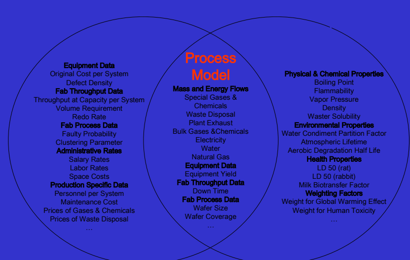
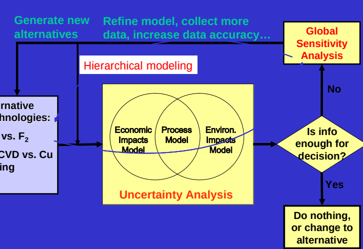
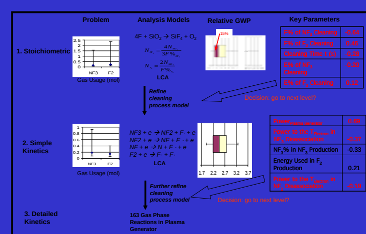
Integrating Environmental Considerations into Technology Selections Under Uncertainty

Y. Nina Chen (yuechen@alum.mit.edu)
Gregory J. McRae
Karen K. Gleason

MIT – Chemical Engineering







ERC Teleseminar 2004

Why are Technology Choices Complex?

Example: Choosing a chamber cleaning gas (NF_3 vs. F_2?)

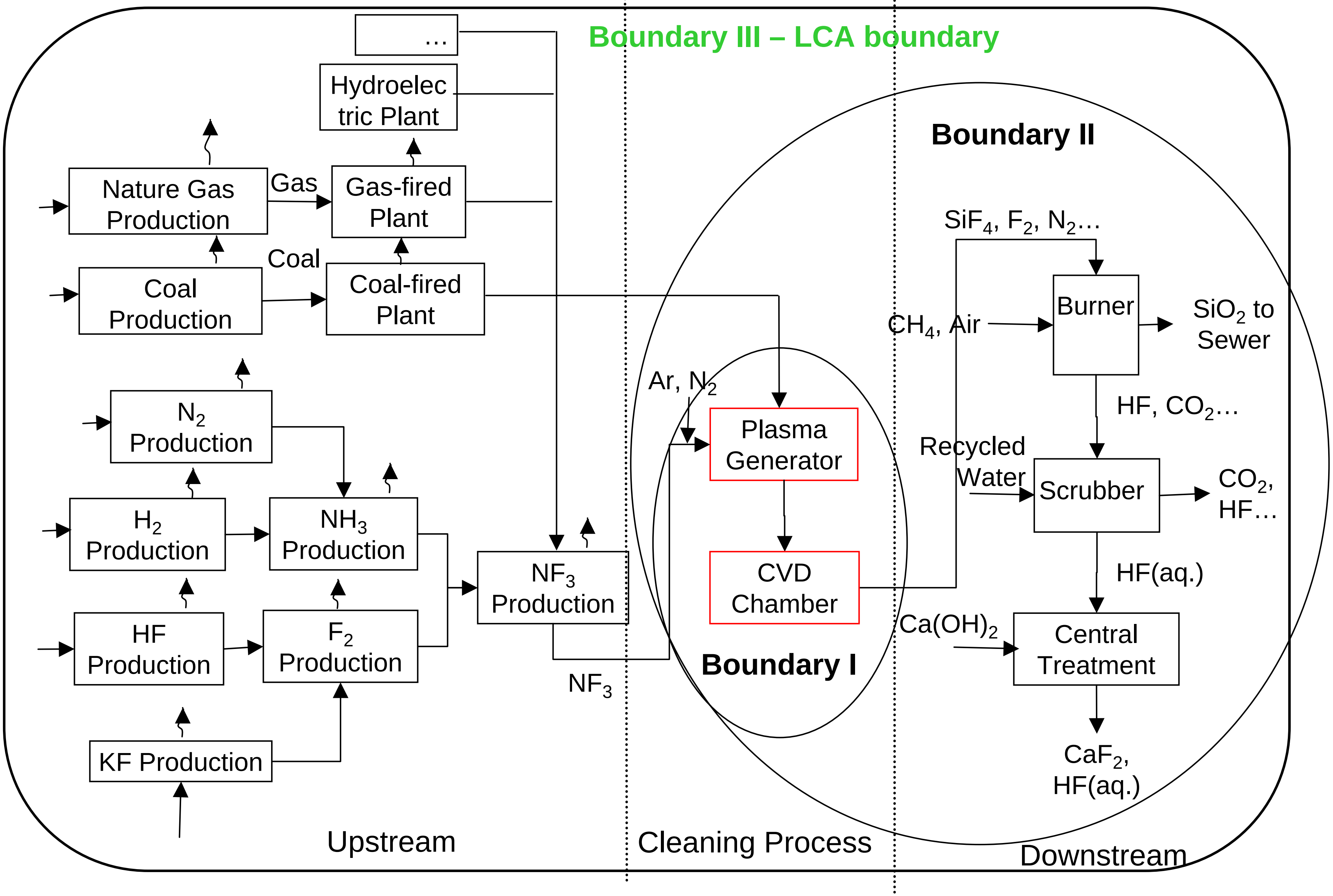
Decision Criteria	NF_3	F_2	Reference
Fluorine usage rate at the same etch rate (mole/min)	0.15	0.11	This work
Cost/mole of Fluorine	$2	$0.8	[1, 2]
LCA Global Warming Effect (kg CO_2 equivalent/kg)	3.3	2.4	This work
Toxicity LC_{50} (ppm)	6700	180	[3,4]
Safety	Inert gas	Very reactive	

The Problem: How to choose between technologies

- When there are conflicting decision criteria
- Many uncertainties

[1] MicroGenTM, 2003 [2] Raux, S.; 2004 [3] MSDS of NF_3, 2003 [4] MSDS of F_2, 2003

Boundary of Life Cycle Analysis (LCA)



Challenges Facing Integration of Life Cycle Analysis to Process Design

- Large amount of data are required
- Large uncertainties are imbedded in environmental evaluation

  Example: ~1 order of magnitude in air pollutant emission factors
  2 ~ 3 orders of magnitude in cancer toxicity indicators
  3 ~ 6 orders of magnitude in non-cancer toxicity indicators

- Limited time allowed for evaluations while regular LCA methods require large amount of time.
  - Typical innovation cycle of semiconductor industry: 2 years.
- Large disconnection in the tools used for ESH analysis and process / equipment design despite significant overlapping of information needed for both.

Overlapping Data Requirements

Economic Evaluations

Equipment Data
Original Cost per System
Defect Density
Fab Throughput Data
Throughput at Capacity per System
Volume Requirement
Redo Rate
Fab Process Data
Faulty Probability
Clustering Parameter
Administrative Rates
Salary Rates
Labor Rates
Space Costs
Production Specific Data
Personnel per System
Maintenance Cost
Prices of Gases & Chemicals
Prices of Waste Disposal
…

Process Model

Mass and Energy Flows
Special Gases & Chemicals
Waste Disposal
Plant Exhaust
Bulk Gases &Chemicals
Electricity
Water
Natural Gas
Equipment Data
Equipment Yield
Fab Throughput Data
Down Time
Fab Process Data
Wafer Size
Wafer Coverage
…

Environmental Evaluations

Physical & Chemical Properties
Boiling Point
Flammability
Vapor Pressure
Density
Waster Solubility
Environmental Properties
Water Condiment Partition Factor
Atmospheric Lifetime
Aerobic Degradation Half Life
Health Properties
LD 50 (rat)
LD 50 (rabbit)
Milk Biotransfer Factor
Weighting Factors
Weight for Global Warming Effect
Weight for Human Toxicity
…

There are many areas of overlap in data. We need tools that can connect them.

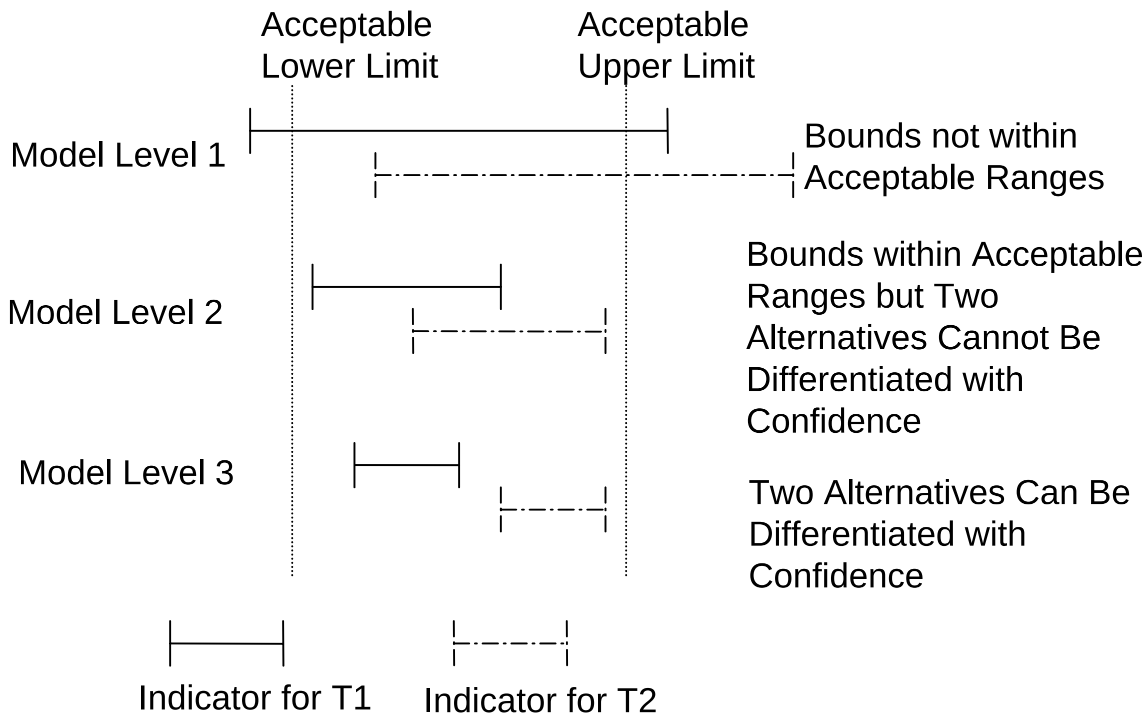
Key Message *– Outcomes are Important*

There are always uncertainties in technology evaluations, the real issue is to identify and act on those activities that influence outcomes.

