Robust Design of Chemical Processes under Uncertainty through Stochastic Optimization

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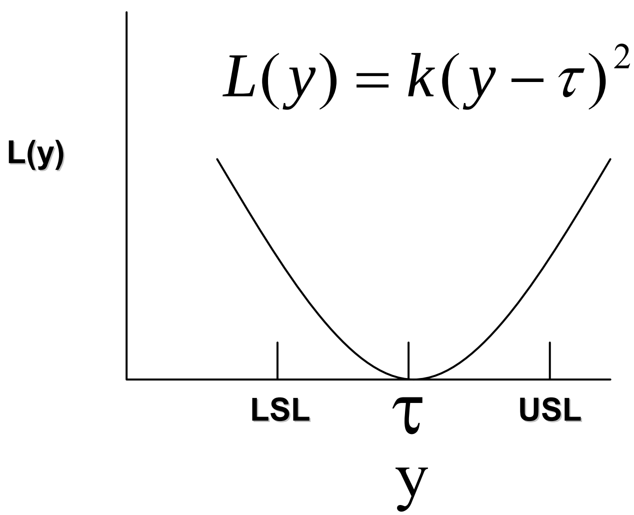
Introduction

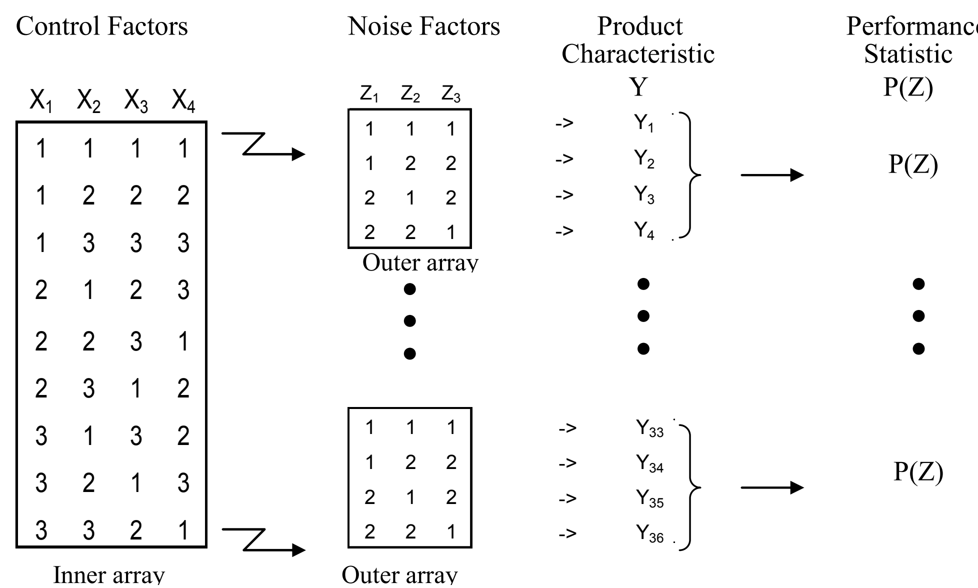
Robustness

A process is said to be robust if it is capable of dealing with variability in its inputs.

Robust Parameter Design Methodology (Taguchi)

Used to identify the setting of variables that make the product or process more robust to input variation



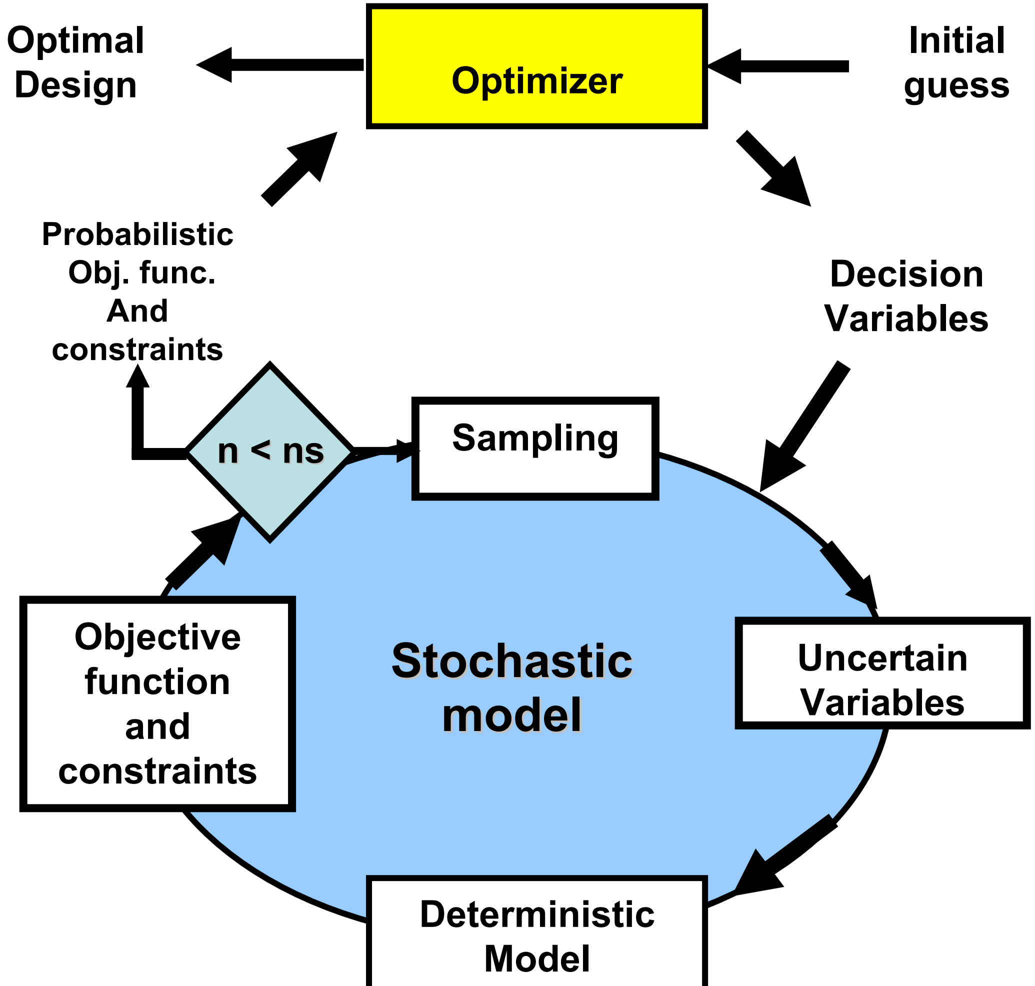


Limitations

- No physical process thus limiting experimentation.
- High capital cost for prototypes and pilot plants.
- High operating cost for multiple runs.
- Mean and variance of quality variable must be independent.

Stochastic Approach

An alternative approach to robust parameter design is to couple an optimizer directly with a computer simulation model using stochastic descriptions of the noise factors.



$$\text{Optimize } E(Z) = E(z(\mathbf{d},\boldsymbol{\theta}))$$

Subject to

$$E(h(\mathbf{d},\boldsymbol{\theta})) = 0$$

$$E(g(\mathbf{d},\boldsymbol{\theta})) \leq 0$$

$$E(z(\mathbf{d},\boldsymbol{\theta})) = \int_{-\infty}^{+\infty} z(\mathbf{d},\boldsymbol{\theta}) f(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

$$\sigma^2 = \int_{-\infty}^{+\infty} (z(\mathbf{d},\boldsymbol{\theta}) - E(z(\mathbf{d},\boldsymbol{\theta}))^2 f(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

Estimating Expected Values Via Sampling

Monte Carlo Methods

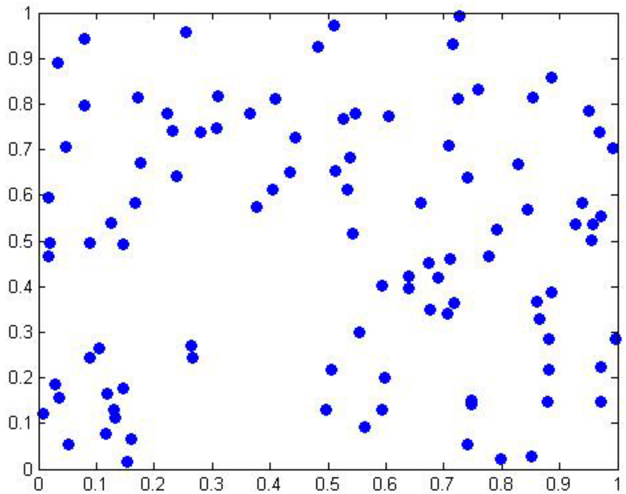
- Monte Carlo Sampling — $\text{std. error} = \dfrac{\sigma}{\sqrt{n}}$
- Latin Hypercube Sampling

