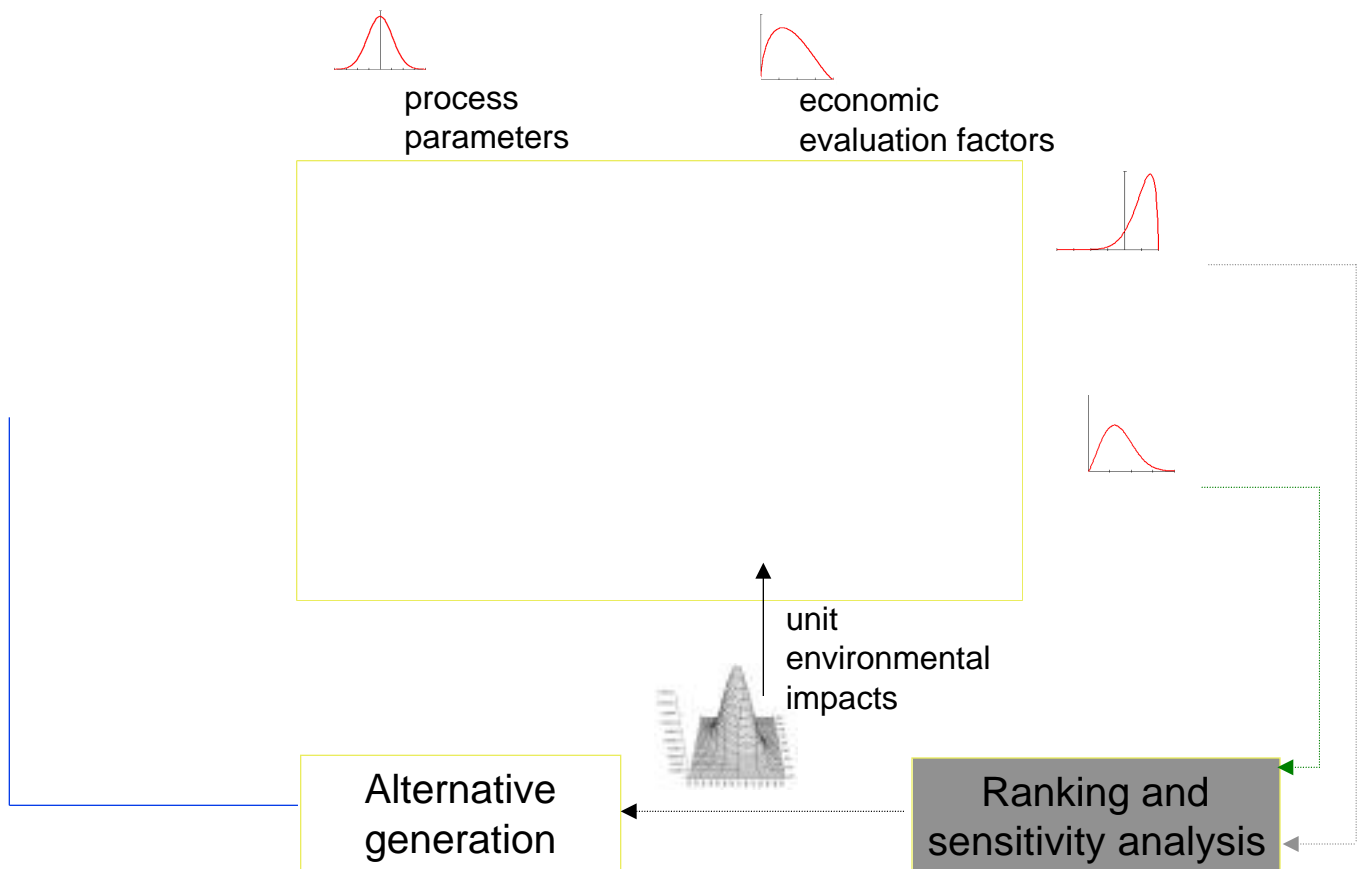
● Middle Management

- What is optimal product/project portfolio?
- How can new products be identified?
- How should projects and resources be managed across work processes?

● Work Process Leaders

- How can the efficiency of work processes be improved?
- How should resources be deployed to meet company goals?