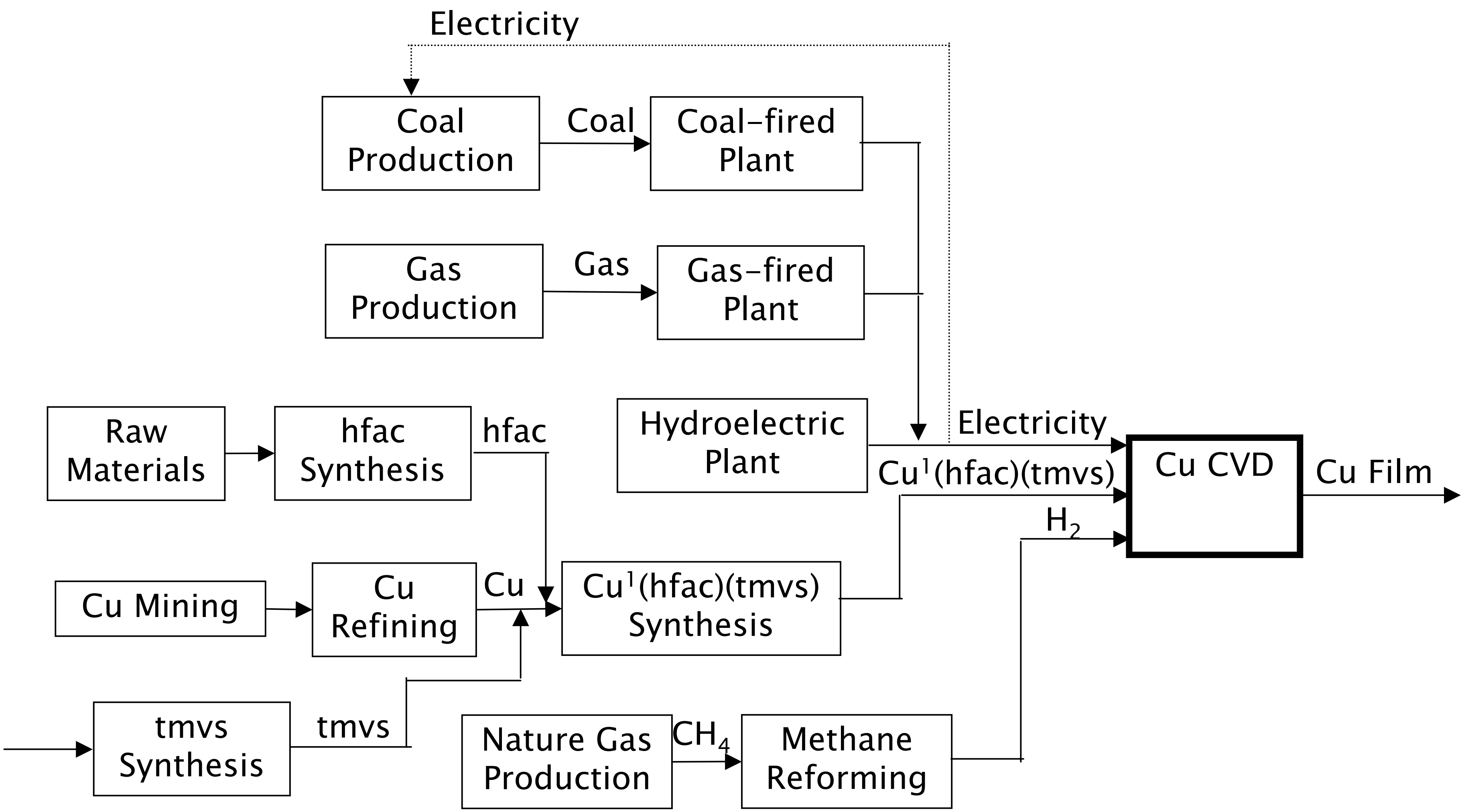
Essence of "Decision Problem"

- How can we capture (efficiently) the uncertainties in outcomes given uncertainties in inputs?
- How much information do we need in order to make a decision?
- Where should we allocate resources (modeling, experiments,...) to reduce risk in decision outcomes?

