Technology Choices in the Presence of Uncertainties

An Update on the Economic and Environmental Issues Influencing the Choice of NF_3 vs. F_2 as a Chamber Cleaning Gas

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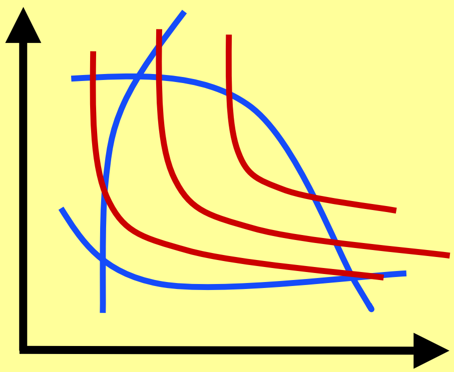
Some on Perspectives Business Optimization



$$\min \quad f(x,\theta)$$
$$s.t. \quad g(x,\theta) = 0$$
$$h(x,\theta) \leq 0$$

Conventional

Minimize the cost subject to meeting technical and environmental regulations

Better (but rarer) Formulation

Maximize profit subject to meeting technical and environmental constraints

Even Better Formulation

Maximize corporate performance

What are the implications of viewing environment, safety,… as objectives rather than as constraints on operations?

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	0.17	This work
Cost/mole of Fluorine	\$6	\$0.8	[1]
LCA Global Warming Effect (kg CO_2 equivalent/kg)	3.3	2.4	This work
Toxicity LC_{50} (ppm)	6700	180	[2,3]

The Problem: How to choose between technologies

- When there are conflicting decision criteria
- Many uncertainties

The Essence of the "Decision Problem"

1. How do we value alternatives? (cost, profit, first-to-market,…)
2. How much information do we need in order to get the sign right?
3. Where to allocate resources (modeling, experiments,…) to reduce risk in decision outcomes?

Key Message

ESH – Environment, Safety and Health

COO – Cost of Ownership

They must be seamlessly integrated for effective decision making

Overlapping Data Requirements

Cost of Ownership

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

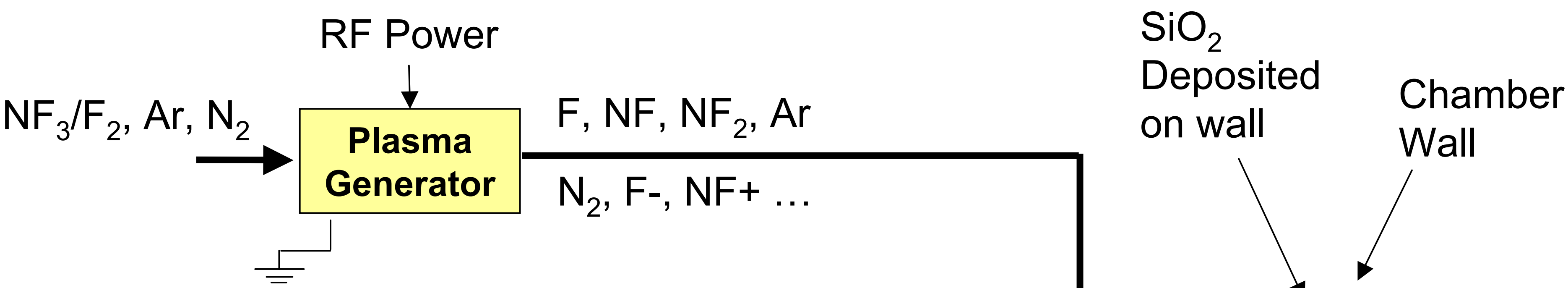
Mass and Energy Flows
Special Gases & Chemicals
Waste Disposal
Plant Exhaust
Bulk Gases &Chemicals
Electricity
Water
Natural Gas
Equipment Data
Equipment Yield
Fab Throughput Data
Down Time
Fab Process Data
Wafer Size
Wafer Coverage