Decision Making in Presence of Uncertainty



Framing of a Design Optimization Problem

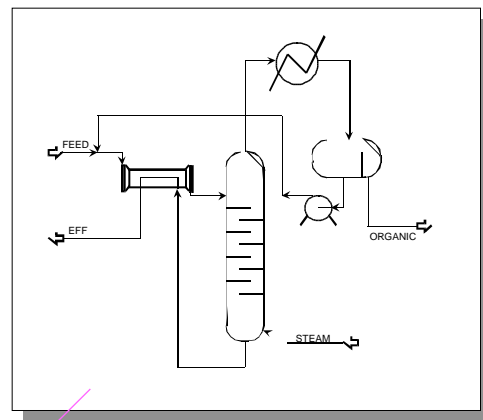
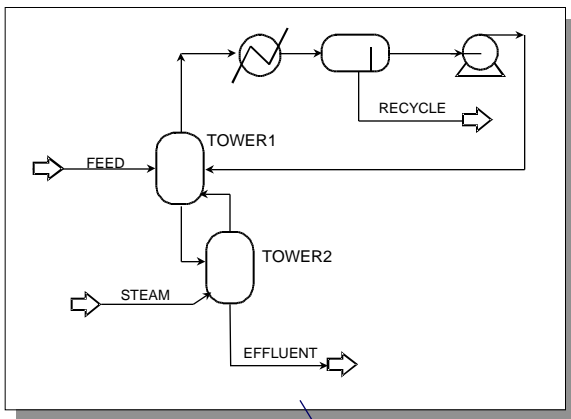
Objective: $\min_{\mathbf{x}, \mathbf{z}} \mathbb{M}_{\theta} [F(\mathbf{x}, \mathbf{y}, \mathbf{z}; \theta)] + C(\cdot, \cdot, \cdot)$

Cost function
Value of information

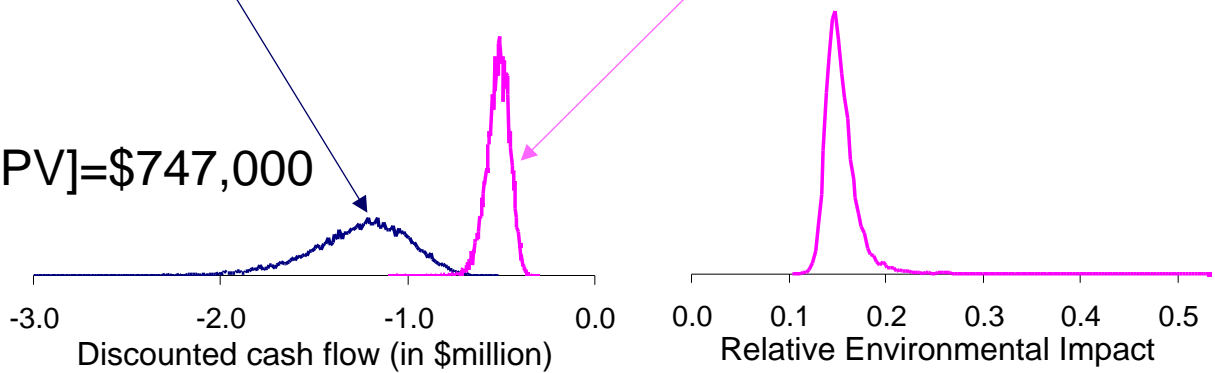
Equality: s.t. $\mathbb{P}_{\theta} \{ - \leq G(\mathbf{x}, \mathbf{y}, \mathbf{z}; \theta) \leq + \} = 1 -$
 (e.g., stochastic algebraic or differential equations)

Inequality: $\mathbb{P}_{\theta} \{ H(\mathbf{x}, \mathbf{y}, \mathbf{z}; \theta) \leq 0 \} = 1 -$
 (e.g., stochastic flexibility index, or risk assessment)