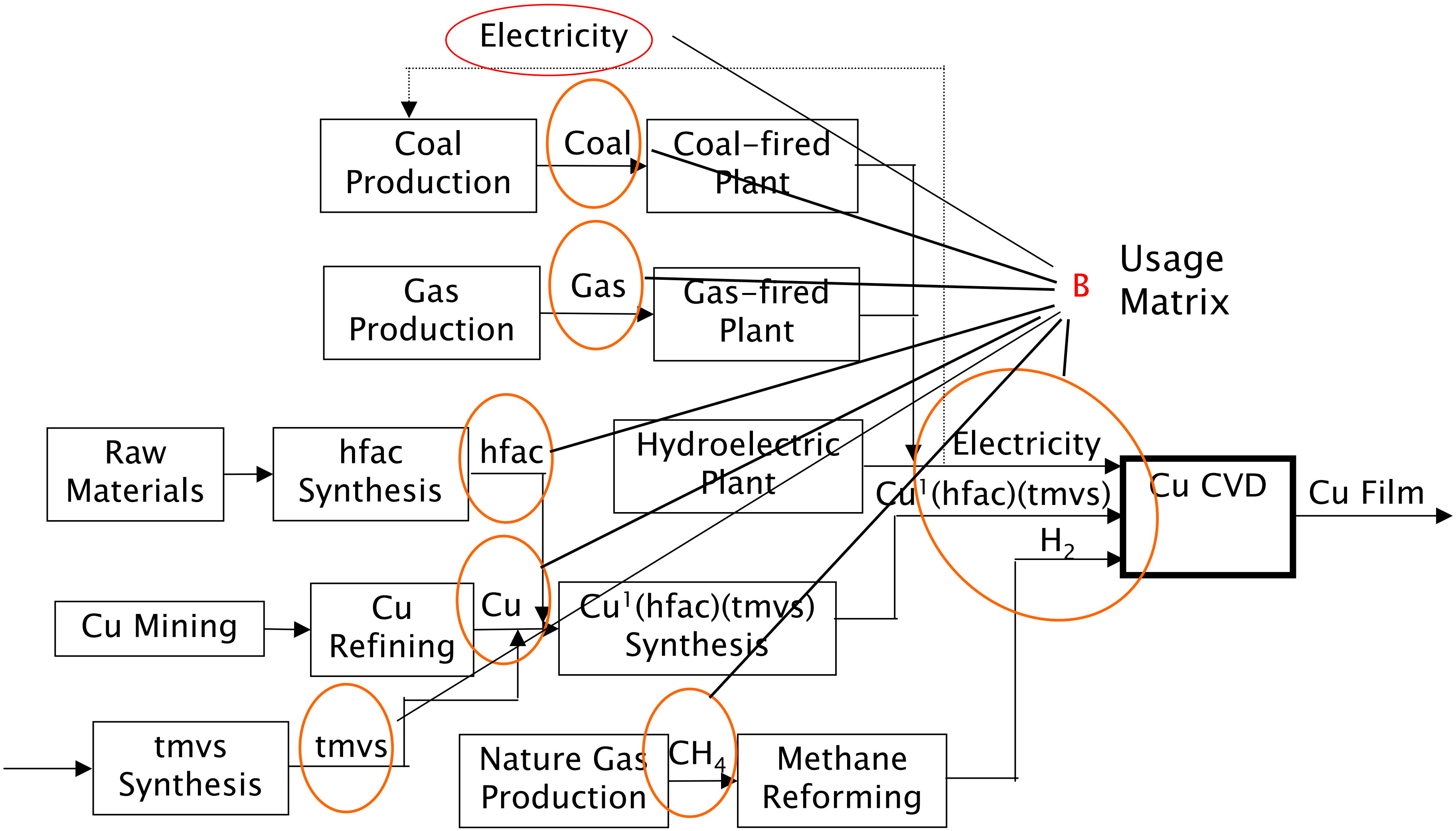
Hierarchical Modeling of Alternatives



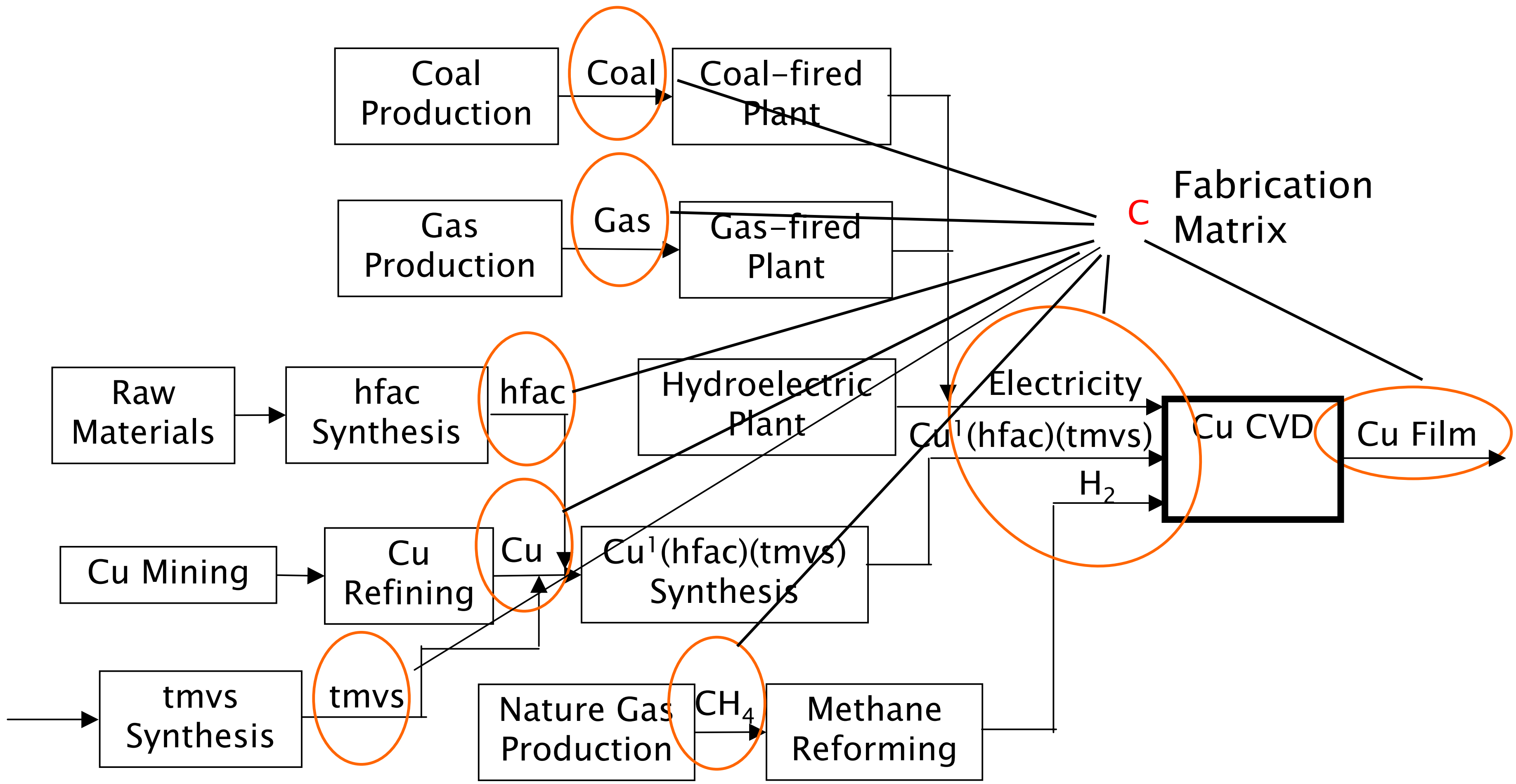
Process-Product Input Output LCA – an example



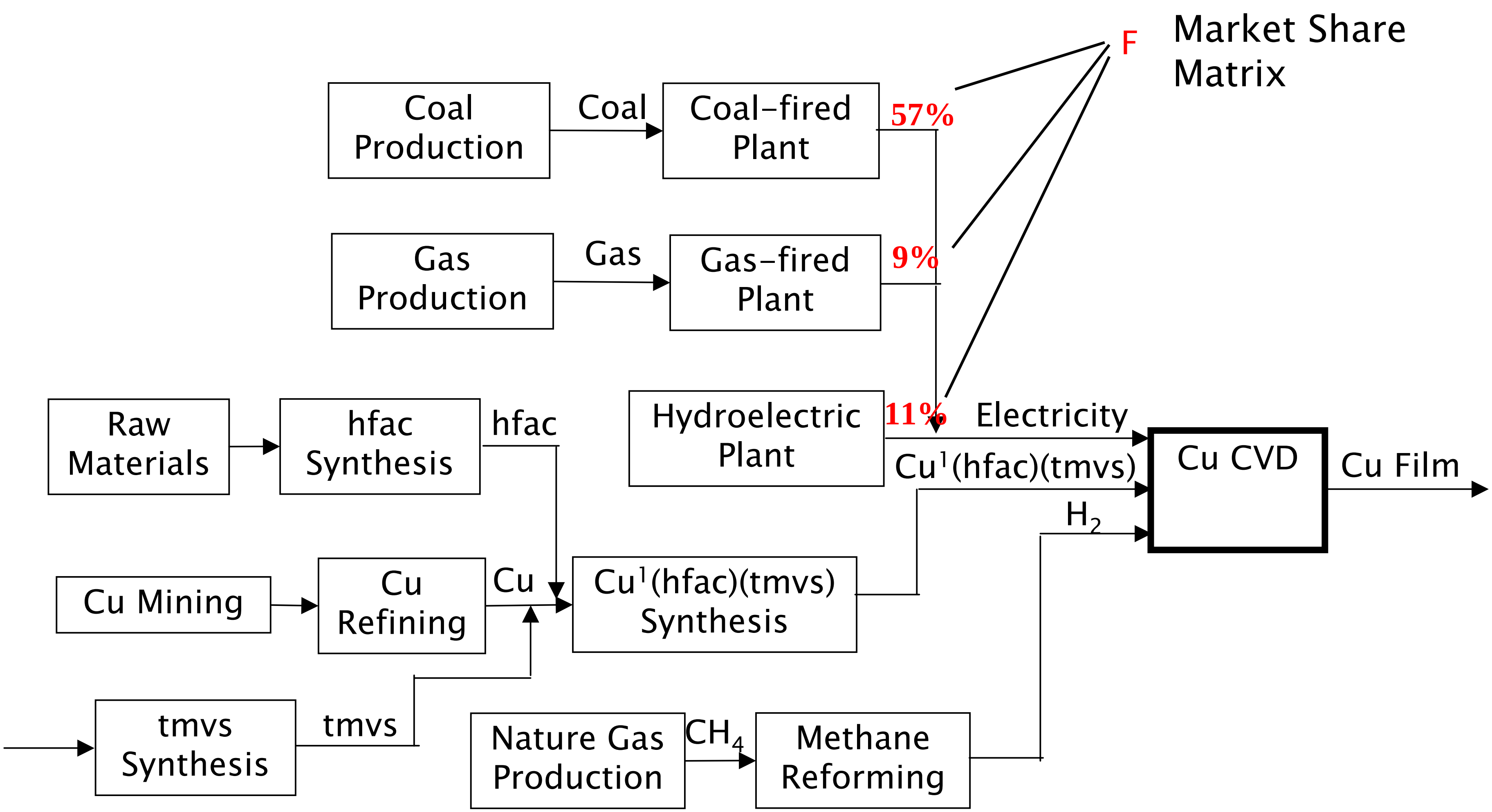
Model Input One: Usage Matrix (B)



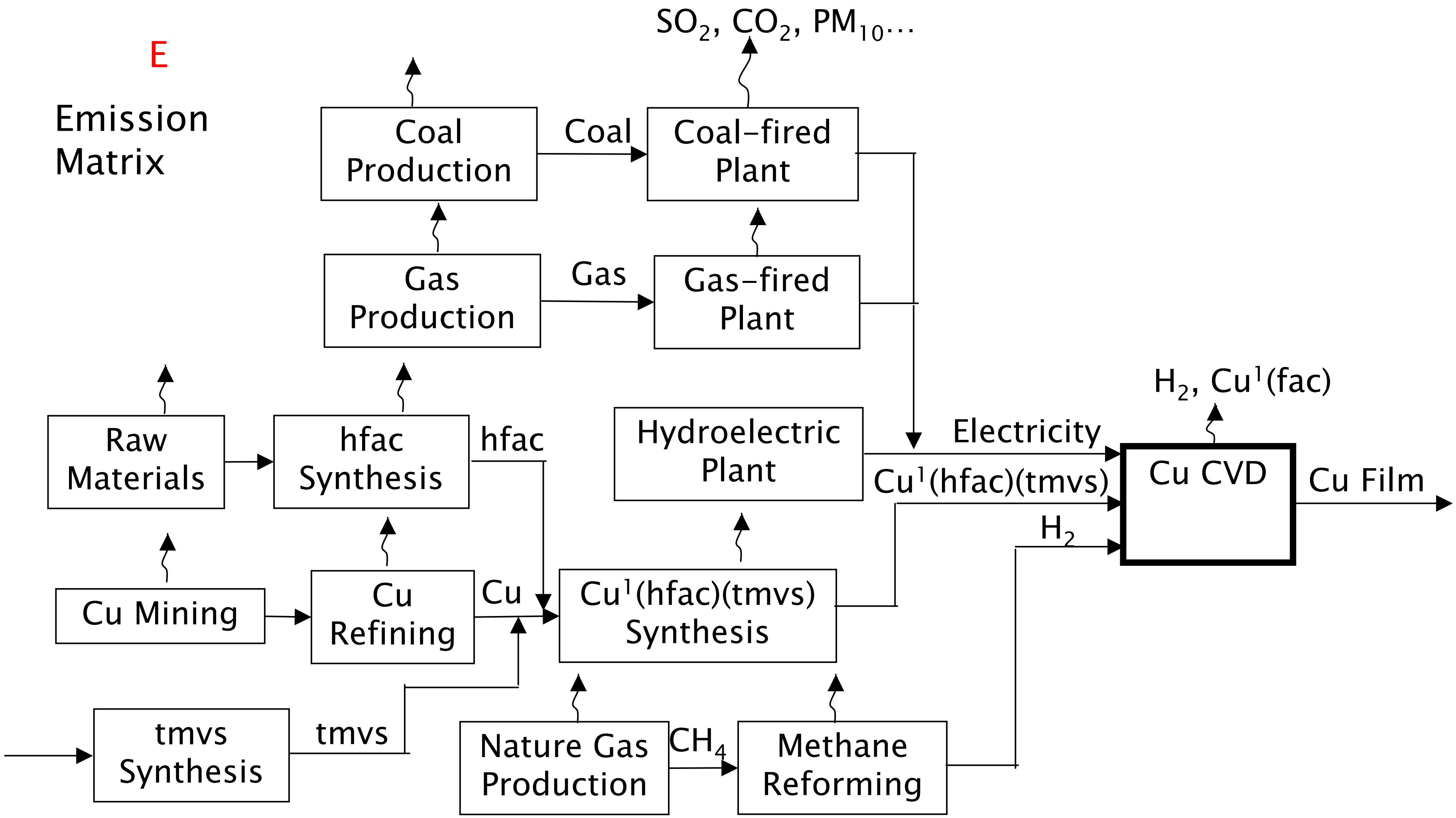
Model Input Two: Fabrication Matrix (C)