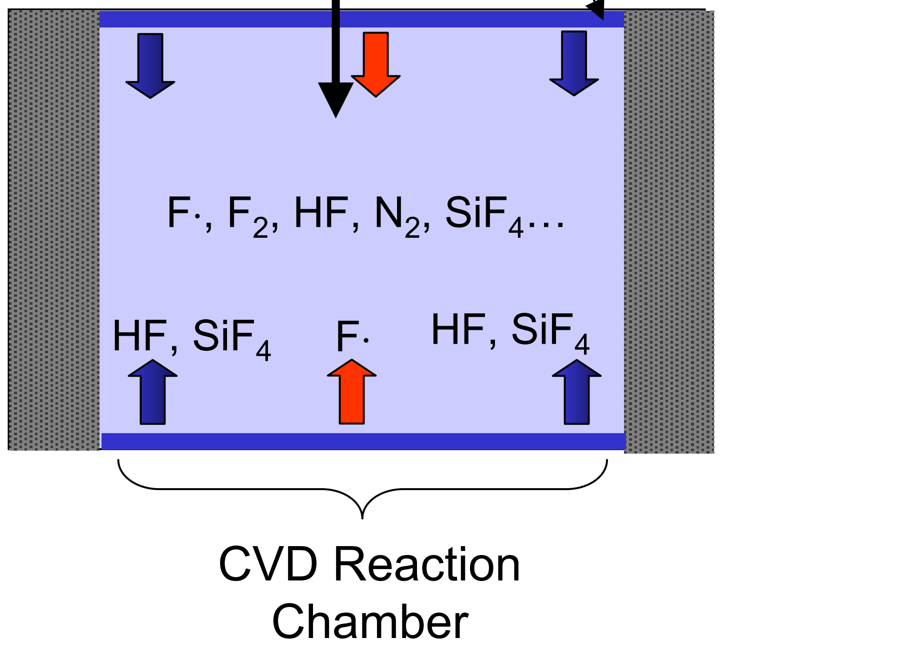
Environmental Evaluation

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

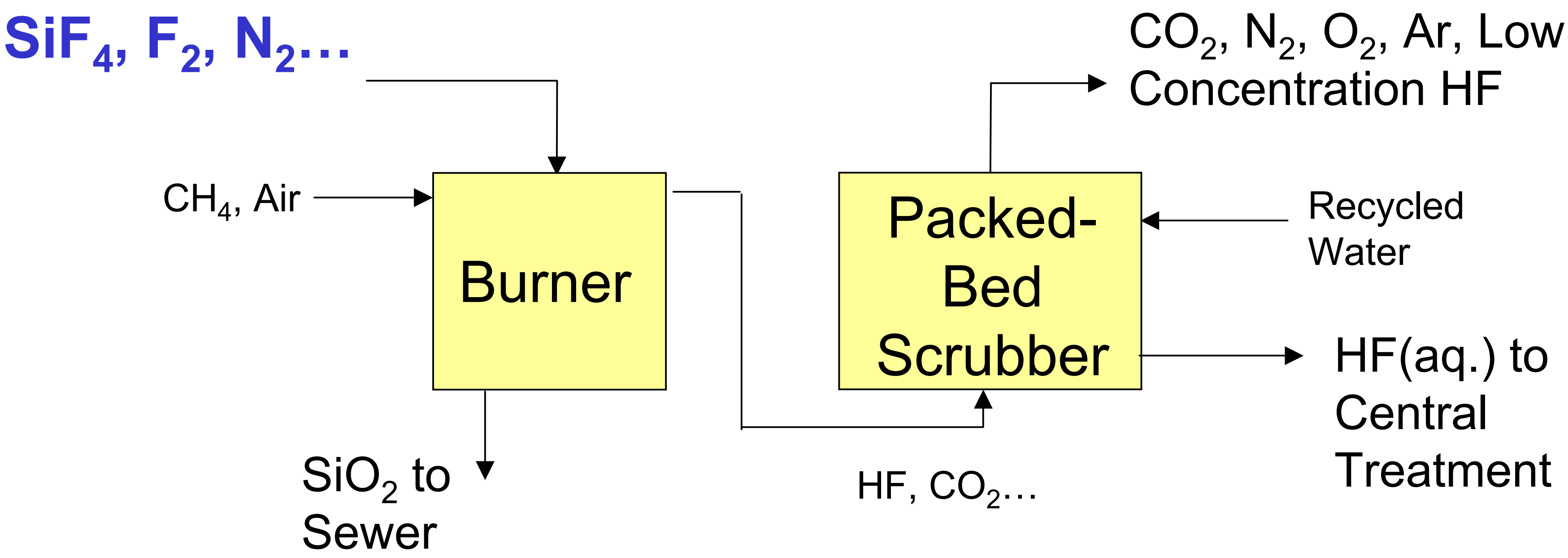
Chamber Cleaning with NF_3/F_2





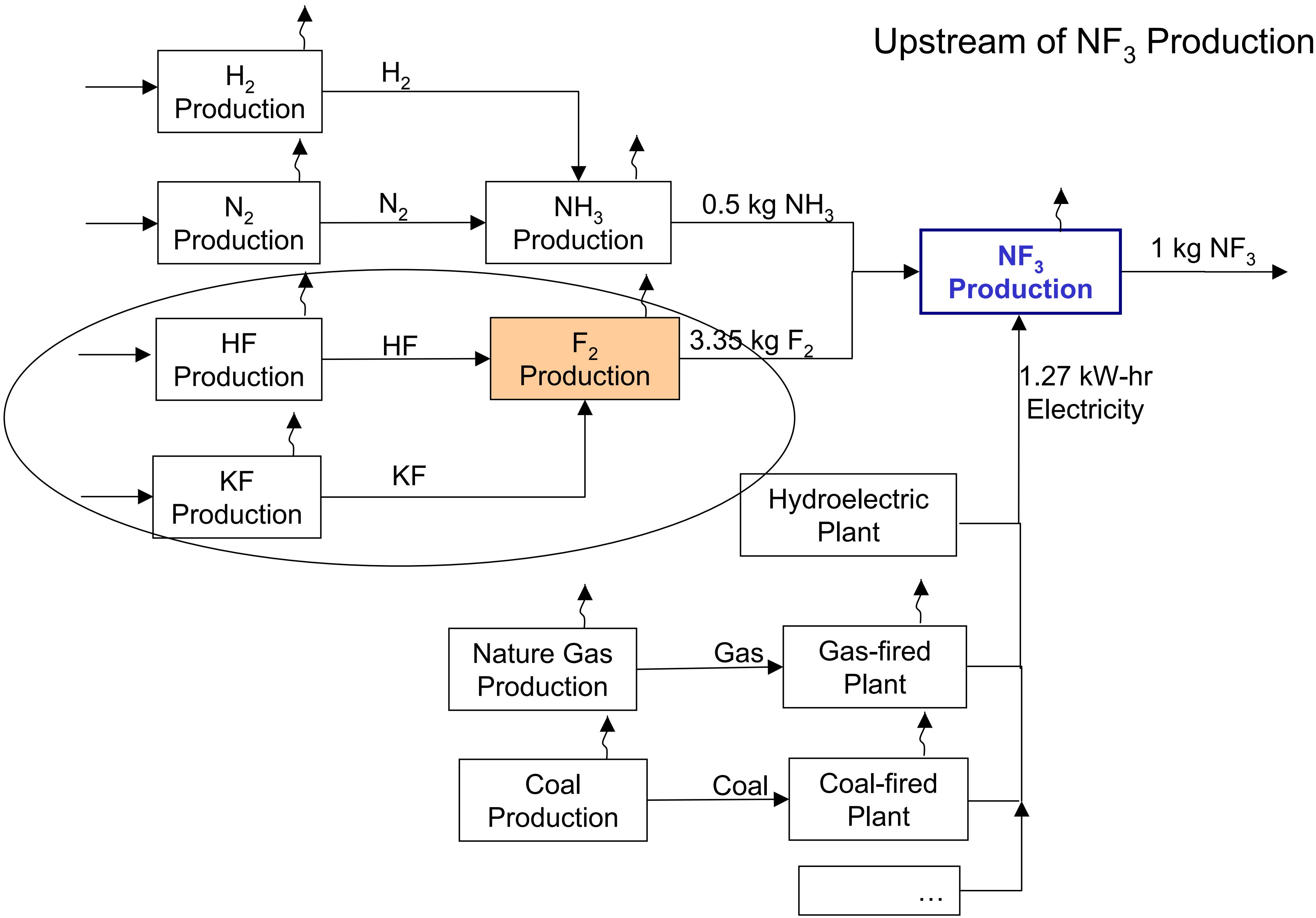
- Merits of NF3
  - High disassociation rate
  - High removal rate
  - High etch rate
- Drawback of NF3
  - High cost
- Merits of F_2
  - Low cost
- Drawbacks of F_2
  - High toxicity
  - High reactivity
  - POU generation creates explosive H_2
- **Comparison criteria: cleaning performance, environmental impacts, cost**

Including Downstream Treatment



- Fuel Usage – Similar
- Water Usage – 548 gallon/yr for NF_3, 566 gallon/yr for F_2
  – Insignificant compared to 1 million gallon/day

Including Upstream Processes

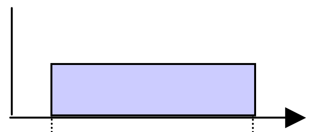
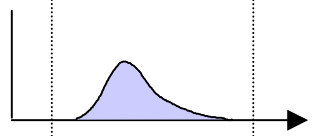
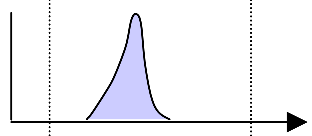
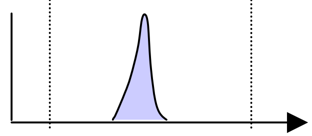


The Essence of the "Decision Problem"

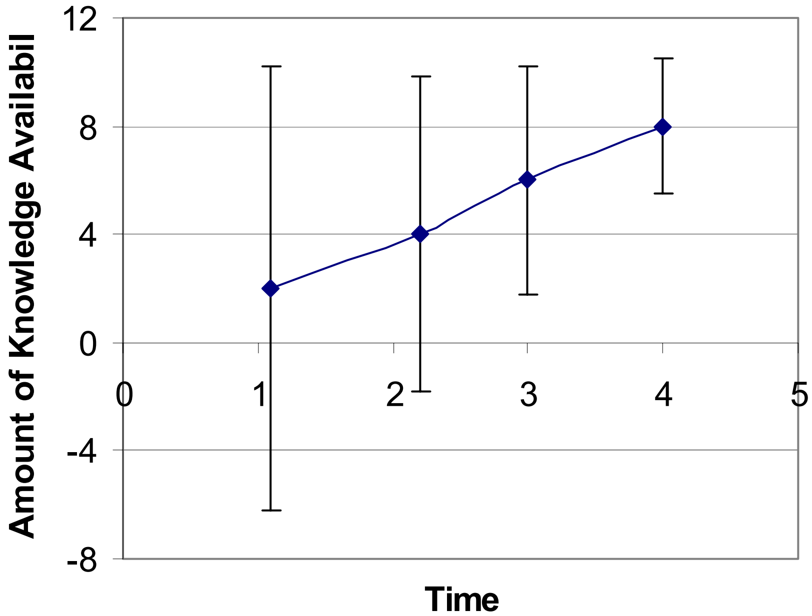
1. How much information do we need to know in order to get the sign right?