Quasi-Monte Carlo Methods

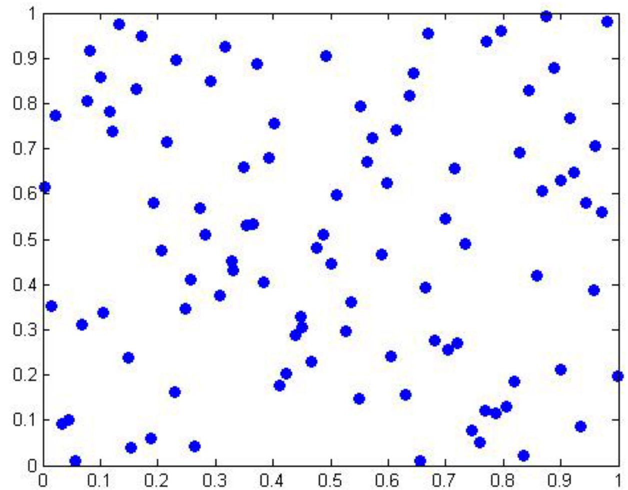
- Hammersley Sequence Sampling

(All three methods:) Estimate Of Precision

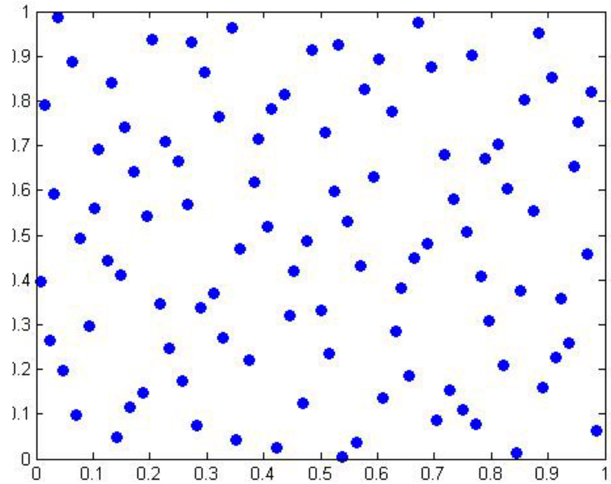
Distribution of 100 Sample Points from a Uniform Distribution in a 2-Dimensional Unit Space



Monte Carlo Sampling (MCS)



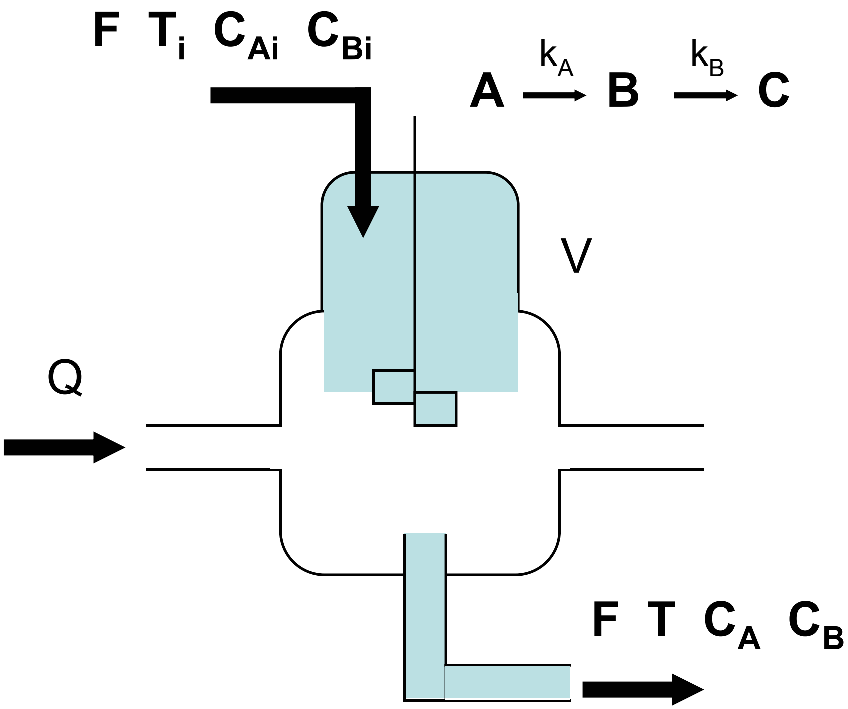
Latin Hypercube Sampling (LSS)



Hammersley Sequence Sampling (HSS)

Design of a Continuous Stirred-Tank Reactor

Boudriga (1990); Diwekar and Kalagnanam (1997)



Objectives:

$$P_B = r_B V = 60 \text{ mol/min} \quad \textbf{(Target)}$$

$$\text{Variance} = \sigma^2_{R_B} \quad \textbf{(Minimum)}$$

Uncertain Variables:

- Inlet Concentrations (C_{Ai}, C_{Bi})
- Inlet Temperature (T_i)
- Reactor Volume (V)
- Flow rate (F)
- Heat Input (Q)

Decision Variables:

Nominal Values of uncertain variables

$$\mu_{C_{Ai}}\ \mu_{C_{Bi}}, \mu_{Ti}, \mu_V, \mu_F, \mu_Q$$

Design Equations

Equality Constraints

(Material and Energy Balance)

$$\tau = \frac{V}{F}$$

$$C_A = \frac{C_{Ai}}{1 + k_A^0 e^{-E_A/RT} \tau}$$

$$C_B = \frac{C_{Bi} + k_A^0 e^{-E_A/RT} C_A}{1 + k_B^0 e^{-E_B/RT} \tau}$$

$$-r_A = k_A^0 e^{-E_A/RT} C_A$$

$$-r_B = k_B^0 e^{-E_B/RT} C_B - k_A^0 e^{-E_A/RT} C_A$$

$$Q = F\rho C_P (T - T_i) + V(r_A H_{RA} + r_B H_{RB})$$

$$r_B V = 60$$

Inequality Constraints

(Process constraints)

$$1000 \leq \mu_{CAi} \leq 5000$$

$$100 \leq \mu_{CBi} \leq 500$$

$$290 \leq \mu_{Ti} \leq < 330$$

$$0.01 \leq \mu_V \leq 0.09$$

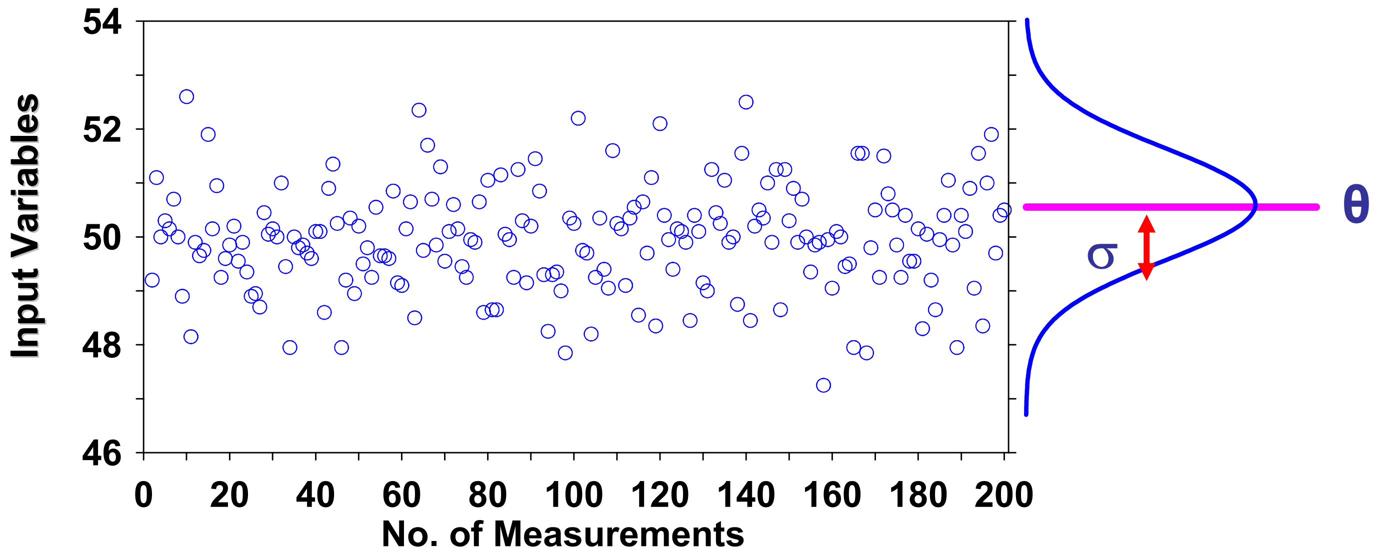
$$0.012 \leq \mu_F \leq 0.17$$

$$290 \leq \mu_T \leq 330$$

Characterization of Input Uncertainty/Variability

Input uncertainties are represented by a Gaussian p.d.f.