Model Input Three: Market Share Matrix (F)



Model Input Four: Emission Matrix (E)



Model Input Five: Characterization Matrix (H)

- Characterization matrix (H)

	Unit	GWP100 *kg CO2 equivalent/kg*	Respiratory Effect *kg PM10 equivalent/kg*	Human Toxicity Potential (non- cancer) *DALYs/kg*	. . .
CO_2	*kg*	1			
SO_2	*kg*	-23.3	0.15	4.21E-9	
PM_{10}	*kg*	-8.3	1		
⋮					
Valuation Factor w	*$*	3e-2	40	85000	

Based on willingness to pay

Mathematical Model

- Model Input Six: Price vector (p)
- Allocation matrix (G): for multiple product processes

$$G_{ji} = \begin{cases} \dfrac{p_i}{\sum_k C_{kj} p_k} & \forall C_{ij} \neq 0 \\ 0 & \forall C_{ij} = 0 \end{cases}$$

G_{ji}: the amount of throughput of process j that is attributed to one unit of product i made in process j

- Throughput matrix (D)

$$D_{ji} = F_{ji} G_{ji}$$

D_{ji}: the amount of throughput of process j that is attributed to the demand of one unit of product I at current price and market share

- Direct product requirement (q_{direct})

$$q_{direct} = (I + BD)d$$

- Total product requirements

$$q = (I + A_{prod} + A_{prod}A_{prod} + A_{prod}A_{prod}A_{prod} + \ldots)d = (I - A_{prod})^{-1}d$$

where $A_{prod} \equiv BD$

Mathematical Model

- Total process throughput requirements (x)

$$x = Dq$$

- Life cycle environmental exchanges inventory (e)

$$e = Ex$$

- Impact valuation by process ($\Omega_{process}$)

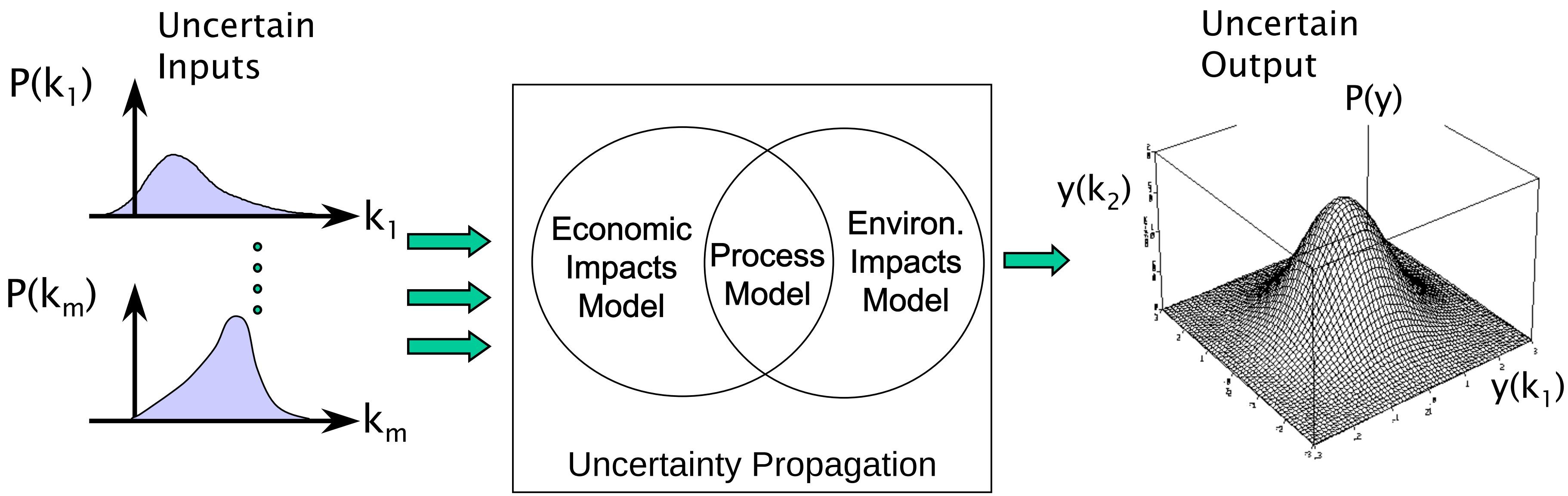
$$\Omega_{process} = \mathrm{Diag}(x)\, E^T\, H\, w$$

- Impact valuation by emission ($\Omega_{emission}$)

$$\Omega_{emission} = \mathrm{Diag}(e)\, H\, w$$

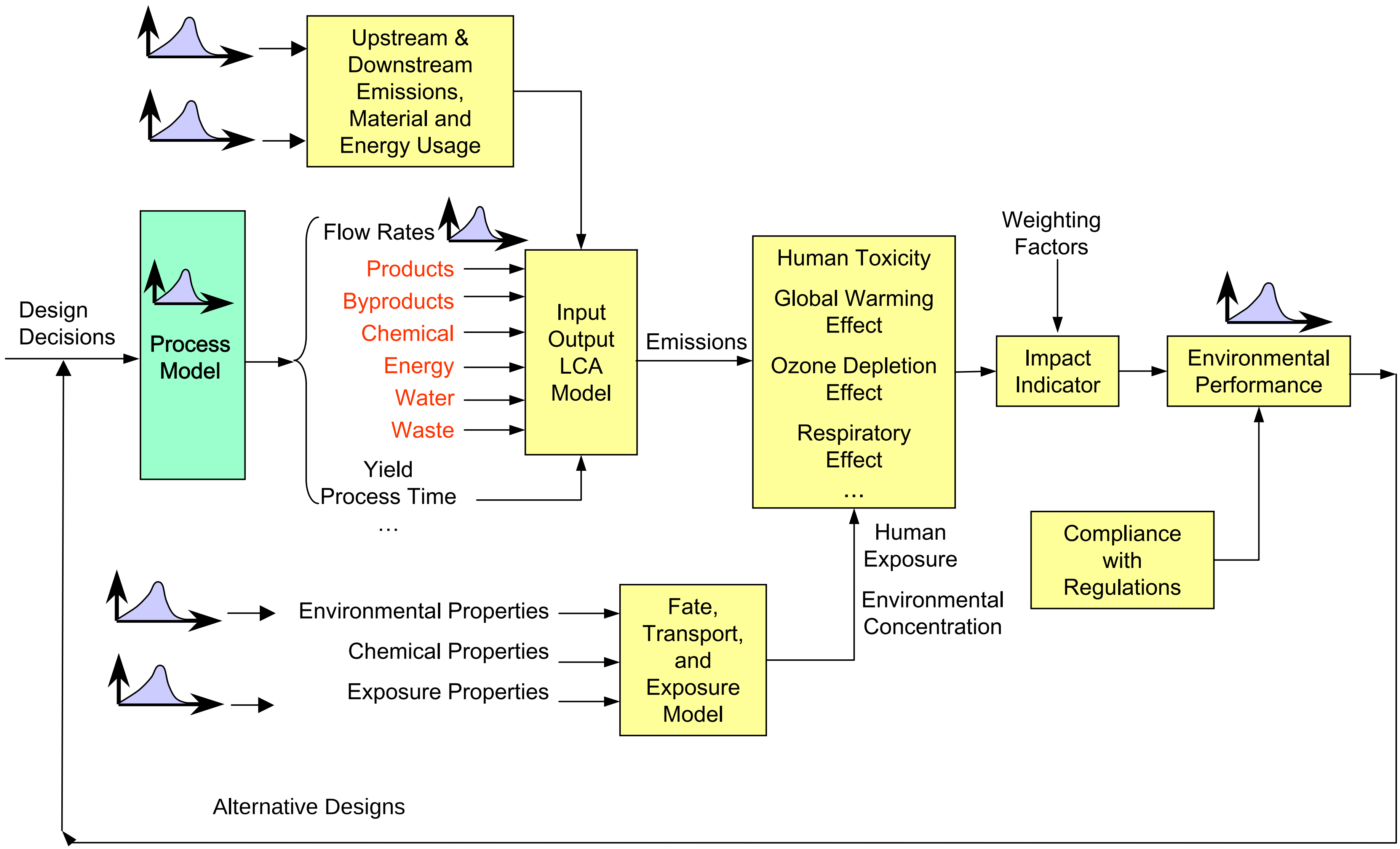
Large Uncertainties in Inputs?