2. How do we decide where to allocate resources for more analyses, experiments and/or better data?

Process Modeling Hierarchy and Resource Needs

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

Knowledge Availability along Design Process

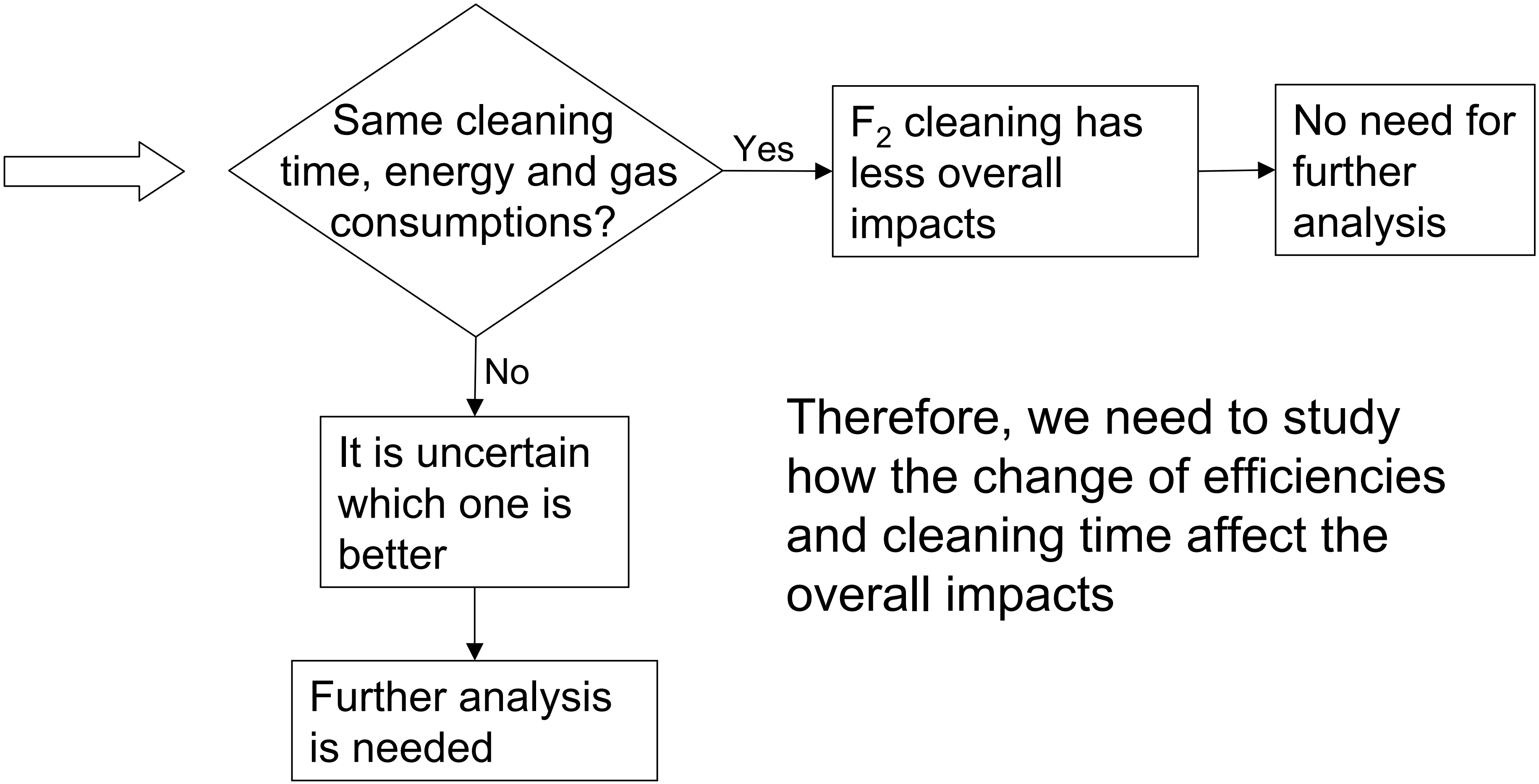


- At the early design stage, little information is available.
- There is large uncertainty associated with available knowledge.
- Time and resources are limited for the designer.

- **Where should time and resources be allocated for the data collection effort?**

Start Comparison with Little Information

- With little information of the process, direct comparison of the criteria is impossible.
- Currently available knowledge: $2NH_3 + 3F_2 \rightarrow 2NF_3 + 3H_2$



Therefore, we need to study how the change of efficiencies and cleaning time affect the overall impacts

Hierarchical Modeling – First Process Modeling Level

Starting from estimations of cleaning gases and 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

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

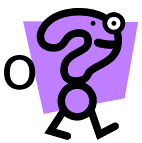
where for NF_3 cleaning

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

for F_2 cleaning

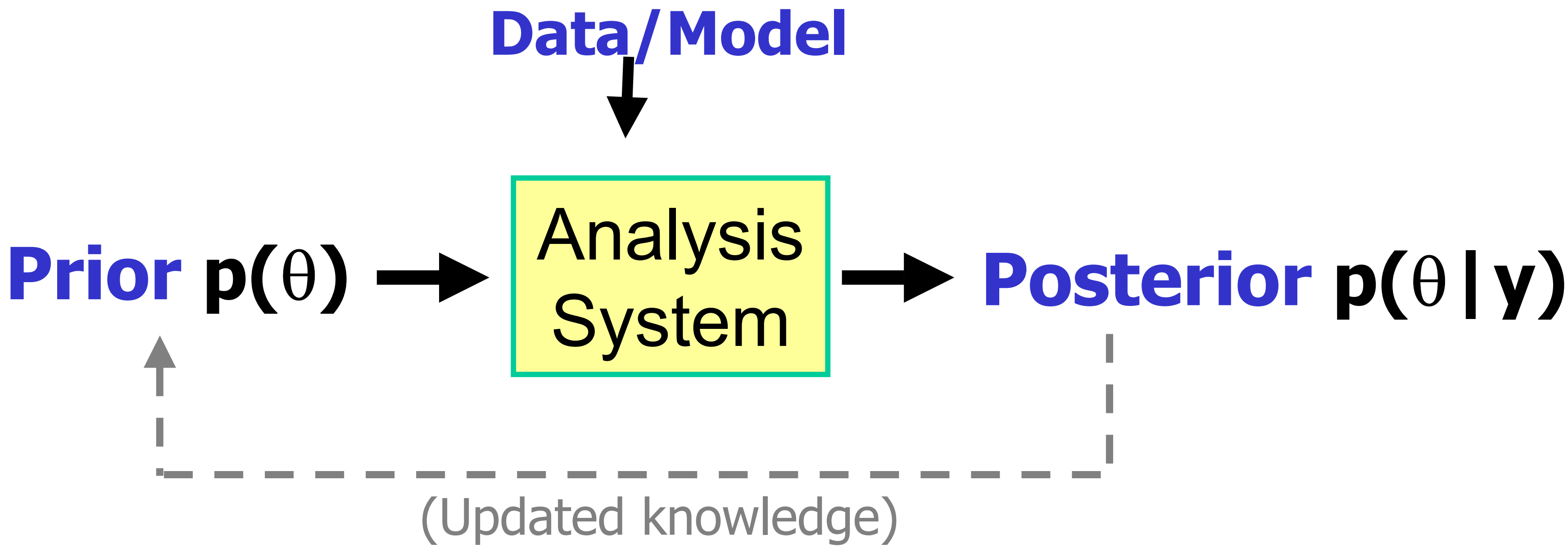
$$F\%_{F_2} = \left(4 \cdot N_{SiF_4} + N_{HF}\right) / \left(2 \cdot N_{F_2}\right) \cdot 100\%$$

- Little process specific information is known for F%, ξ_E, and t

What to do 

Use probability distribution functions to describe them 

Bayes Theorem – *Learning from Data/Models*



T. Bayes (1702-1761)

$$p(\theta \mid y) = \frac{p(y \mid \theta)\, p(\theta)}{p(y)}$$

Advantages of a Bayesian Approach

1. Can use prior knowledge and physical constraints in the analysis
2. Provides a formal framework for combining measurements of different quality
3. Gives the pdf's of the solution
4. New algorithms (MCMC) can solve non-linear problems
5. Broad applications including decision analysis