Stochastic Optimization and Decision Making



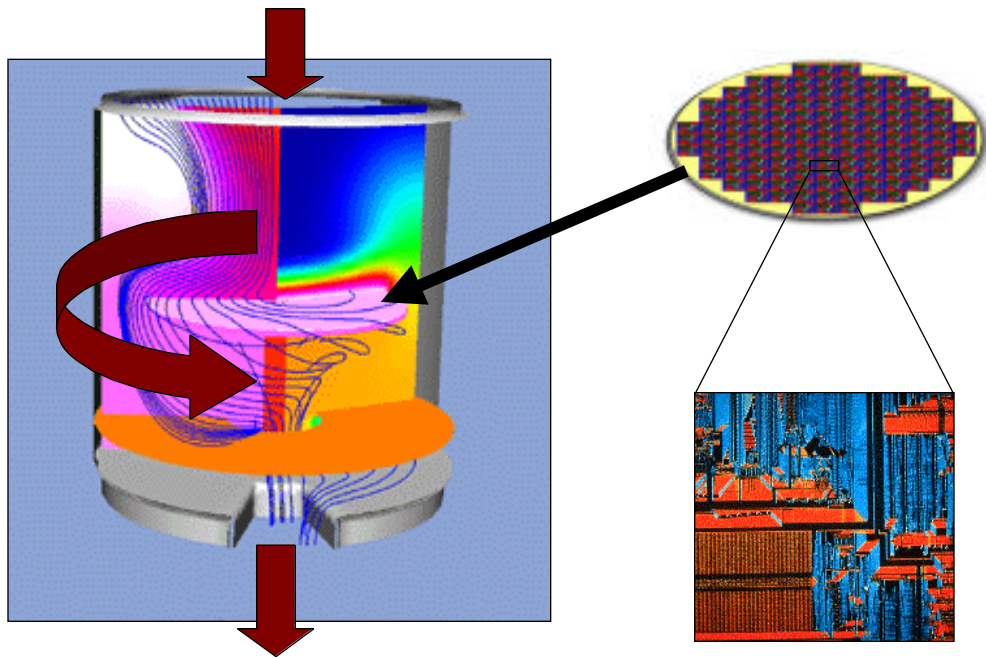
$E[\text{NPV}] = \$747,000$



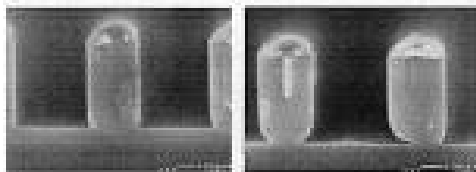
win-win solution!

Example: Manufacturing of Semiconductors

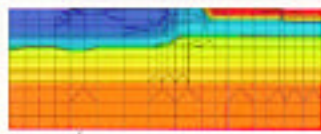
CVD Reactor



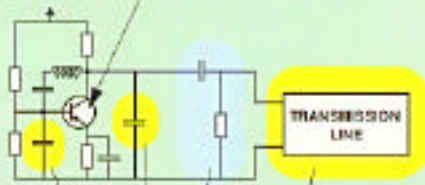
A Hierarchy of Models (All with Uncertainties)



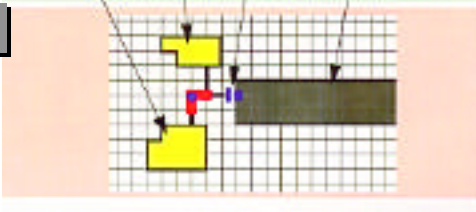
Device Model



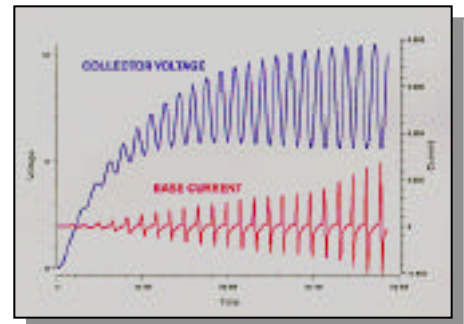
Circuit Model



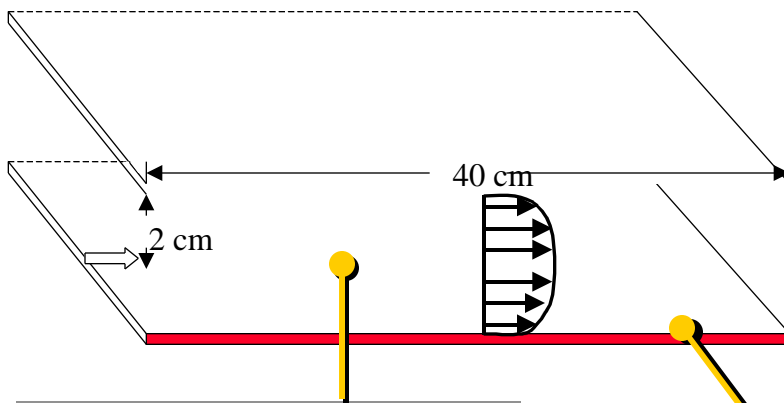
Circuit Board



Transient Response



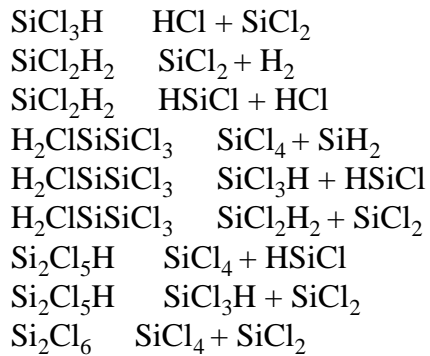
AMAT Centura CVD Reactor



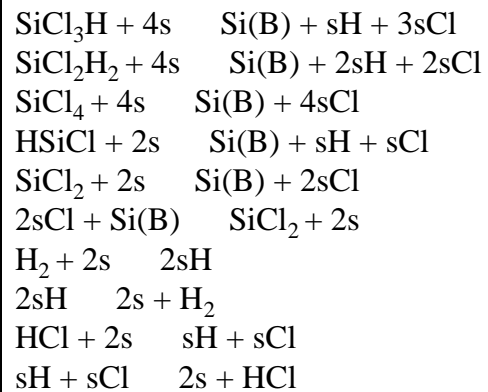
Operating Conditions

Reactor Pressure	1 atm
Inlet Gas Temperature	698 K
Surface Temperature	1173 K
Inlet Gas-Phase Velocity	46.6 cm/sec