$$\mathrm{PDF}(\theta) = \frac{1}{|\Sigma|^{1/2}(2\pi)^{p/2}} \exp\left(-\frac{1}{2}(\theta - \mu_\theta)^T \Sigma^{-1} (\theta - \mu_\theta)\right)$$



Uncertainties are quantified in terms of mean and variance

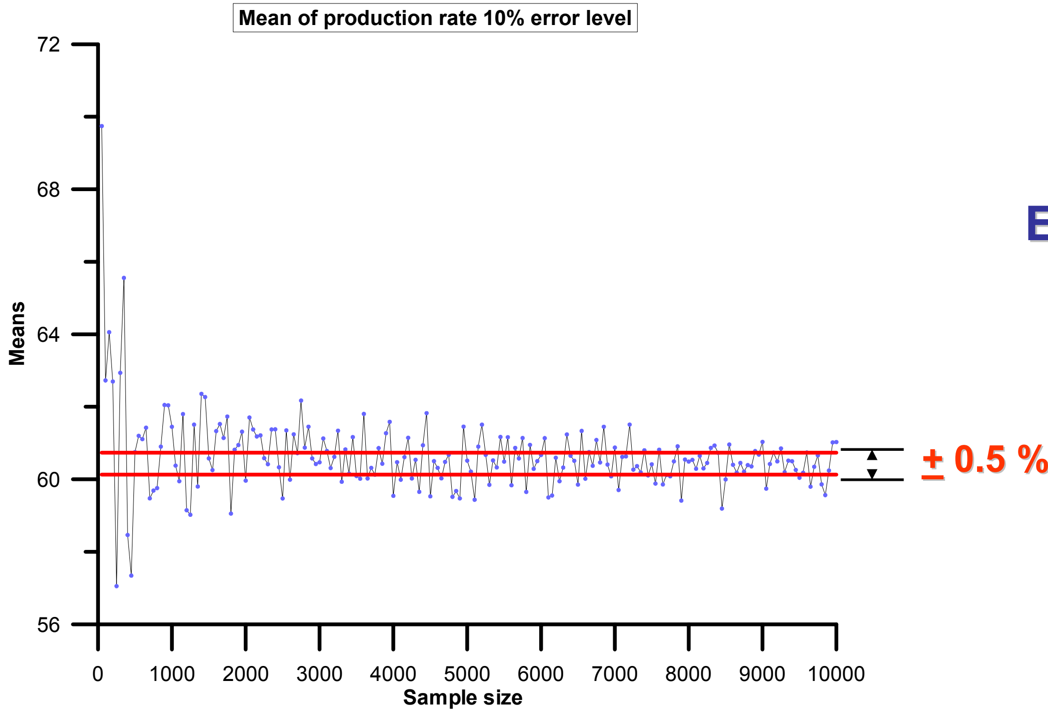
$$\boldsymbol{\theta} = [C_{Ai}, C_{Bi}, T_i, V, F, Q]^T \sim N(\mu_\theta, \Sigma)$$

$$\sigma_{\theta i} = 0.1 * \mu_{\theta i}$$

μ_θ: **Mean**

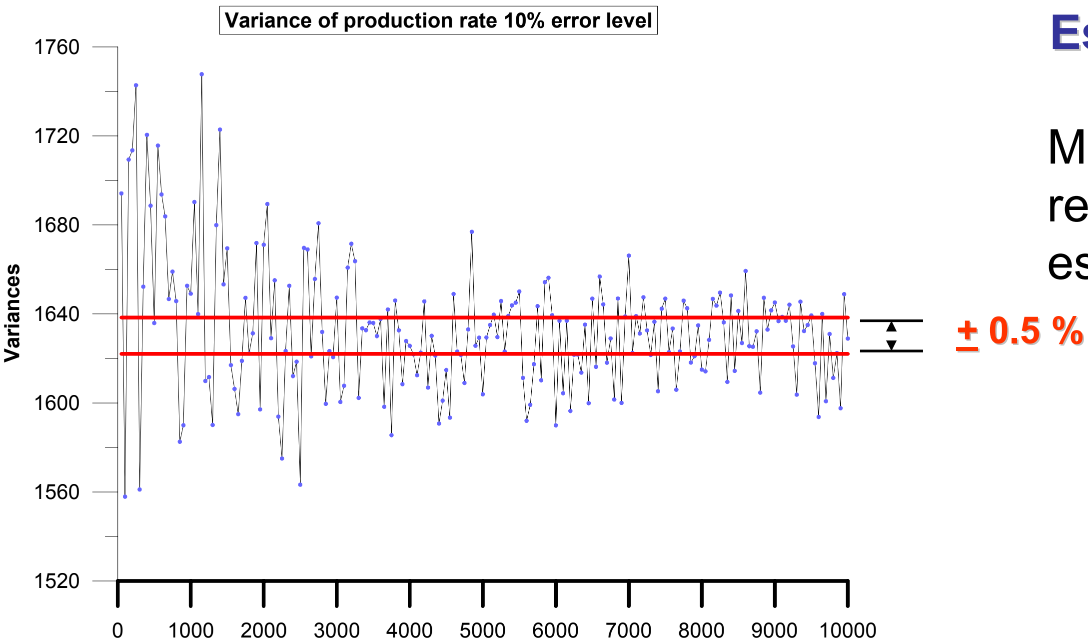
σ_θ: **Standard Deviation**

Monte Carlo Sampling (MCS)



Estimation of the expected mean

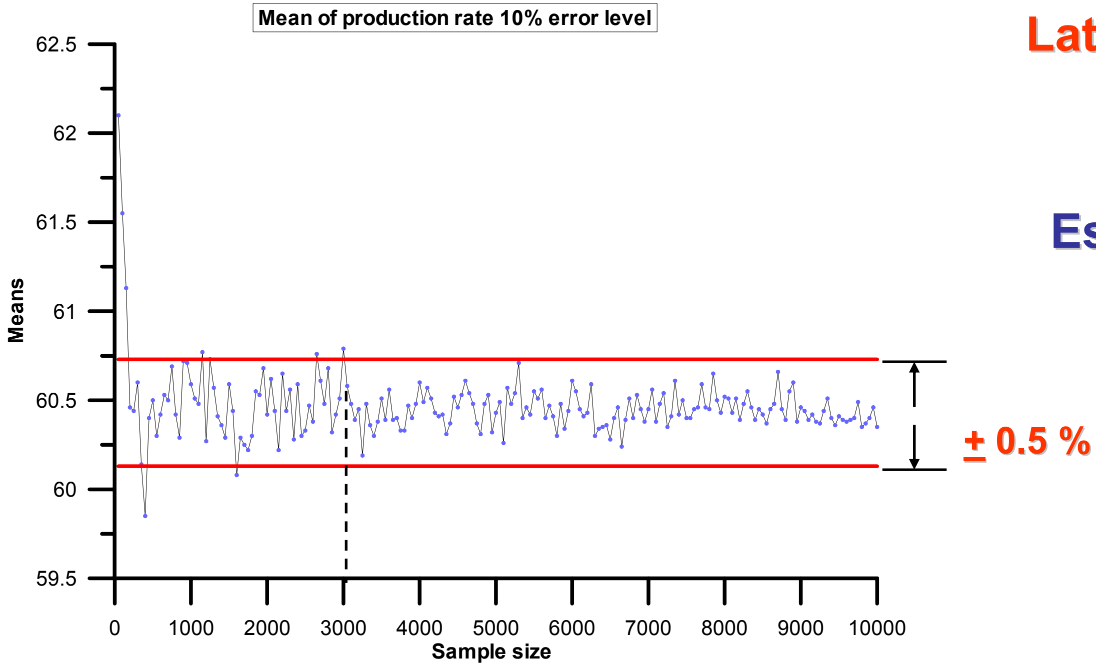
More than 10,000 samples are needed to obtain a precise estimate of the expected mean.