… <u>Both</u> Bayesian and Frequentist views are useful in practice

Assumed Distributions of Efficiencies and Time

- Fluorine Utilization Efficiency
  - F% ~ uniform(10^{-5}, 0.6)

$$f(F\%) = \frac{1}{0.6 - 10^{-5}}$$

- Energy Utilization Efficiency
  - ξ_E ~ uniform(10^{-10}, 0.6)

$$f(\xi_E) = \frac{1}{0.6 - 10^{-10}}$$

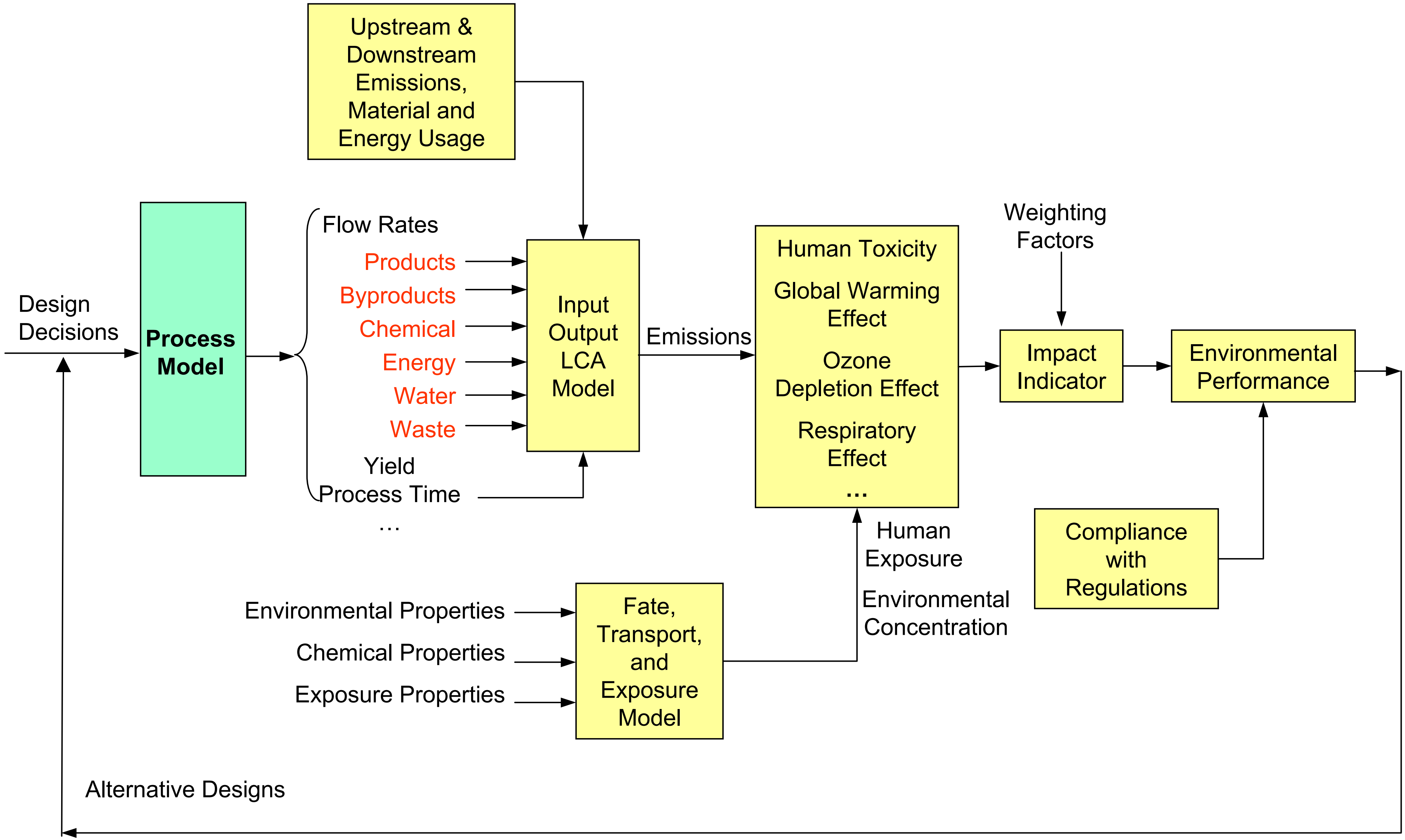
- Cleaning Time
  - t (s) ~ uniform(6E^{-4}, 1200)

$$f(t) = \frac{1}{1200 - 6 \times 10^{-4}}$$

- LCA includes the upstream gas production and downstream disposal treatment

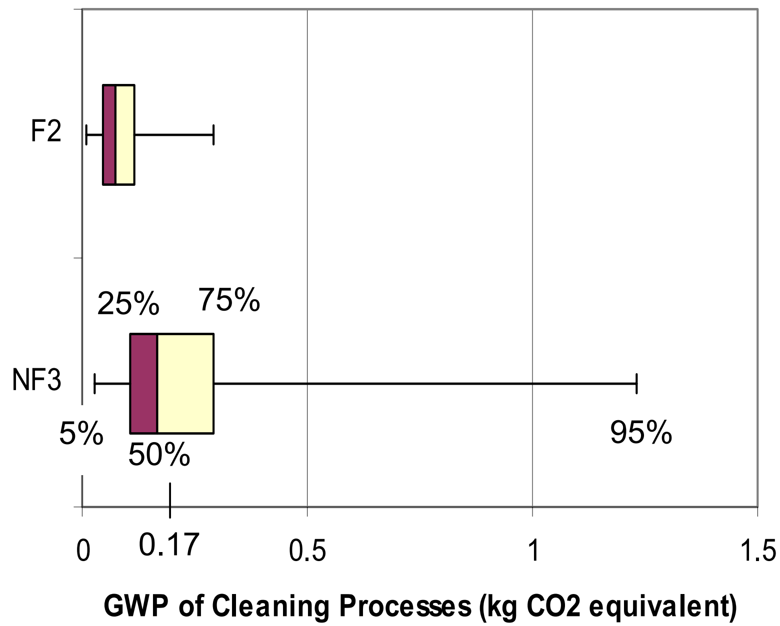
- Advantages of probability distributions:
  - Quantitative
  - Present the uncertainty of the information
  - Can be refined when further knowledge is available