Uncertainty Analysis!



Uncertainty Analysis: Propagating Uncertainty through System Model

Components of life cycle analysis



Which Parameters Drive Outcome?

- Goal: identify parameters that contribute most to uncertainty in outputs in highly non-linear systems with large variations.

- Sensitivity Analysis Methods:
  - Local Sensitivity Analysis
  - Analysis of Variance (ANOVA)
  - Linear Correlation Coefficients

    Assuming linearity
  - Rank Correlation Coefficients

    Assuming monotone
  - Fourier Amplitude Sensitivity Test (FAST)
  - Deterministic Equivalent Modeling Method (DEMM)
  - Sobol's Method

    Variance based, global

Linearity Based Methods

- Local sensitivity analysis
  - Function $Y = g\left(\underline{x}, \underline{\theta}\right)$ is sufficiently smooth near the point $\left(\eta_{\underline{\theta}}\right)$.

$$\sigma_y^2 = \sum_{i=1}^{p} \left(\left. \frac{\partial g}{\partial \theta_i} \right|_{\eta_{\underline{\theta}}} \right)^2 \sigma_{\theta_i}^2 + \sum_{i=1}^{p} \sum_{j=1,\, j \neq i}^{p} \left(\left. \frac{\partial g}{\partial \theta_i} \right|_{\eta_{\underline{\theta}}} \right) \left(\left. \frac{\partial g}{\partial \theta_j} \right|_{\eta_{\underline{\theta}}} \right) r_{ij} \sigma_{\theta_i} \sigma_{\theta_j}$$

Contribution to variance if no correlation

- ANOVA
  - Variance of the output is decomposed into partial variances of increasing dimensionality
  - Based on linear regression: System satisfies the Gauss-Markov Conditions → Outputs are normally distributed

$$Y_{i_1 i_2 i_3} - Y_g = \sum_{k=1}^{3} M_{i_k} + \sum_{k=1,3>j>k}^{3} M_{i_k i_j} + M_{i_1 i_2 i_3}$$

Averaged over three factors

Average of Y

Decomposed contribution of one factor, two factors, and three factors

Correlation Methods

- Linear Correlation Coefficients
  - Ratio of contribution to standard deviation to Y by θ_i alone and contribution of θ_i along with other θ_js.

$$\rho_{\theta,Y} = E\left[\left(\frac{\theta-\mu_\theta}{\sigma_\theta}\right)\left(\frac{\theta-\mu_Y}{\sigma_Y}\right)\right] \qquad \therefore \rho_{\theta_i,Y} = \frac{x_i\sigma_{\theta_i} + \sum_j x_j \frac{Cov(\theta_i,\theta_j)}{\sigma_{\theta_i}}}{\sigma_Y}$$

- Rank Correlation Coefficients
  - Rank-based rather than value based.
  - No assume of linearity, but monotone.

$$r_s = \frac{\sum_{i=1}^{n}\left(rank(x_i)-\frac{n+1}{2}\right)\left(rank(y_i)-\frac{n+1}{2}\right)}{\frac{n(n+1)(n-1)}{12}}$$

Variance Based Methods

- Similar to ANOVA, decompose variance into contributions by factors individually and collectively
  - No assumption of linearity or monotone
  - Model independent
  - Global
  - Example: One factor alone

$$\eta^2 = \frac{\mathrm{Var}_X \mathrm{E}[Y \mid X]}{\mathrm{Var}[Y]}$$

- Fourier Amplitude Sensitivity Test (FAST)
  - Using a single variable search curve is used to cover the multidimensional space of the input factors

Transformation of inputs

$$\theta_i = F_l(\sin \omega_i s), \quad l = 1, 2, \ldots, p$$

Transformation of output

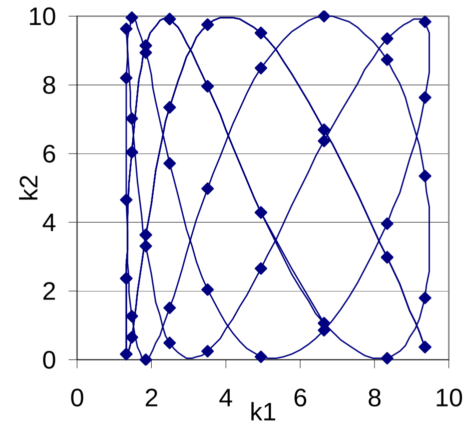
$$Y = \sum_{i=-\infty}^{\infty} \left[A_i(\underline{x}) \cos is + B_i(\underline{x}) \sin is \right].$$

Variance of Y

$$\sigma_Y^2 = 2\sum_{i=1}^{\infty} \left\{ A_i^2(\underline{x}) + B_i^2(\underline{x}) \right\}$$

Contribution of factor ω_i

$$\sigma_{\omega_l}^2 = 2\sum_{p=1}^{\infty} \left\{ A_{p\omega_l}^2(\underline{x}) + B_{p\omega_l}^2(\underline{x}) \right\}$$



Deterministic Equivalent Modeling Method

- Directly approximating distribution of Y by a polynomial expansion

Transformation of inputs $\underline{\theta} = \underline{\theta}\left(\left\{\xi_i(\omega)\right\}\right)$

Transformation of output $\hat{g}(\underline{\theta}) = \sum_{j=1}^{N} a_j Z_j\left(\left\{\xi_i(\omega)\right\}\right)$

Decomposition of Output

$$\hat{g}\left(\theta_1,\ldots,\theta_p\right) = g\left(\theta_1(\xi),\ldots,\theta_p(\xi)\right) = \underbrace{g_0 + \sum_{i=1}^{p} g_{i1} L_1(\xi_i)}_{\text{linear}} + \underbrace{\sum_{i=0}^{p} g_{i2} L_2(\xi_i)}_{\text{2nd order}} + \underbrace{\sum_{i=0}^{p}\sum_{j<i} g_{i1j1} L_1(\xi_i) L_1(\xi_j)}_{\text{bilinear}}$$

$$+ \underbrace{\sum_{i=0}^{p} g_{i3} L_3(\xi_i)}_{\text{3rd order}} + \underbrace{\sum_{i=0}^{p}\sum_{j=1}^{i-1} g_{i2j1} L_2(\xi_i) L_1(\xi_j)}_{\text{2nd order in } \xi_i,\ \text{1st in } \xi_j} + \underbrace{\sum_{i=0}^{p}\sum_{j=1}^{i-1} g_{i1j2} L_1(\xi_i) L_2(\xi_j)}_{\text{1st in } \xi_i,\ \text{2nd in } \xi_j}$$

$$+ \underbrace{\sum_{i=0}^{p-2}\sum_{j=i+1}^{p-1}\sum_{k=j+1}^{p} g_{i1j1k1} L_1(\xi_i) L_1(\xi_j) L_1(\xi_k)}_{\text{trilinear}} + \text{ higher order terms}$$

- Calculating coefficients by forcing error of expansion at collocation points to zero or minimizing error over whole space of inputs

Sobol's Method

- Integrating over other factors to obtain contribution of each factor

$$D_{i_1\cdots i_s}=\int_0^1\cdots\int_0^1 g^2_{i_1\cdots i_s}\left(\theta_{i_1}\cdots\theta_{i_s}\right)f_{\theta_{i_1}\cdots\theta_{i_s}}\left(\theta_{i_1}\cdots\theta_{i_s}\right)d\theta_{i_1}\cdots d\theta_{i_s}$$

Factor $\theta_{j\neq i1\ldots is}$ are fixed.

$$S_{i_1\ldots i_s}=\frac{D_{i_1\ldots i_s}}{D}$$

Global Sensitivity Indices (GSI)