Estimation of the expected variance

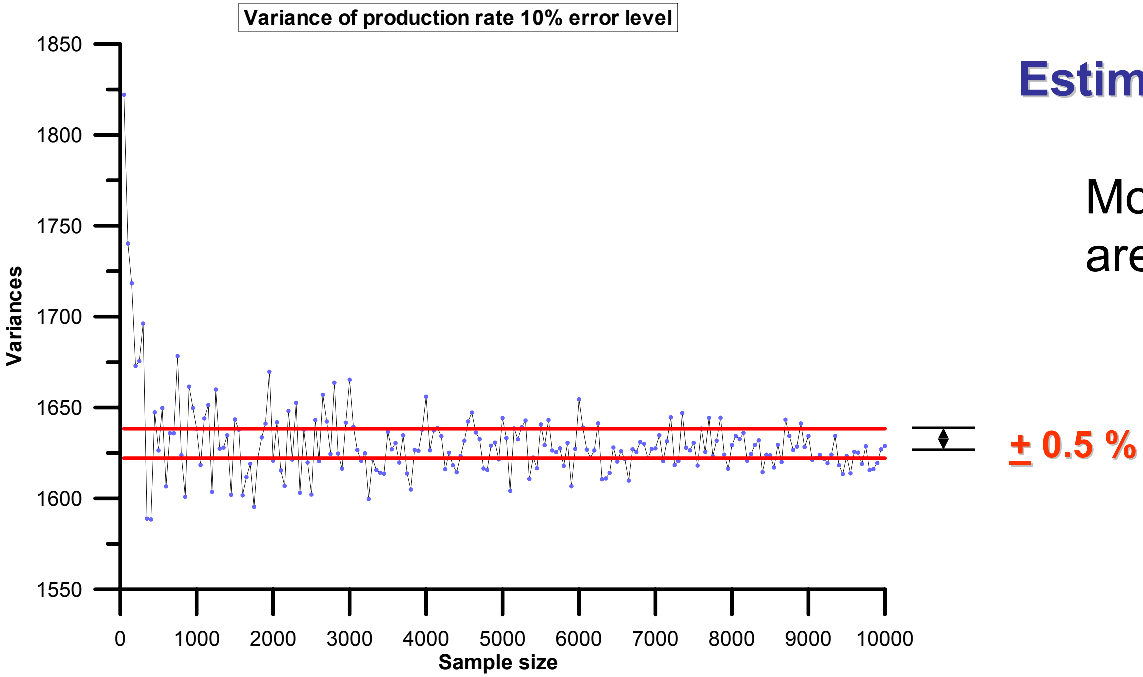
More than 10,000 samples are required to obtain a precise estimate of the expected variance.

Latin Hypercube Sampling (LHS)



Estimation of the expected mean

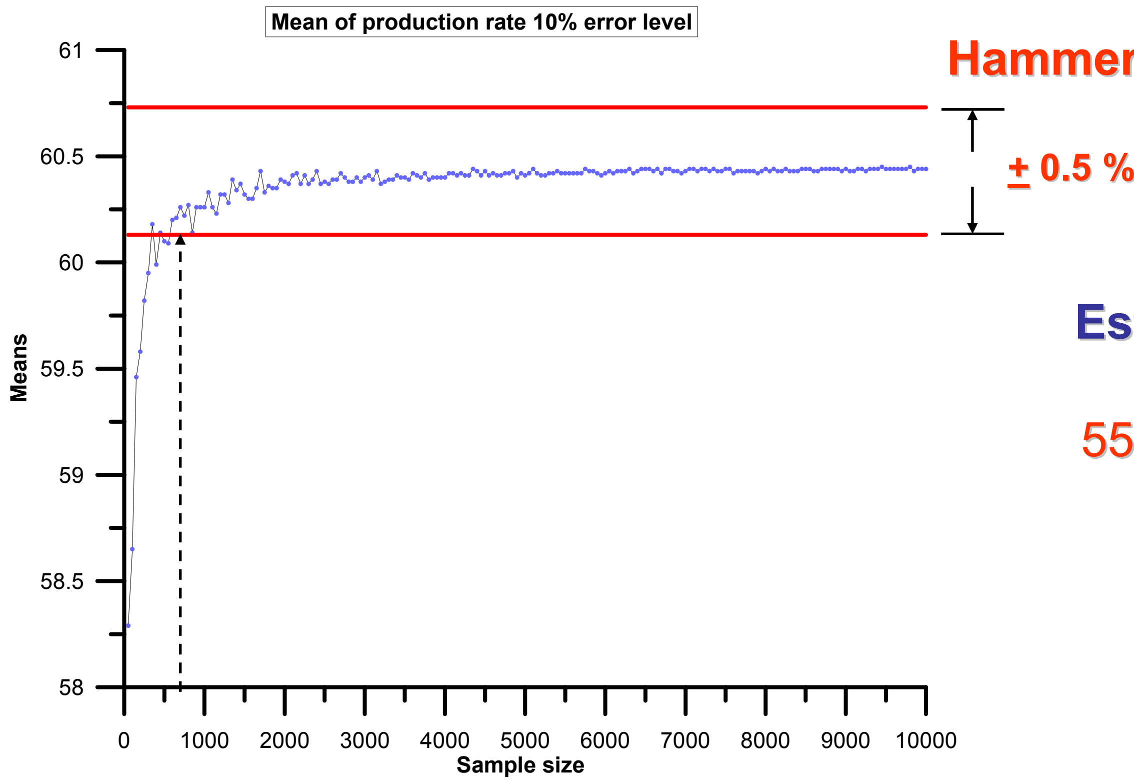
3000 samples or more are needed.



Estimation of the expected variance

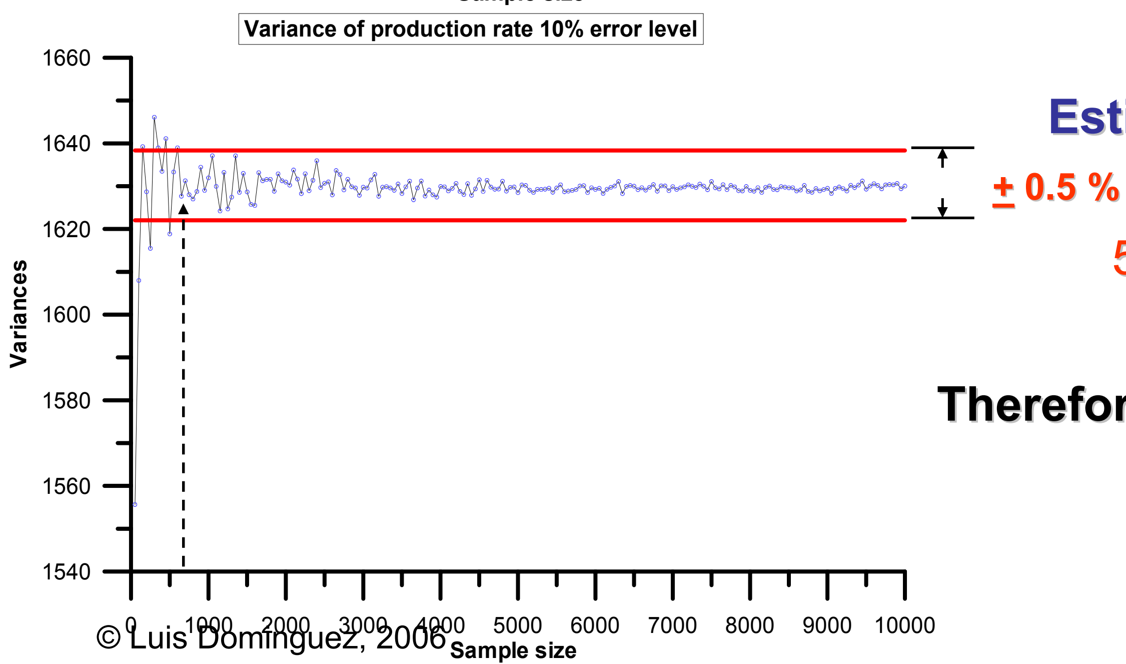
More than 10,000 sampling points are needed.