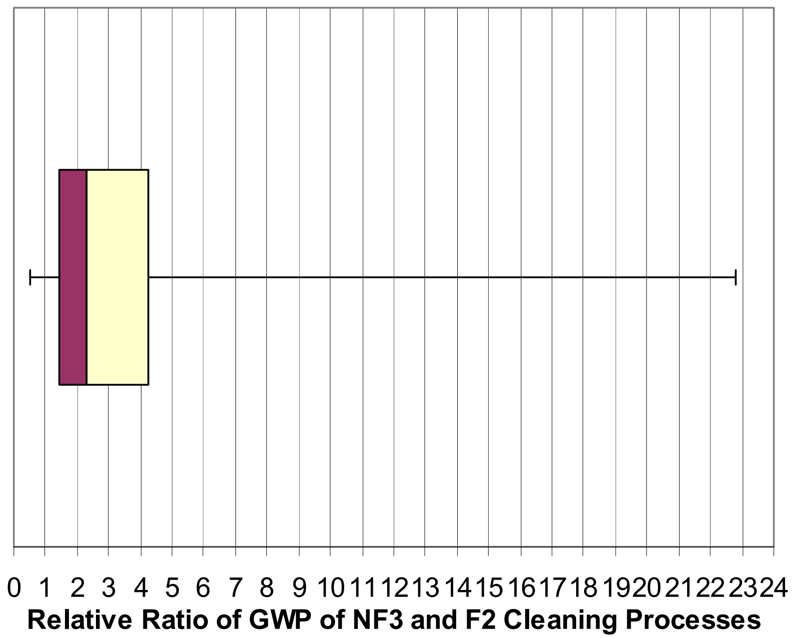
MIT Environmental Evaluation Model



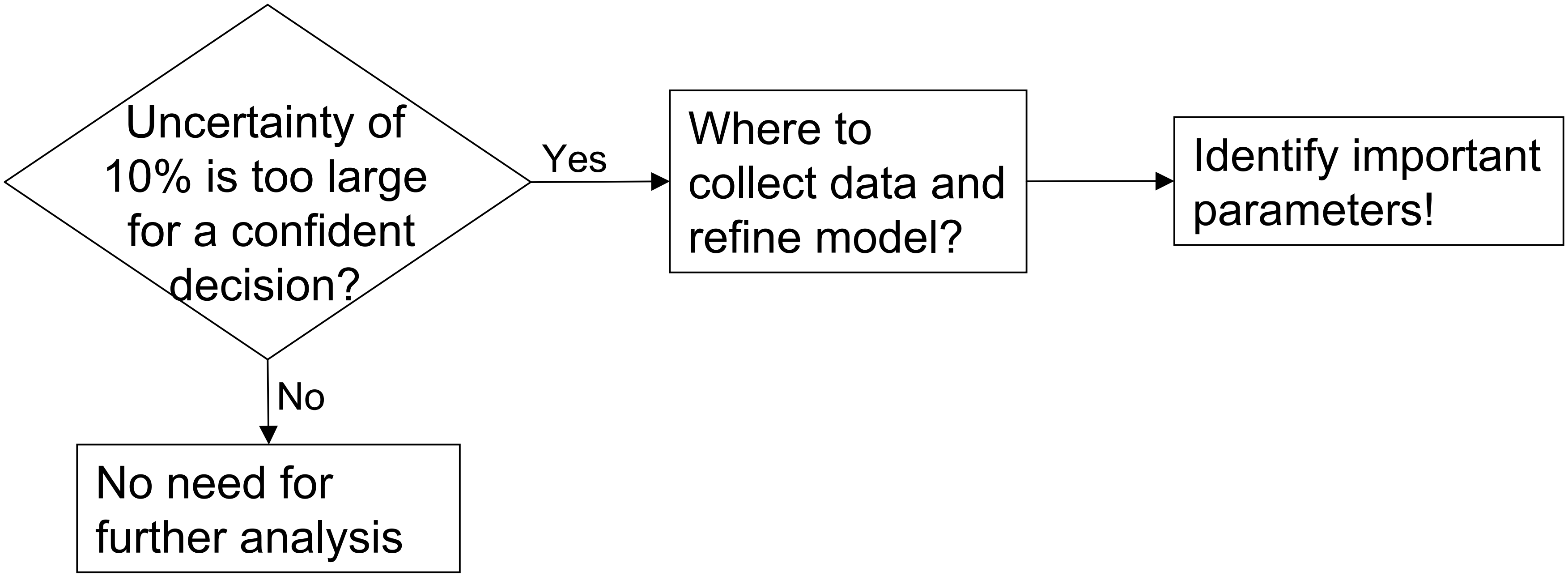
Environmental Impacts from LCA

- Comparison of the global warming potential of the two processes





Where Shall We Go Next?



- Uncertainty can come from
  - Process model
  - Upstream and downstream data
  - LCA model/data

Important Parameters of Affecting Relative GWP

Table I

Parameter	Rank Correlation Coefficient
$F\%_{NF3}$	-0.64
$F\%_{F2}$	0.46
Cleaning Time t (s)	-0.28
ξ_{E_NF3}	-0.20
ξ_{E_F2}	0.12
NF3 Yield in NF3 Production from NH3 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

Process model need to be refined!

Hierarchical Modeling – Second Process Modeling Level

- Lumped Kinetics and PSTR 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.

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

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

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

$$\beta_i \equiv k_i n_e$$

Process Modeling Results

Etch Rate – Falls into industrial experience

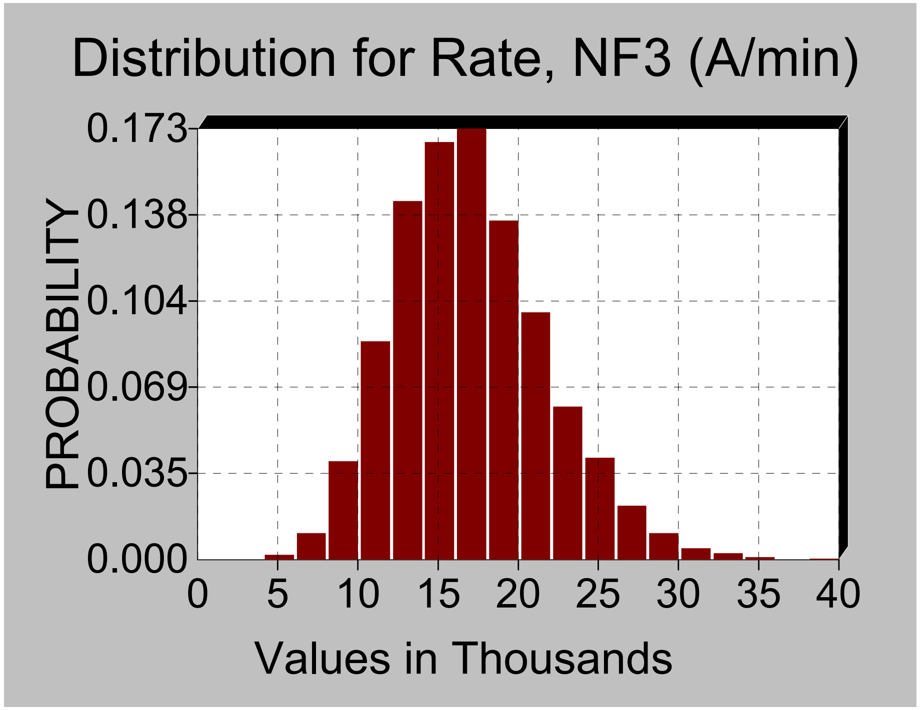
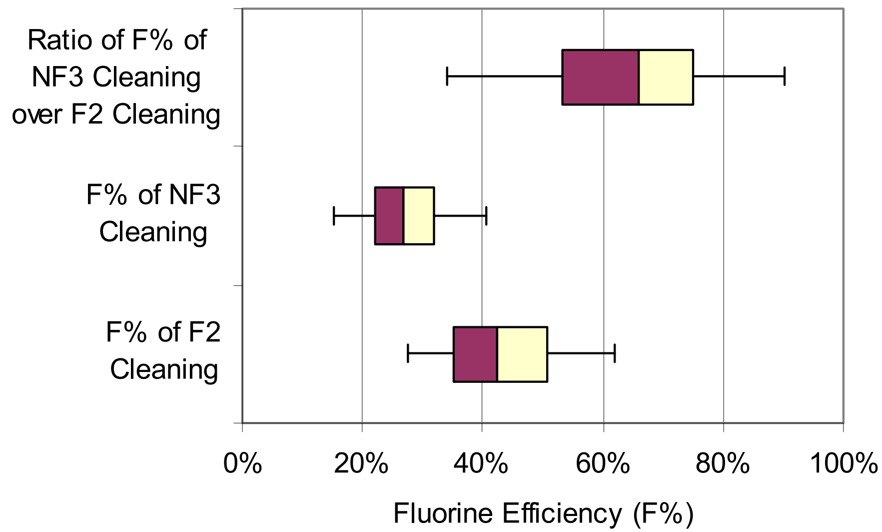