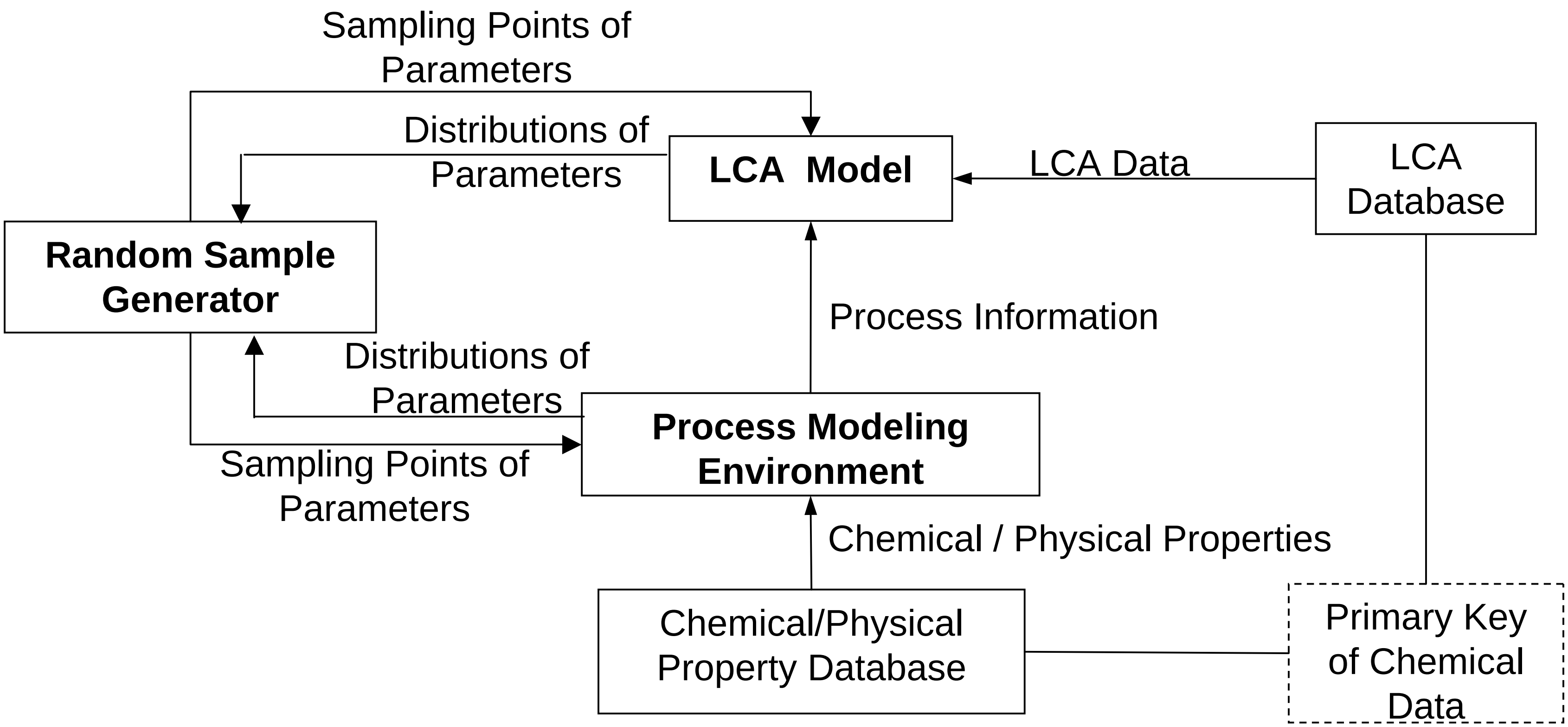
$$S_{Ti}\equiv S_i+S_{i,ci}=1-S_{ci}$$

- GSI – total effect of variable θ_j, including fraction of variance accounted for by θ_j alone and fraction accounted by any combination of θ_j with remaining factors

Comparison of Methods

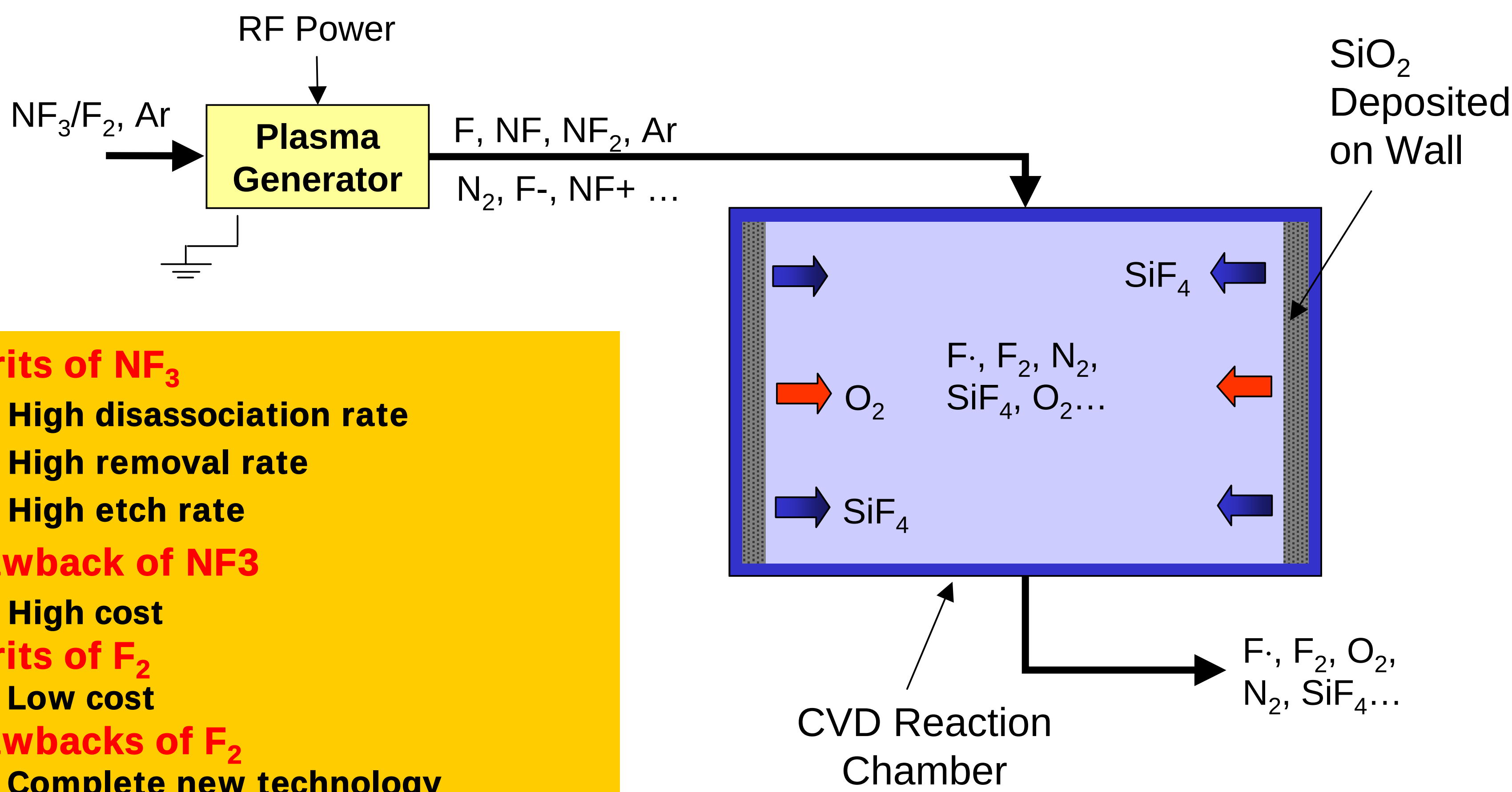
- Capturing global response with wide variation – variance based methods
- Easiness to implement -- correlation methods
- Suggestion: to use correlation methods as a starting point for many inputs, then to use variance based methods for detailed, quantitative analysis.

Integration of Software for LCA and Process Modelling



- Advantages of this integrated system:
  - Reduced cost and time for developing a process modelling environment that is compatible with LCA from scratch.
  - Allows uncertainty analysis on both the LCA models, economic models (not shown here), and process models.

Case Study: Clean Chamber with NF_3 or F_2?



- **Merits of NF_3**
  - **High disassociation rate**
  - **High removal rate**
  - **High etch rate**
- **Drawback of NF3**
  - **High cost**
- **Merits of F_2**
  - **Low cost**
- **Drawbacks of F_2**
  - **Complete new technology**
  - **High toxicity**
  - **High reactivity**
  - **On-site generation creates explosive H_2**

Compare Life cycle impacts for the same cleaning performance

Modeling of Chamber Cleaning Processes

Driving forces of LCA impacts: Cleaning gas usages

Energy consumptions

Cleaning Gases $$N_{NF_3} = \frac{4N_{SiO_2}}{3F\%_{NF_3}}, \quad N_{F_2} = \frac{2N_{SiO_2}}{F\%_{F_2}}$$

Energy $$E_{NF_3} = \frac{N_{SiO_2}E_{b\_NF_3}}{F\%_{NF_3}\xi_{E\_NF_3}} + tP_{plasma}, \quad E_{F_2} = \frac{N_{SiO_2}E_{b\_F_2}}{F\%_{F_2}\xi_{E\_NF_3}} + tP_{plasma}$$

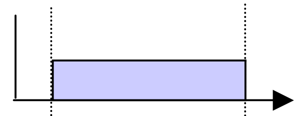
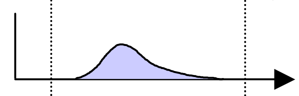
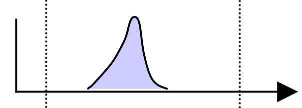
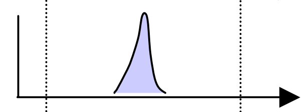
where for NF_3 cleaning $$F\%_{NF_3} = \left(4 \cdot N_{SiF_4} + N_{HF}\right)/\left(3 \cdot N_{NF_3}\right) \cdot 100\ \%$$

for F_2 cleaning $$F\%_{F_2} = \left(4 \cdot N_{SiF_4} + N_{HF}\right)/\left(2 \cdot N_{F_2}\right) \cdot 100\ \%$$

- Little process specific information is known for fluorine yield F%, energy yield ξ_E, and cleaning time t.