Hammersley Sequence Sampling (HSS)



Estimation of the expected mean

550 samples or more are needed.



Estimation of the expected variance

550 samples or more are needed.

Therefore, 550 samples were used in the stochastic optimization.

Objective Functions

Dual Response Approach (Vining and Myers,1990)

$$\text{Min } 20 * [\sigma^2_{P_B}]$$

s.t.

$$\mu_{P_B} = 60$$

MSE Approach (Lin and Tu, 1990)

$$\text{Min MSE}(R_B) = 20 * [\underbrace{\sigma^2_{P_B}}_{\text{Variance}} + \underbrace{(E(P_B) - 60)^2}_{\text{Bias}}] \Longleftrightarrow L(y) = k(y - \tau)^2$$

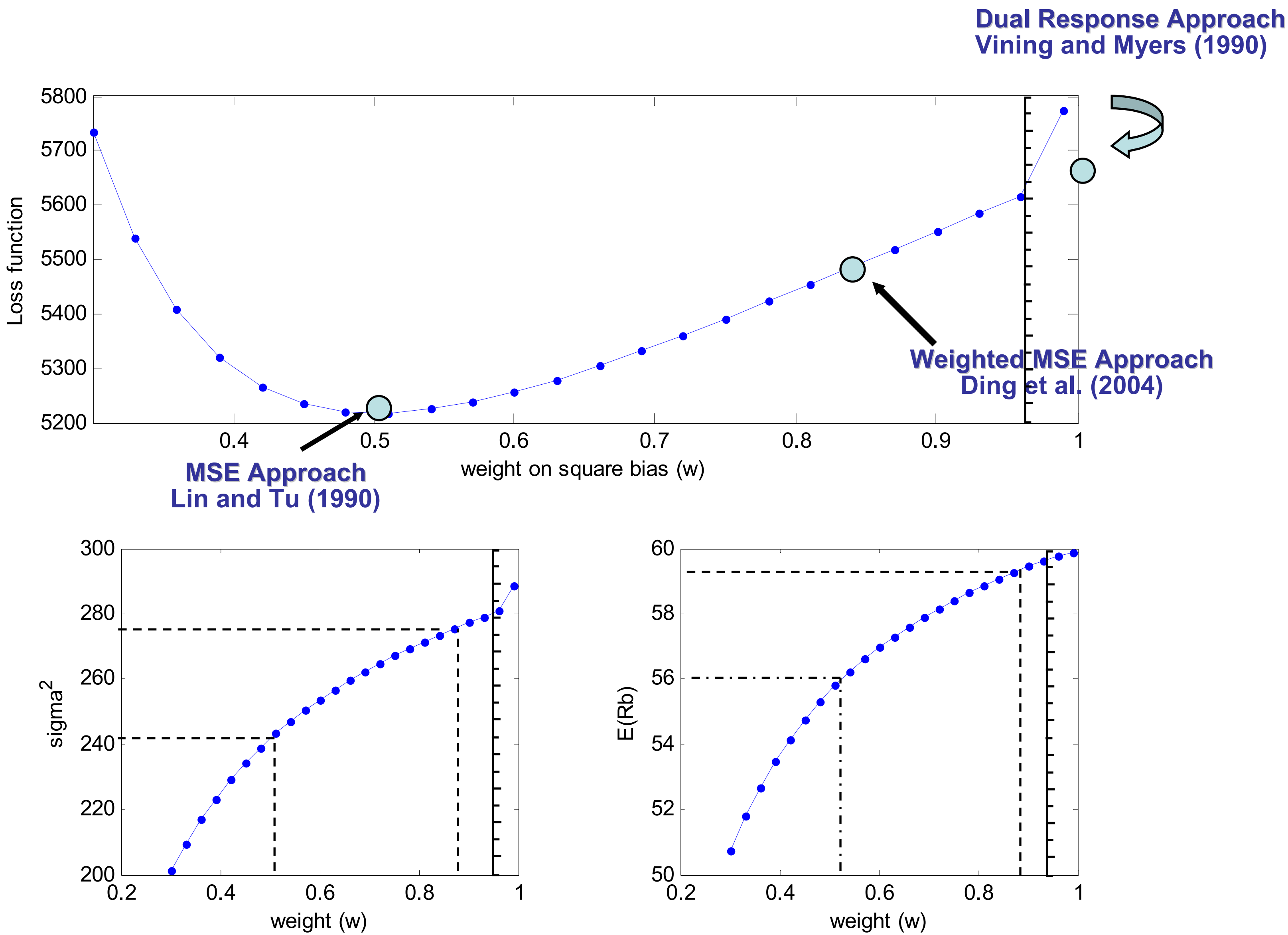
Variance **Bias**

$k = 20$ \$.mol^{-1}.hr

Weighted MSE Approach (Ding et al., 2004)