Table II

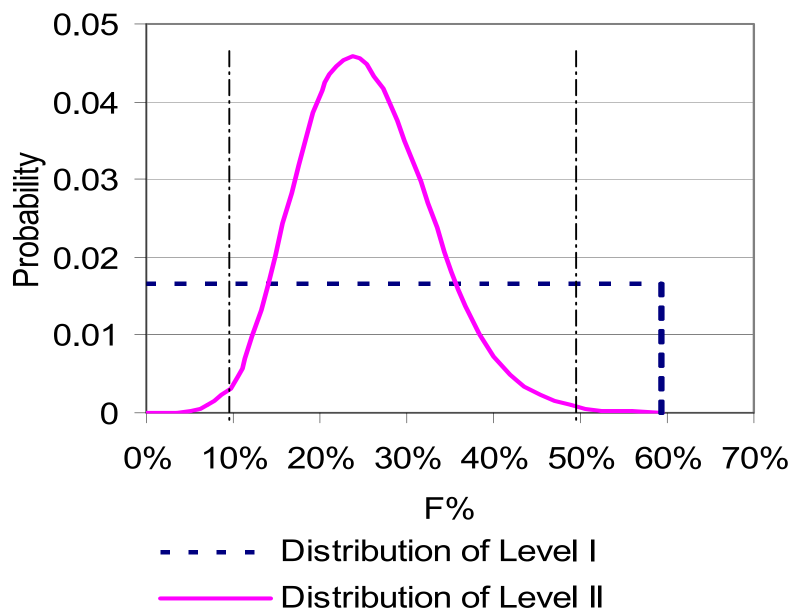
Important Parameters that Affect Etch Rate	Rank Correlation Coefficient
Film surface temperature (K)	0.545
Activation energy in the SiO_2 etch rate equation (J)	-0.403
Power of the electron temperature of NF_3 disassociation reaction in plasma	0.416
Chamber temperature (K)	-0.371
Electron temperature (eV)	0.243

Fluorine Utilization Efficiency Results

- The F_2 cleaning has higher fluorine utilization efficiency

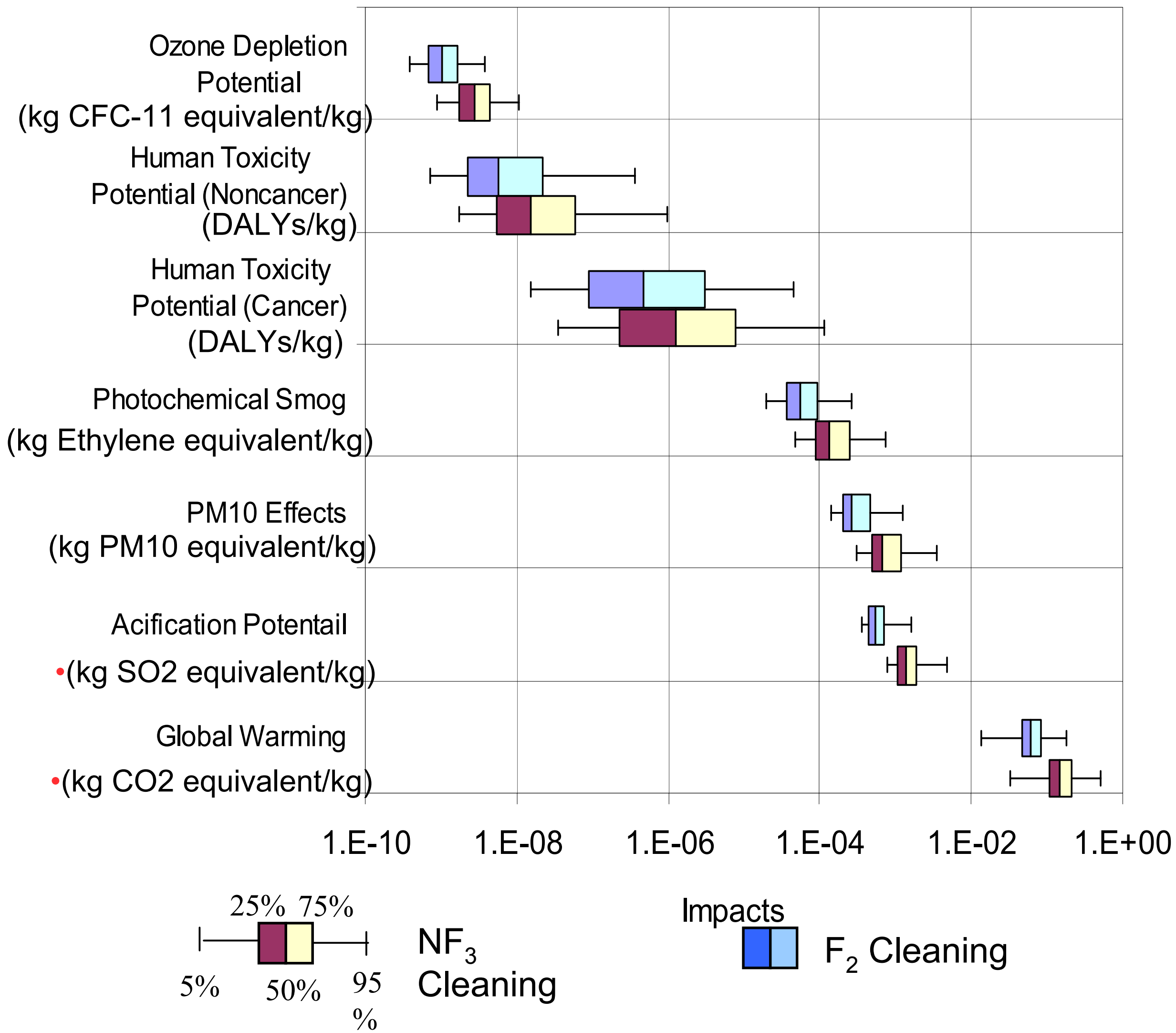


- Narrower distribution compared to the first modeling level (F% ~ uniform(10^{-5}, 0.6))