What to do 

Process Modeling Hierarchy and Resource Needs

	Process Model Hierarchy	Distributions of Yield	Resources Needed
1	Simple stoichiometric yield		1
2	Lumped kinetics (3 reactions)		10
3	Detailed kinetics (60 reactions)		100
4	Model based experiments		1000

Distributions Used in Process and LCA

- Fluorine Utilization Yield

  F% ~ uniform(10^{-5}, 0.6)
- Energy Utilization Yield

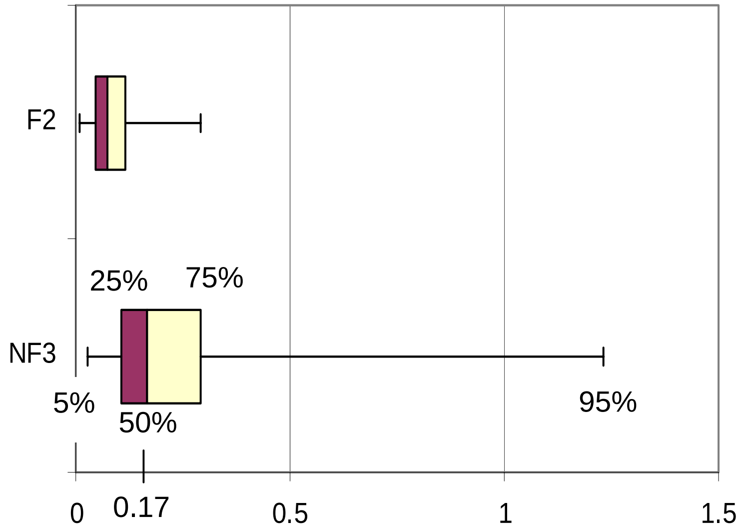
  ξ_E ~ uniform(10^{-10}, 0.6)
- Cleaning Time

  t(s) ~ uniform(6E^{-4}, 1200)

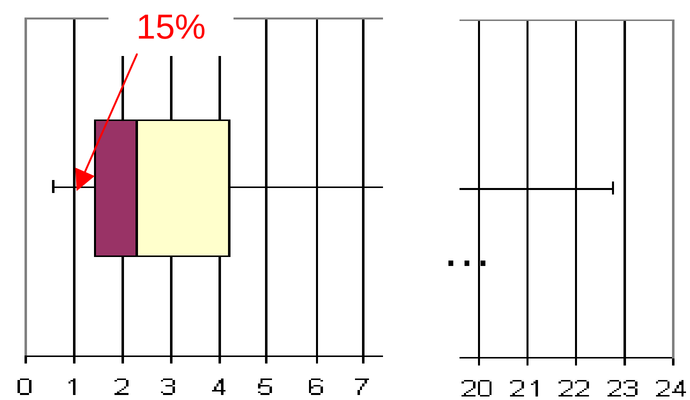
- Examples of distributions of other variables
  - Environmental impact characterization factors:
    Lognormal, normal
  - Upstream resources consumption factors
    Lognormal, normal, triangular

Environmental Impacts from LCA

- Comparison of the global warming potentials (GWP) of the two processes



GWP of Cleaning Processes (kg CO_2 equivalent)



Relative Ratio of GWP of NF3 and F2 Cleaning Processes

We can be 85% sure that the F_2 cleaning has lower a global warming impact than the NF_3 cleaning.

Do we still need a more detailed model?

Important Parameters of Affecting Relative GWP

Parameter	Spearman Rank Correlation Coefficient
Fluorine Yield of NF_3 Cleaning	-0.64
Fluorine Yield of F_2 Cleaning	0.46
Cleaning Time t (s)	-0.28
Energy Yield of NF_3 Cleaning	-0.20
Energy Yield of F_2 Cleaning	0.12
NF_3 Yield in NF_3 Production from NH_3 and HF	-0.11
H_2S Emission from Oil-Fired Power Plant (kg/ kW-h Energy)	-0.083
Electricity Used in Diesel Fuel Production (MJ/kg)	0.078
GWP of $C_2H_3Cl_3$ (kg CO_2 equivalent/kg)	0.067
GWP of CH_2Cl_2 (kg CO_2 equivalent/kg)	0.061

If we need more precise results,
process model need to be refined!

Hierarchical Modeling – 2nd Process Modeling Level

- Lumped kinetics and Perfectly Stirred Tank Reactor model
- Key assumptions
  - Free electrons are generated mainly by ionization $Ar+e \rightarrow Ar^{+}+2e$
  - Electron loss and production are linear to electron concentration
  - Diffusion of electrons dominates the transport of electrons.

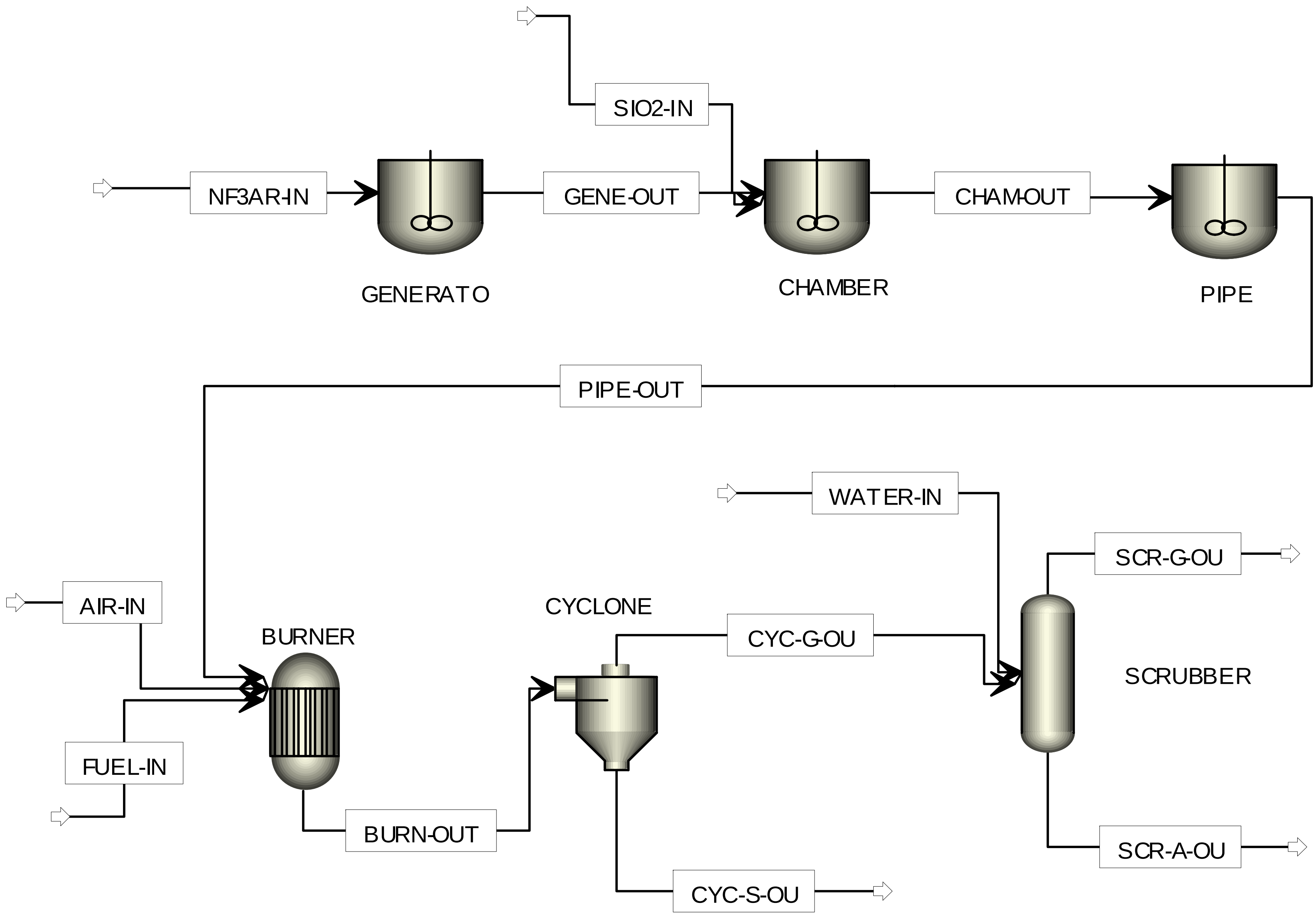
$NF_3 + e \rightarrow NF_2 + F\cdot + e$	$k_3=2.06E^{-17}\, T_e^{1.7}\exp(-37274/T_e)$
$NF_2 + e \rightarrow NF + F\cdot + e$	$k_2=1.57E^{-17}\, T_e^{1.8}\exp(-27565/T_e)$
$NF + e \rightarrow N + F\cdot + e$	$k_1=1.57E^{-17}T_e^{1.8}\exp(-27565/T_e)$
$F_2 + e \rightarrow F^- + F\cdot$	$k=1.02E^{-5}T_e^{-0.9}\exp(1081.8/T_e)$
$4F\cdot + SiO_2 \rightarrow SiF_4 + O_2$	$r=\left(8.97\pm 0.82\right)\times 10^{-13} n_F T_s^{1/2}\exp\left(-\frac{0.163\,eV}{kT_s}\right)$

$$n_{F,NF_3} = \frac{\beta_3 \tau n_{NF_3,in}}{1+\beta_3\tau} + \frac{\beta_2\beta_3\tau^2 n_{NF_3,in}}{(1+\beta_2\tau)(1+\beta_3\tau)} + \frac{\beta_1\beta_2\beta_3\tau^3 n_{NF_3,in}}{(1+\beta_1\tau)(1+\beta_2\tau)(1+\beta_3\tau)}$$