$$\text{Min MSE}(P_B) = 20 * [(1 - w)\sigma^2_{P_B} + w(E(P_B) - 60)^2]$$

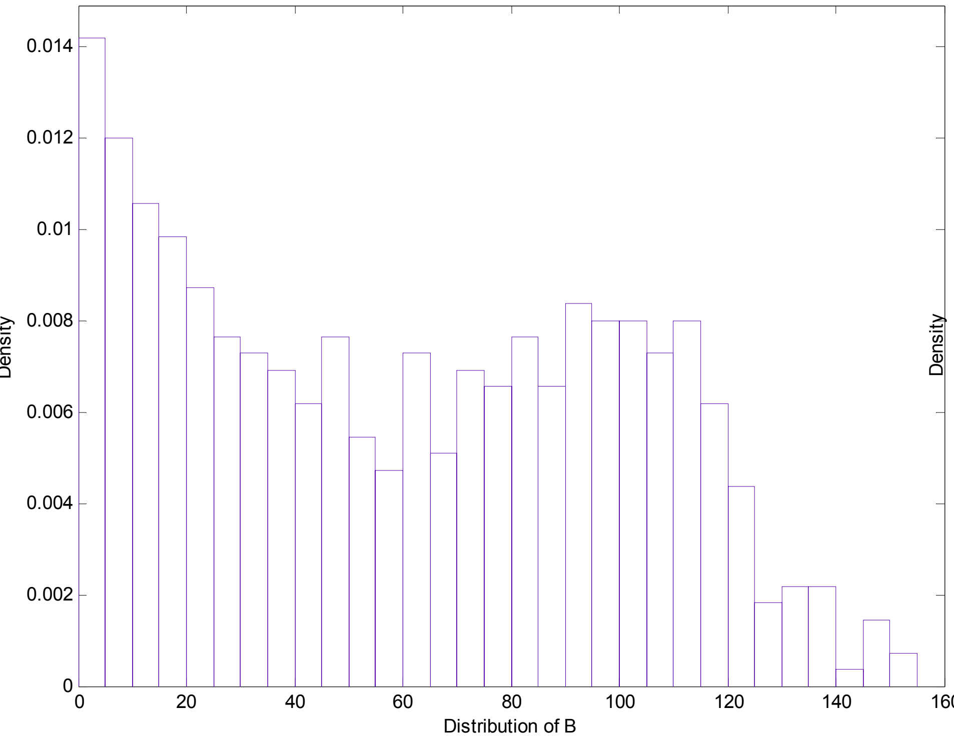
Effect of Weight on Objective Function

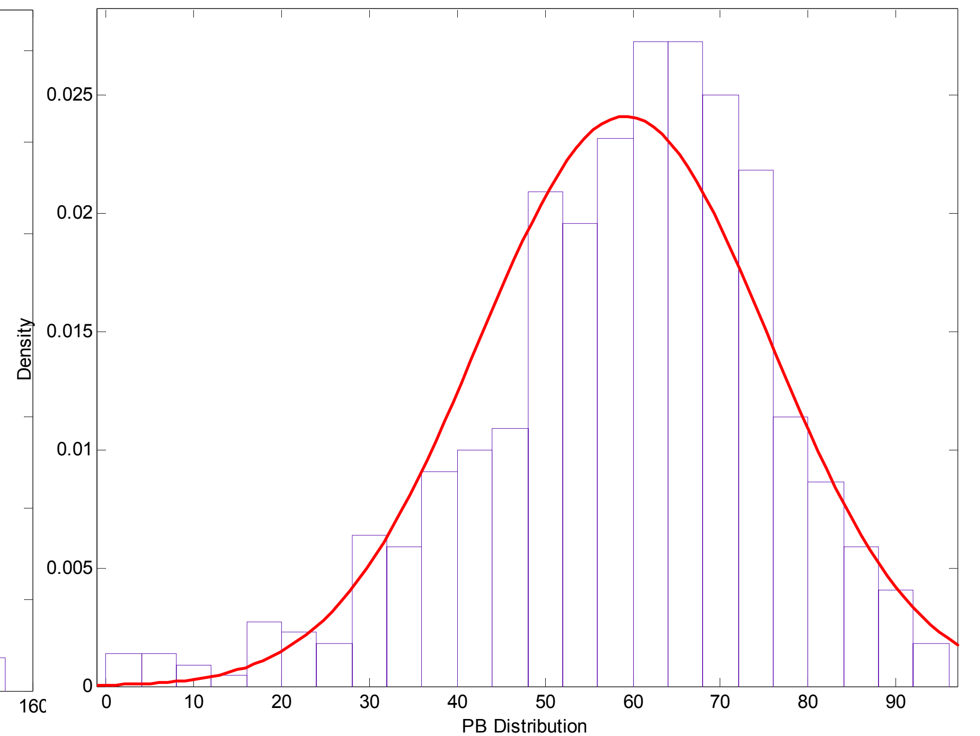


Distribution of Response Before and After Robust Design

Weighted MSE Approach
(Ding et al., 2004)

BEFORE	AFTER





μ_{PB}	60.43
σ^2_{PB}	1630
σ_{RB}	40.37

μ_{PB}	59.06
σ^2_{PB}	273.47
σ_{RB}	16.53

Limitations

- Approach only focuses on minimization of transmitted variability from the inputs to the objective function with or without consideration of a target value for the quality variable.
- Capital and operating costs are not considered.
- There is a potential for violation of input/state constraints during stochastic operation. (Expected values meet constraints but realizations may not.)

Design of a Chemical Plant

Mathematical Form:

$$\left.\begin{aligned} &\text{Min } C(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) \\ &\text{w.r.t.} \quad \mathbf{d},\mathbf{z},\mathbf{x} \\ &\text{s.t.} \quad h(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) = 0 \\ &\qquad\; g(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) \le 0 \\ &\qquad\; \mathbf{d} \in D, \quad \mathbf{z} \in Z, \quad \mathbf{x} \in X, \quad \boldsymbol{\theta} \in \Theta \end{aligned}\right\} \quad \textbf{NLP}$$

d, x, z : design, control and state vectors

Two approaches that tackle the problem of designing Chemical Processes under uncertainty

Deterministic/Multiperiod Approach

$$\Theta = \left\{ \boldsymbol{\theta} : \boldsymbol{\theta}_i^L \le \boldsymbol{\theta}_i \le \boldsymbol{\theta}_i^U, \quad i = 1,2,..N_p \right\}$$

Stochastic Approach

$$\Theta = \left\{ \boldsymbol{\theta} : \boldsymbol{\theta}_i \in j(\boldsymbol{\theta}) \right\}$$

Expectation of Objective function

Uncertainty in the parameters is characterized as a joint probability density function (PDF)

$$E_{\boldsymbol{\theta}\in\Theta}\left\{ \min_{\mathbf{z}} C(\mathbf{d},\mathbf{z},\boldsymbol{\theta}) \middle| f(\mathbf{d},\mathbf{z},\boldsymbol{\theta}) \le 0 \right\} = \int_{\boldsymbol{\theta}\in\Theta} C^*(\mathbf{d},\boldsymbol{\theta}) j(\boldsymbol{\theta}) d\theta$$

where

$$C^*(\mathbf{d},\boldsymbol{\theta}) = \min_{\mathbf{z}} \left\{ C(\mathbf{d},\boldsymbol{\theta}) \;\middle|\; f(\mathbf{d},\mathbf{z},\boldsymbol{\theta}) \le 0 \right\}$$

Simplified form

$$\min \int_{\boldsymbol{\theta}\in\Theta} C^*(\mathbf{d},\boldsymbol{\theta}) j(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

$$\text{w.r.t. } \mathbf{d}$$

$$\text{s.t. } \forall\boldsymbol{\theta}\in\Theta \left\{ \exists\mathbf{z} \left(\forall j \in J [f_j(\mathbf{d},\mathbf{z},\boldsymbol{\theta})] \le 0] \right) \right\}$$

$$\mathbf{d}\in D, \quad \mathbf{z}\in Z, \quad \boldsymbol{\theta}\in\Theta$$

Inclusion of Robustness and Quality in the Design of Chemical Plants

(Bernardo et al 2001)

Robustness criterion 1: Penalty term in objective function based on Taguchi loss function

$$P_q = k(y - y^*)^2$$

$$C_q(\mathbf{d}, \mathbf{z}, \mathbf{x}, \mathbf{y}, \mathbf{y}^*, \boldsymbol{\theta}) = C(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) - P_q(\mathbf{y}, \mathbf{y}^*)$$

Taguchi S/N ratio	k value
Nominal-the-best Symmetric	Same k for all y
Nominal-the-best	$k = k_1$ if $y < y^*$ $k = k_2$ if $y \geq y^*$
Larger-the-better	$k = k_1$ if $y < y^*$ $k = 0$ if $y \geq y^*$
Smaller-the-better	$k = 0$ if $y < y^*$ $k = k_2$ if $y \geq y^*$

Robustness criterion 2: Explicit restriction on robustness metrics

$$r(m_y) \leq \gamma$$

$$\mu_{\mathbf{y}} = E_\Theta(\mathbf{y})$$

$$\sigma_{\mathbf{y}}^2 = E_\Theta\left\{\mathbf{y} - \mu_{\mathbf{y}})^2\right\}$$

Robustness metric	Robustness Criteria	
Mean Variance	Minimum mean Maximum variance	$\mu_y \geq \mu_{min}$ $\sigma_y^2 \leq \sigma_{max}^2$

Single-Stage Stochastic Optimization Formulation

$$\min \quad \frac{1}{N_p}\sum_{i=1}^{N_P} C_q(\mathbf{d}, z_i, x_i, y_i, y_i{*}, \boldsymbol{\theta}_i)$$

$$\text{w.r.t.} \quad \mathbf{d}, z_i, x_i, y_i$$

$$\text{s.t.} \quad C_q(\mathbf{d}, z_i, x_i, y_i, y_i{*}, \boldsymbol{\theta}_i) = C(\mathbf{d}, z_i, x_i, \boldsymbol{\theta}_i) - P_q(y_i, y_i{*})$$