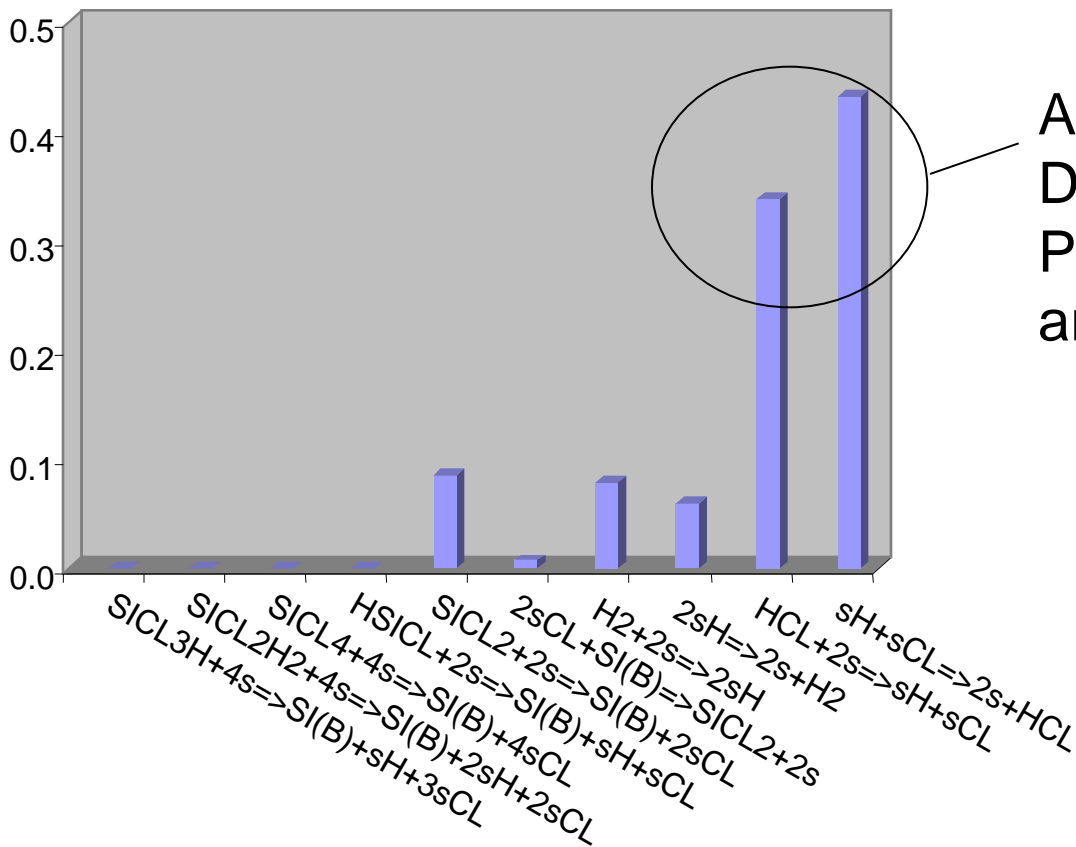
Gas Phase Reactions



Surface Reactions



TCS Lower Wall Deposition Rate (ANOVA)



Significance for Process Modeling

Practical Applications

- Helps identify key variables
- Helps shape experimental design strategy
- Assessment of effects of process variable uncertainty
- Identification of robust operating “ states”
- etc.



New method provides a direct way to focus on reducing uncertainty in outcomes

Conclusions/Recommendations

- Uncertainty analysis is a fertile and much needed area for multi-disciplinary research
- ➔ ● There are many research opportunities
 - ✓ Database design for representation of uncertainties
 - ✓ New algorithms for uncertainty propagation
 - ✓ Decision making metrics in the presence of uncertainties
 - ✓ Treatment of structural uncertainties
 - ✓ Valuation of cost of “ safety factors”
- ➔ ● Estimates of uncertainties in model inputs are desperately needed

Uncertainty \neq Ignorance