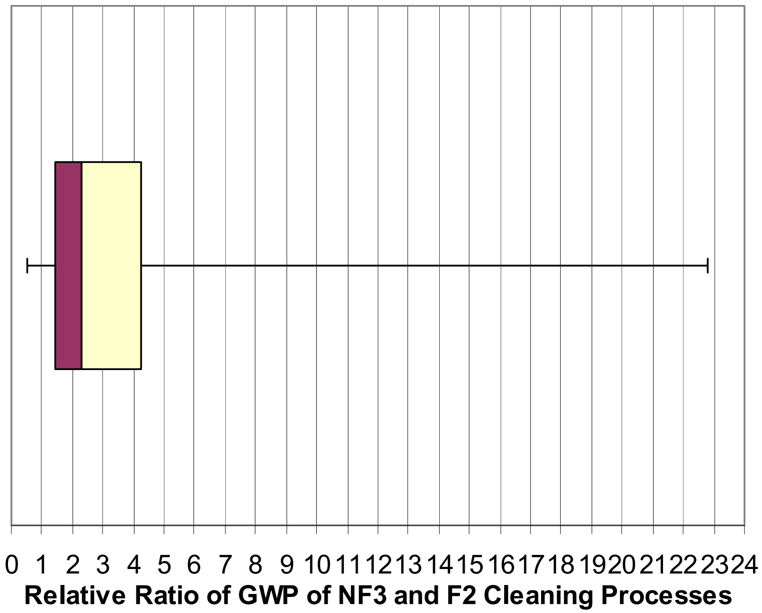
LCA Results at Second Process Level

- Narrower distributions of the impacts

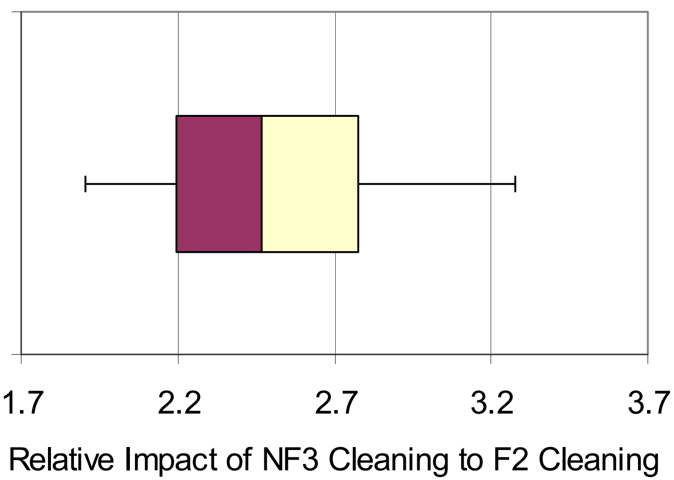


Relative Impact of GWP

First Process Modeling Level

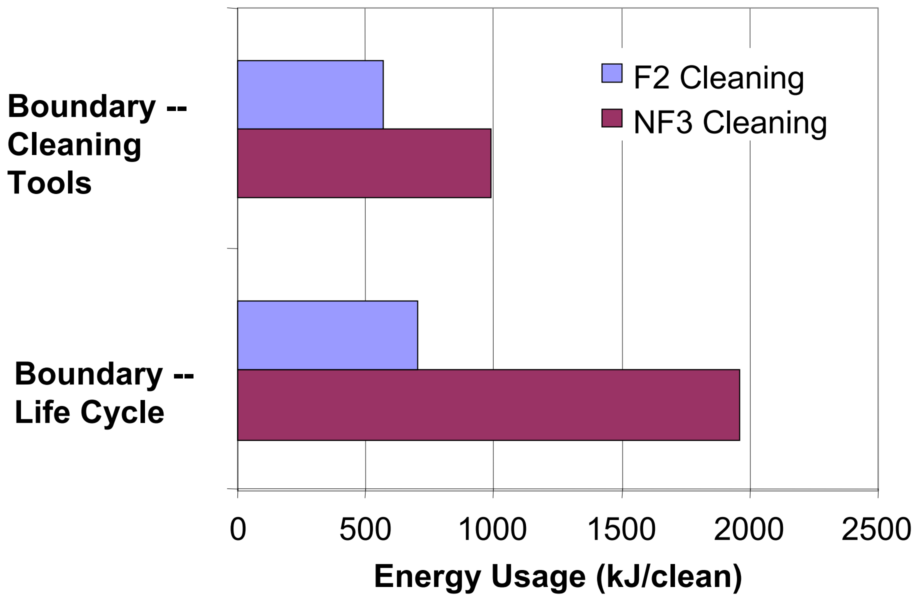


Second Process Modeling Level



- The increase of modeling detail decreases the uncertainty of the outputs.
- Even though there is much uncertainty in the inputs, by directly addressing the uncertainty and using relative ratio, the two processes can be clearly differentiated.

Boundary Effect



- Energy used outside the fab consists half of the total energy consumption for the NF_3 cleaning process.

⇨ Reducing the power needed for the plasma generator

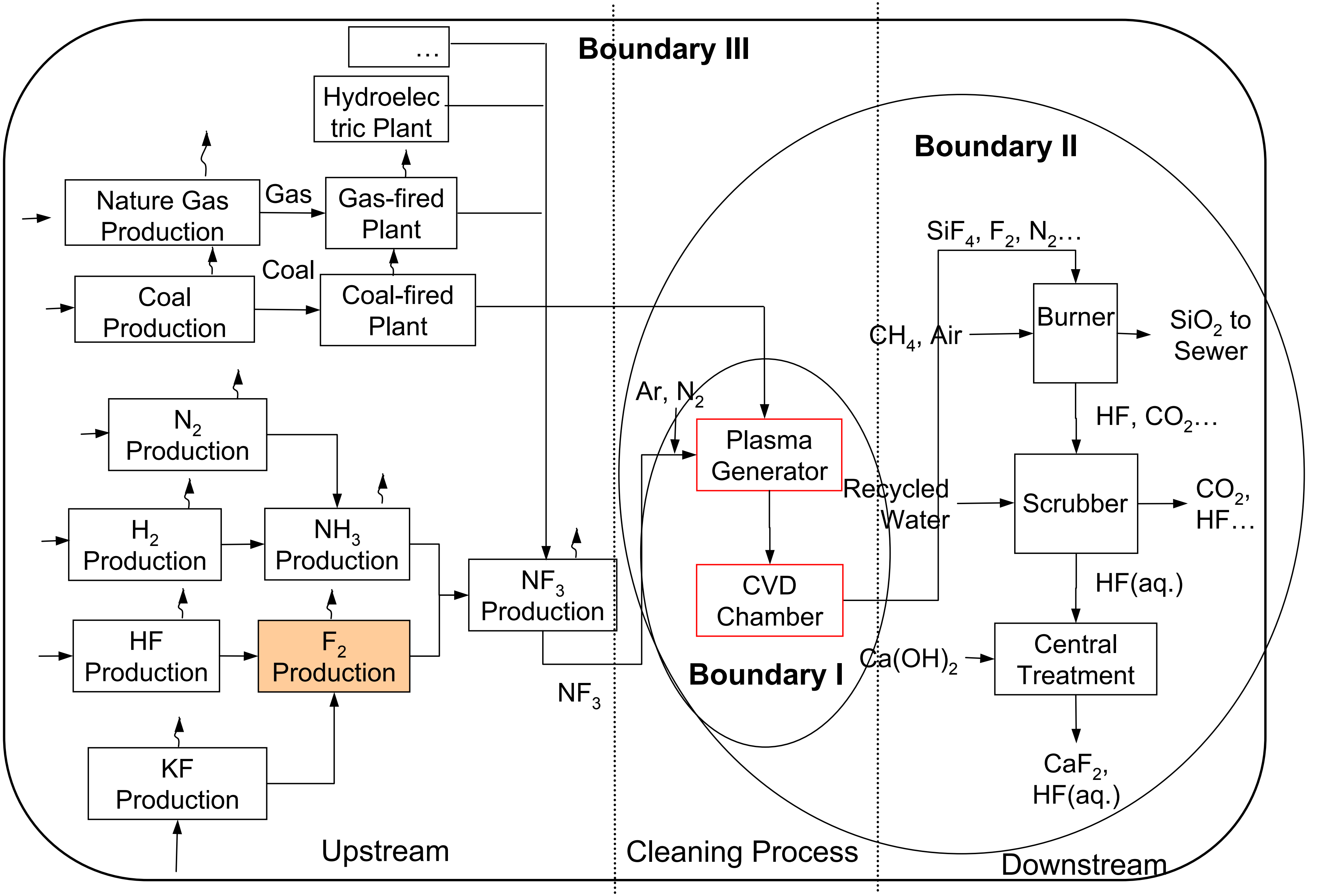
+

Producing NF_3 and other upstream materials more efficiently

=

Less impacts from energy generation, which is a major impact source!