$$\mathbf{h}(\mathbf{d}, z_i, x_i, \boldsymbol{\theta}_i) = 0$$

$$\mathbf{g}(\mathbf{d}, z_i, x_i, \boldsymbol{\theta}_i) \le 0$$

$$\mu_y = \frac{1}{N_p}\sum_{i=1}^{N_p} y_i$$

$$\frac{1}{N_p - 1}\sum_{i=1}^{Np}(y_i - \mu_y)^2 \le \gamma$$

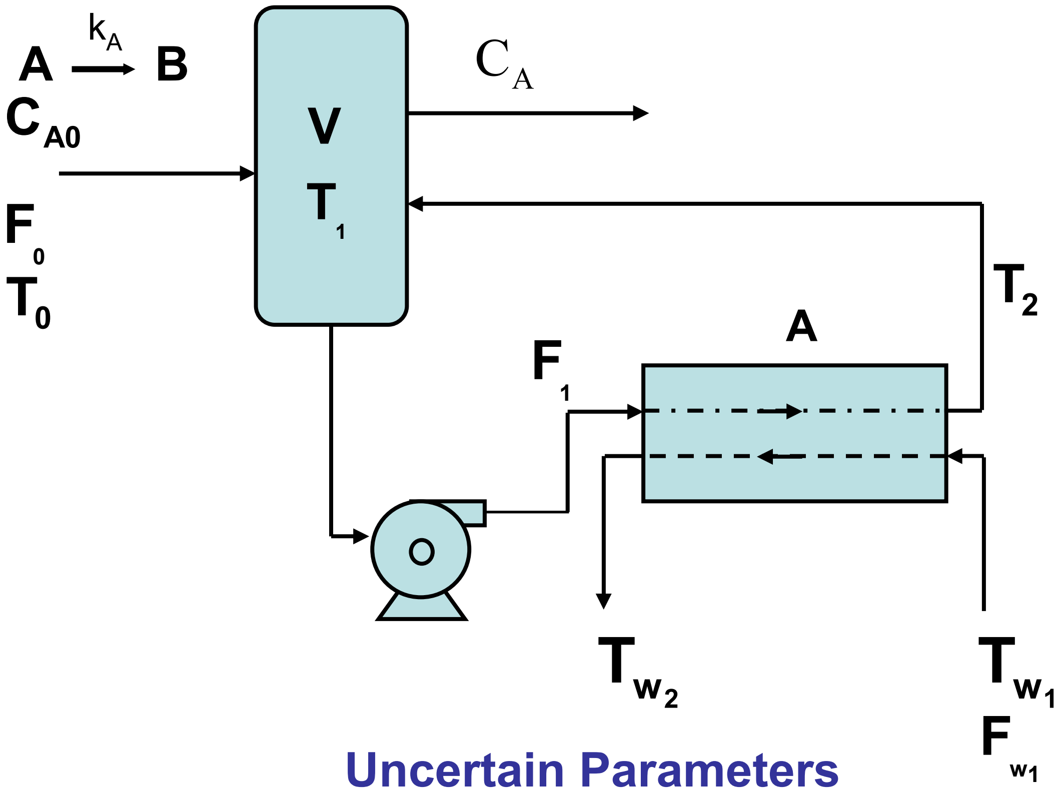
$$\mathbf{d} \in D, \quad \boldsymbol{\theta}_i \in \Theta, \quad z_i \in Z, \quad x_i \in X, \quad y_i \in Y$$

$$i = 1,\ 2,\ \ldots.,\ N_p$$

Design of a RHE system

Georgiadis and Pistikopoulos (1999); Bernardo et al. (2001)

$$\text{Capital} + \text{Operating Costs} = 691.2V^{0.7} + 873.6A^{0.6} + 1.76F_W + 7.056F_1$$



Decision Variables

$$d = [A,\ \ V]^T$$
$$z = [F_1,\ F_w]^T$$
$$y = [X_A]^T$$
$$x = [T_1\ ,\ \ T_2,\ \ T_{w2}]^T$$

Characterization of Uncertain Parameters

$$\theta = [F_0, T_0, T_{w_1}, k_R, U]^T \sim N(\mu, \Sigma)$$

$$\sigma_i = \varepsilon_i * \mu_i$$

Uncertain Parameters

	Parameter	Unit	μ_i	σ_i	99.8 % C. I.	
F_0	Flow rate of the feed	kmol/hr	45.36	2.93	36.30	54.41
T_0	Temperature of the feed	K	333	4.31	319.68	346.31
Tw_1	Cooling water inlet temperature	K	293	3.79	281.28	304.71
k_R	Arrhenius rate constant	hr^{-1}	45	0.77	42.62	47.37
U	Overall heat transfer coefficient	kJ.m-^{2}.h. K	1635	105.82	1308.01	1964.98
C_{A0}	Initial concentration at the feed	kmol.m-^{3}	32.04	2.07	25.64	38.43

Design Equations and Objective

Minimize **Capital + Operating + Quality Costs** (Penalty)

$$691.2V^{0.7} + 873.6A^{0.6} + 1.76F_W + 7.056F_1$$

$$P_q = k(X_A - 0.9)^2$$

Subject to

Material and Energy Balance

$$F_0 x_A - Vk_R e^{-\frac{E}{RT_1}}(1 - x_A) = 0$$

$$(-\Delta H)F_0 x_A + F_0 C_p (T_0 - T_1) - F_1 C_p (T_1 - T_2) = 0$$

$$F_1 C_p (T_1 - T_2) = AU\Delta T_{lm}$$

$$\Delta T_{lm} = \frac{(T_1 - T_{w_2}) - (T_2 - T_{w_1})}{\ln\left[\frac{T_1 - T_{w_2}}{T_2 - T_{w_1}}\right]}$$