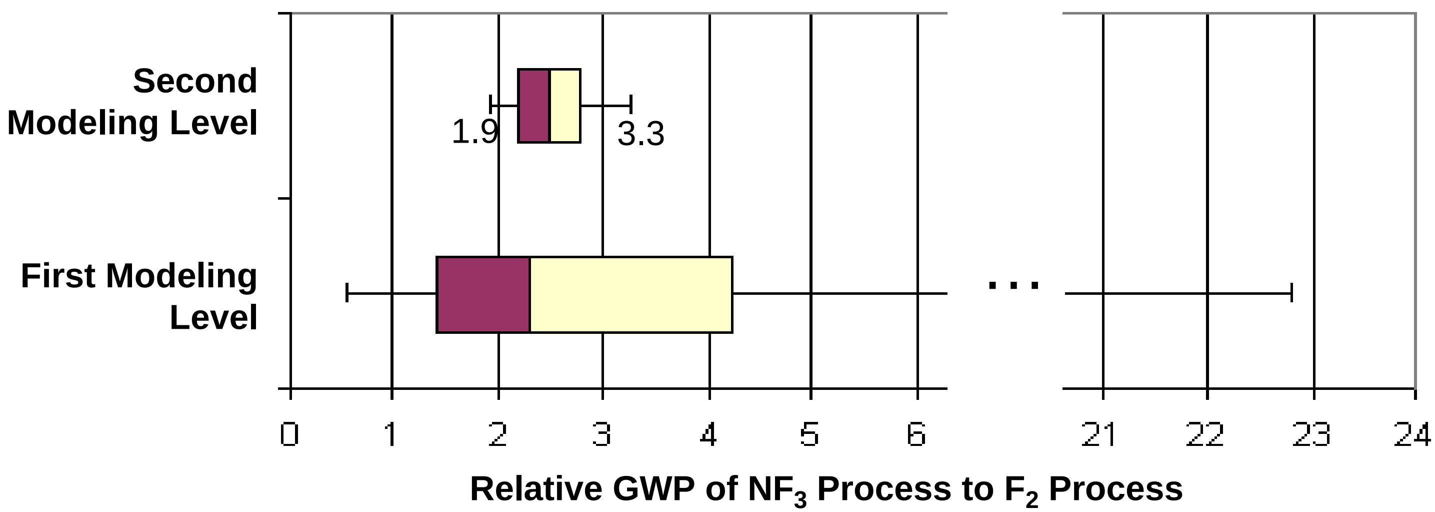
$$n_{F,F_2} = \frac{\beta_{F_2}\tau n_{F_2,in}}{1+\beta_{F_2}\tau}$$

$$\beta_i \equiv k_i n_e$$

Aspen Plus Flow Sheet with Downstream Treatment



Relative Impact of GWP at 2nd Process Modeling Level

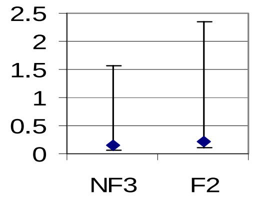


- 2~3 orders of magnitude of uncertainties in inputs does not necessarily leads to low confidence in decision
- Increase of modeling detail decreases the uncertainty of the outputs
- **But the decision is still the same – F_2 is better!**
- **Required confidence level should determine depth of analysis**

Hierarchical Modeling Can Save Time and Money

Problem	Analysis Models	Relative GWP	Key Parameters

1. Stoichiometric



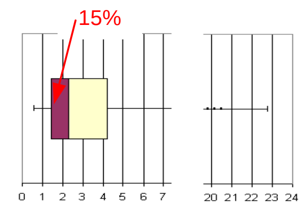
Gas Usage (mol)

$4F + SiO_2 \rightarrow SiF_4 + O_2$

$$N_{NF_3} = \frac{4N_{SiO_2}}{3F\%_{NF_3}}$$

$$N_{F_2} = \frac{2N_{SiO_2}}{F\%_{F_2}}$$

LCA

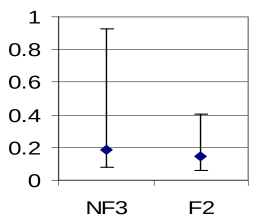


F% of NF_3 Cleaning	-0.64
F% of F_2 Cleaning	0.46
Cleaning Time t (s)	-0.28
E% of NF_3 Cleaning	-0.20
E% of F_2 Cleaning	0.12

Decision: go to next level?

Refine cleaning process model

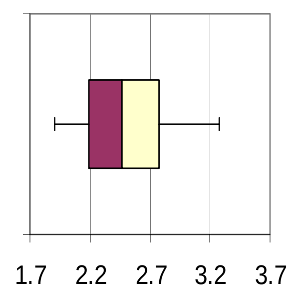
2. Simple Kinetics



Gas Usage (mol)

NF3 + e → NF2 + F· + e
NF2 + e → NF + F · + e
NF + e → N + F · + e
F2 + e → F- + F·

LCA



$Power_{Plasma\ Generator}$	0.69
Power to the $T_{Electron}$ in NF_3 Disassociation	-0.37
NF_3% in NF_3 Production	-0.33
Energy Used in F_2 Production	0.21
Power to the $T_{Electron}$ in NF_2 Disassociation	-0.19

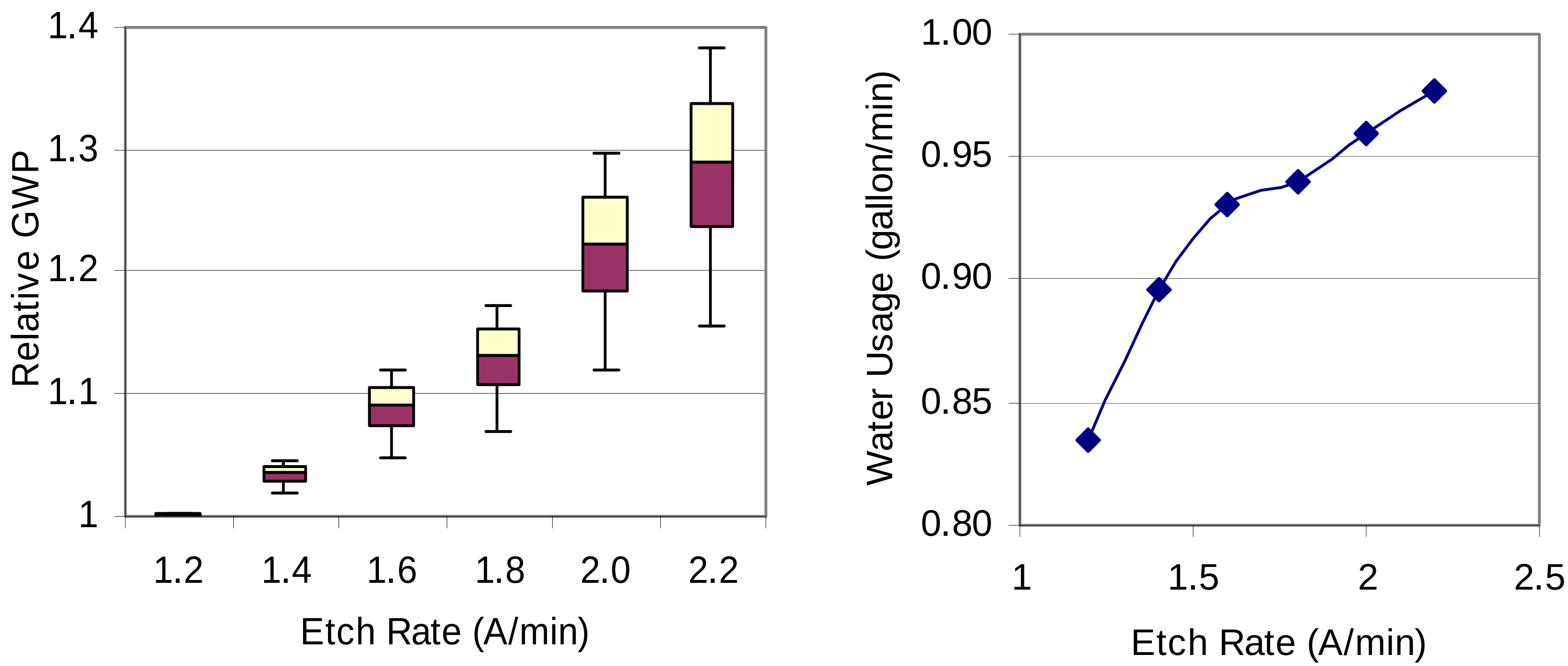
Decision: go to next level?

Further refine cleaning process model

3. Detailed Kinetics

163 Gas Phase Reactions in Plasma Generator

Integrated System Support Process Design



- Integrated system can also be used for studying how process design influences environmental impacts, downstream treatment design, and etc.

Conclusions

- Large uncertainty in the inputs does not necessarily lead to low confidence in decisions.
- Hierarchical modeling in combination with uncertainty analysis are efficient ways to support the decision making and resource allocation process.
- Integrated evaluation system facilitates the integration of environmental, economical, and technical evaluations.

UNCERTAINTY ≠ IGNORANCE

Acknowledgement

- Laura Losey, David Bouldin, Mike Kasner, Tim Yeakley, and Tina Gilliland **– Texas Instruments**
- Larry Novak **– Novak Consulting, LLC**
- Alejandro Cano-Ruiz and Pauline Ho **– Reaction Design**
- Daren Dance **– WWK**
- Joe Van Gompel **– BOC Edwards**
- Holly Ho **– TSMC, Taiwan**
- ERC – **Funding**