$$F_1 C_p (T_1 - T_2) = F_w C_{p_w} (T_{w_2} - T_{w_1})$$

Process Constraints

$$311 \le T_2 \le 389$$

$$311 \le T_1 \le 389$$

$$294 \le T_{w_2} \le 323$$

$$T_1 - T_{w_2} \ge 11.1$$

$$T_2 - T_{w_1} \ge 11.1$$

$$T_1 - T_2 \ge 0$$

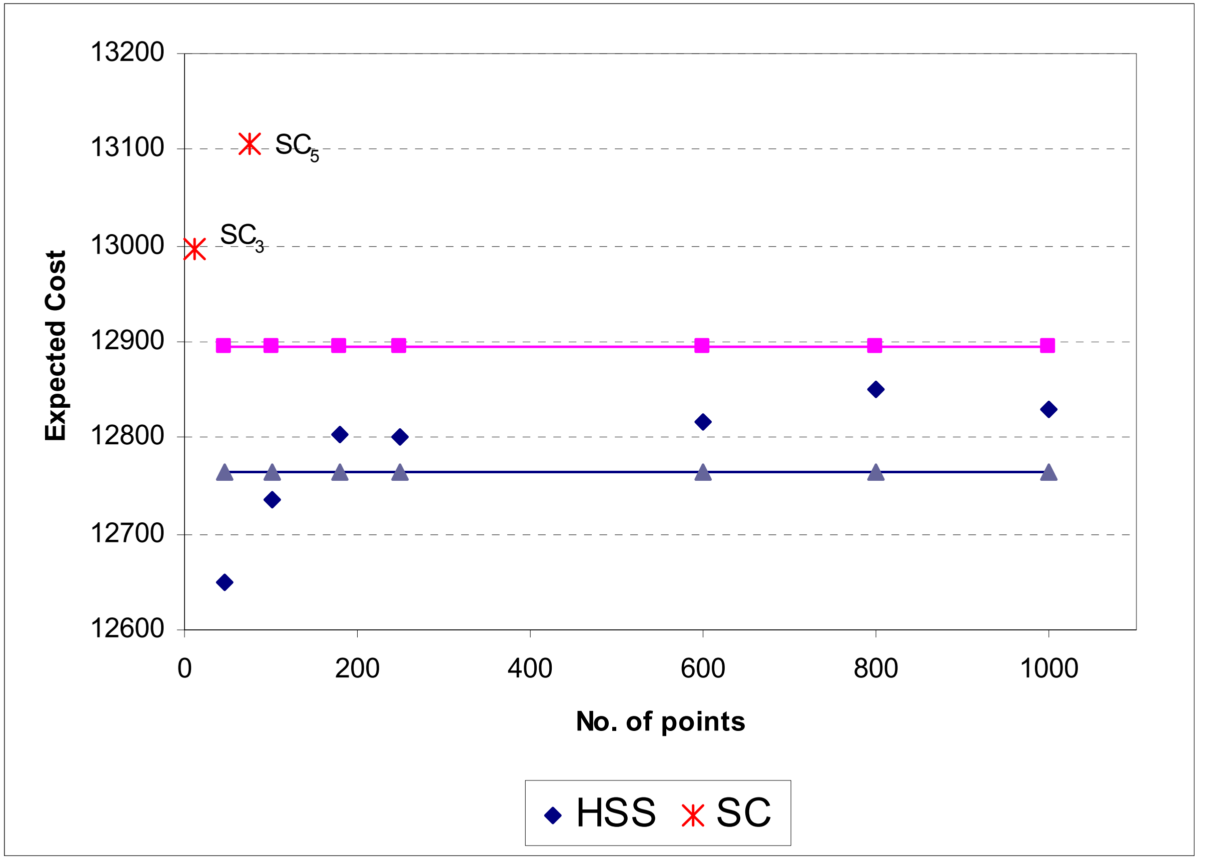
$$T_{w_2} - T_{w_1} \ge 0$$

Quality Constraints

$$x_A \ge 0.9$$

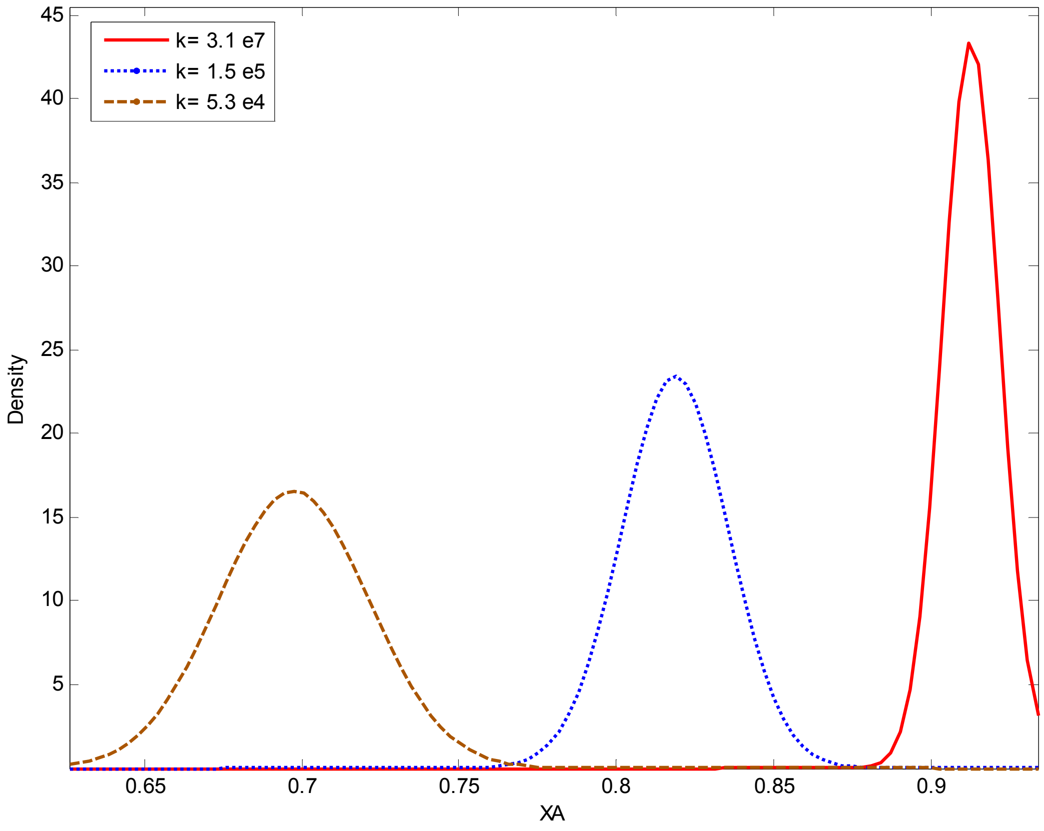
Estimation of overall expected Cost

Using HSS and cubatures degree 3 and 5



Results

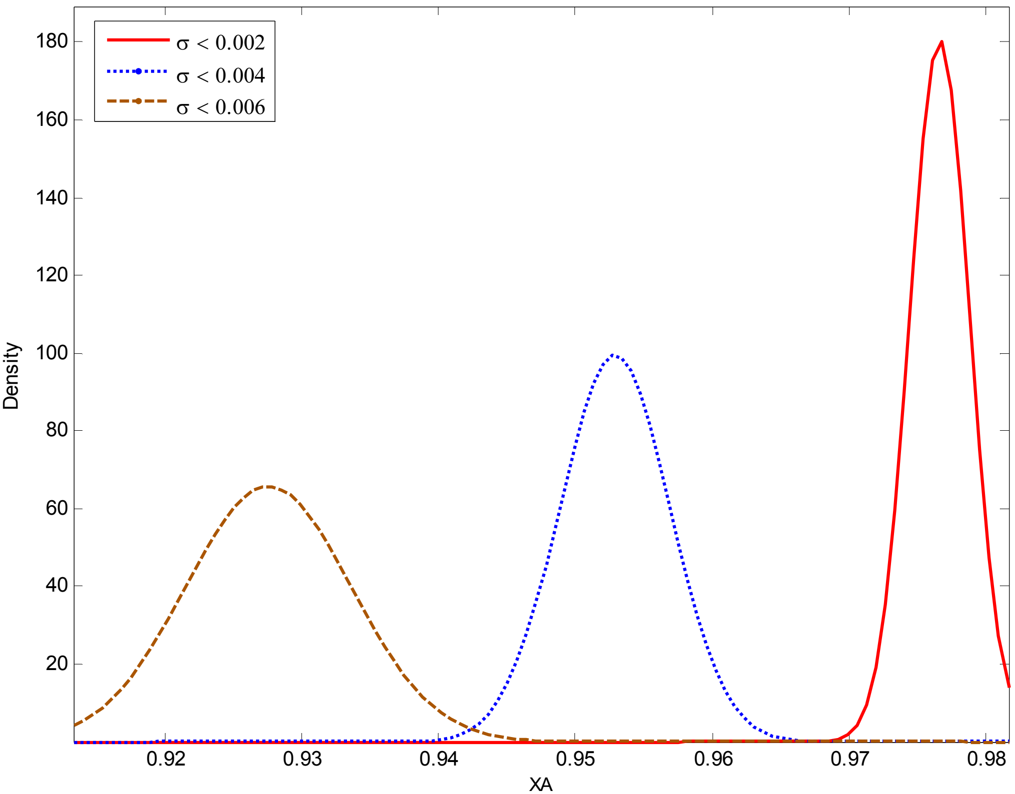
(Penalty term in Objective Function)



k	$5.3x10^4$	$1.5x10^5$	$3.1x10^7$
E[Cost] ($\$.year^{-1}$)	9603.00	11199.483	13066.71
Capital Cost	2673.19	3546.199	4806.26
E[Op Cost]	4722.09	6620.14	8126.11
E[Penalty]	2207.72	1036.137	134.33
A (m^2)	3.69	5.11	6.18
V (m^3)	1.15	2.25	5.23
μ_{XA}	0.70	0.82	0.91
σ_{XA}	0.024	0.017	0.009

Results

(Penalty term + Explicit restriction on robustness Metrics)



	Robustness Criteria		
	$\sigma_{XA} \leq 0.006$	$\sigma_{XA} \leq 0.004$	$\sigma_{XA} \leq 0.002$
E[Cost] $/year	13094.93	13927.88	16823.59
Capital Cost	4544.65	5299.41	7101.19
E[Op. Cost]	8484.70	8628.47	9722.40
E[Loss]	65.58	0	0
A (m^2)	5.80	6.62	7.05
V (m^3)	4.68	6.59	13.55
μ_{XA}	0.90	0.92	0.96
σ_{XA}	0.006	0.004	0.002

Conclusions

- **Concerning sampling techniques to estimate E [Cost function]**

  - Hammersley Sequence Sampling proved to be the most efficient technique:

    - better uniformity properties

    - fewer samples are required

- **Concerning Robust Design criteria**

  - Using the weighted MSE approach a trade-off between low variability and closeness to target is found.

- **Concerning Integrated Design and Stochastic Optimization**

  - A single-stage stochastic approach allows capital and operating cost as well as quality cost to be accounted for at the design stage.

Acknowledgements

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- CONACyT
- Professors and staff in the department at OU

Thank you !!

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Questions ?