Importance of Considering Multi-Boundaries

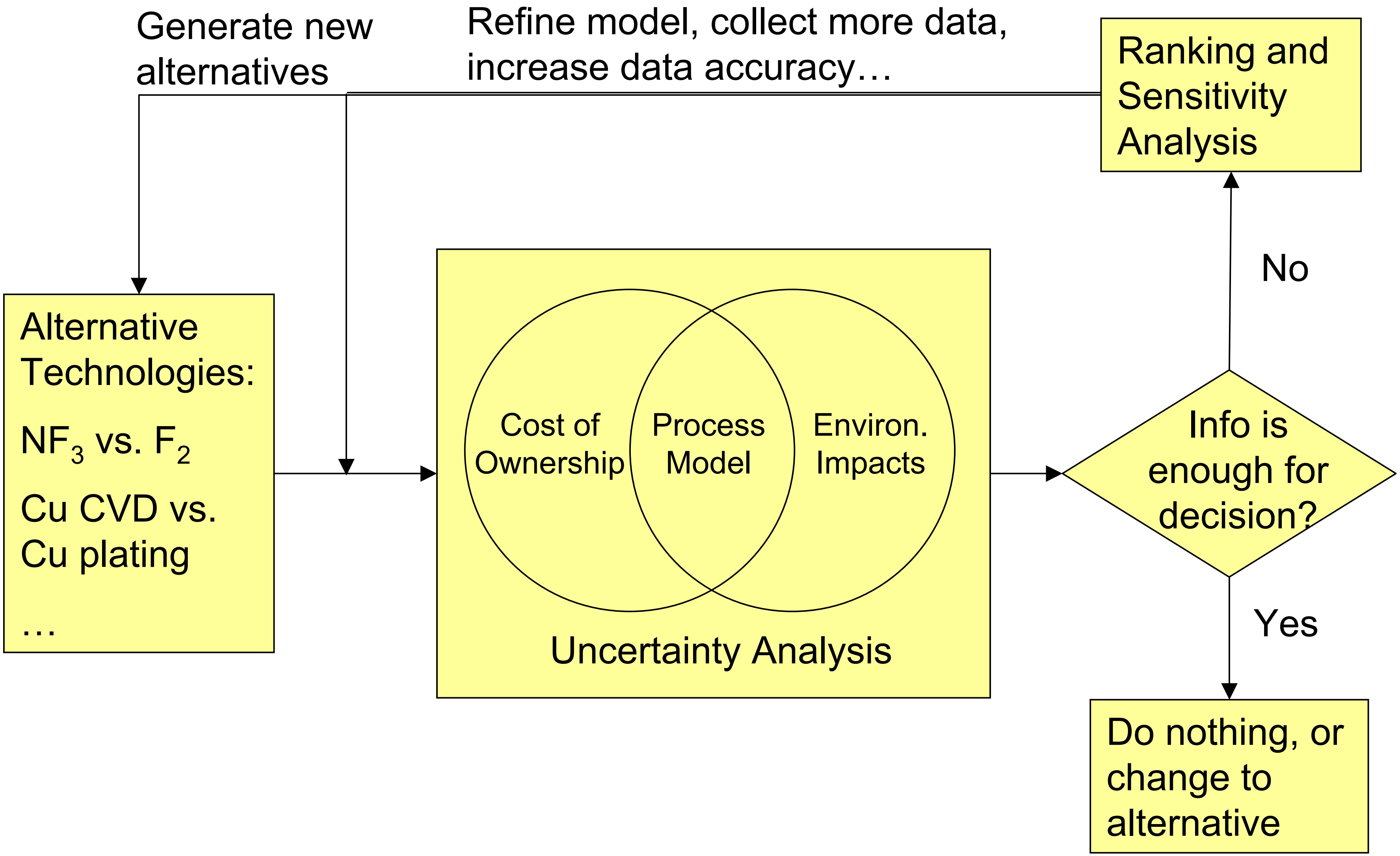


Again, Where Shall We Go Next?

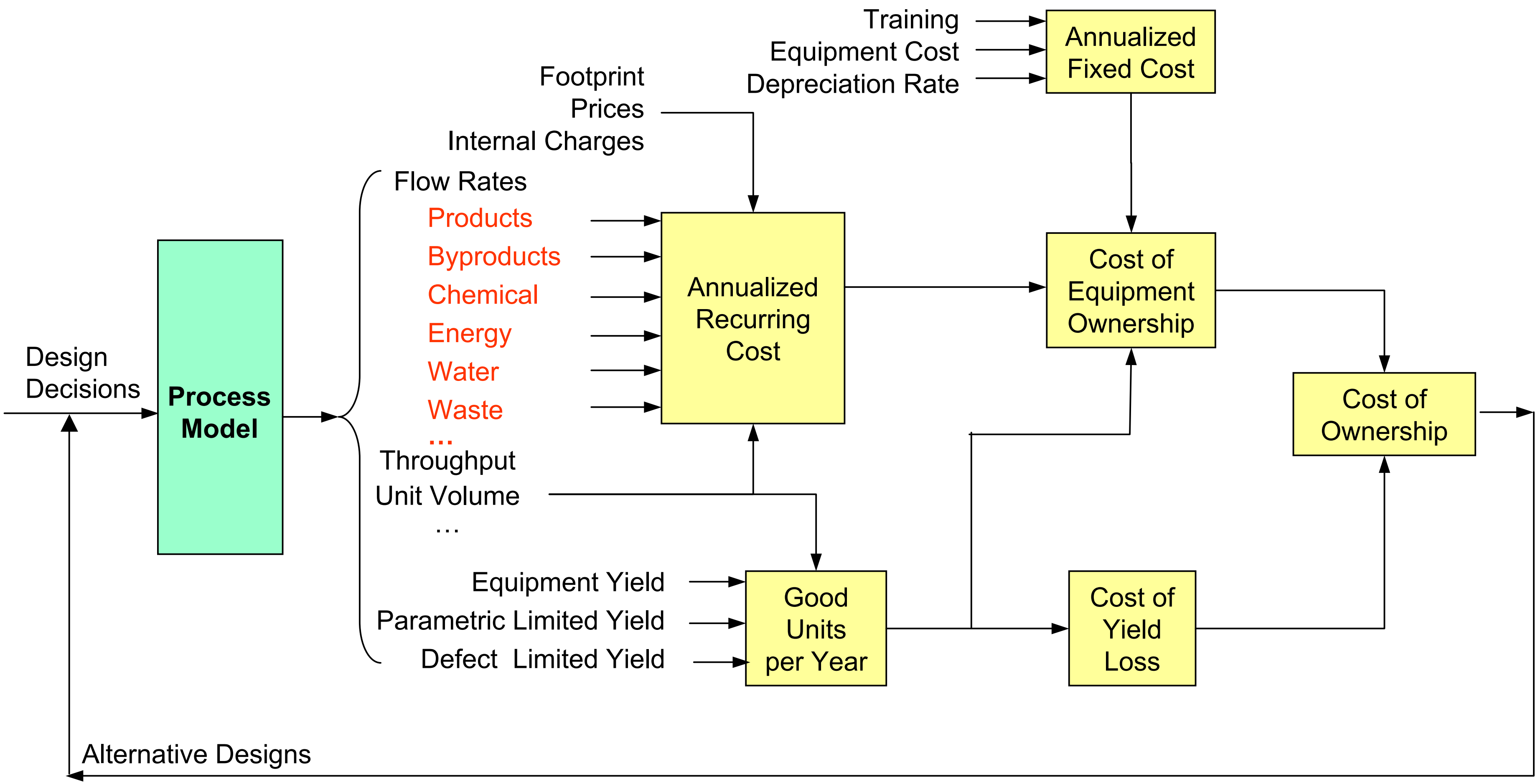
Table III

Important Parameter of Relative GWP at Second Process Modeling Level	Rank Correlation Coefficient
Power Used in Plasma Generator (W)	0.69
Power to the Electron Temperature in NF_3 Disassociation Reaction	-0.37
NF_3 Yield in NF_3 Production from NH_3 and HF	-0.33
Energy Used in F_2 Production (J)	0.21
Power to the Electron Temperature in NF_2 Disassociation Reaction	-0.19
Electron Temperature in the Plasma Source (eV)	-0.13
Temperature of Surface to be Cleaned (K)	-0.087
NH_3 Flow Rate in NF_3 Production (sccm)	-0.085
Pre-exponential Term of F_2 disassociation Reaction in the Plasma	-0.066
Stir Rate in NF_3 Production (W/m^3)	0.058

Framework of Decision-Making Process



SEMI Cost of Ownership (CoO) Model



Preliminary Results of Cost-of-Ownership

- Key Assumptions
  - No yield loss for both processes
  - Fixed costs of chamber and plasma source are the same
  - POU fluorine generator depreciate linearly in 5 years
  - Cleanings are done 200,000 times per year
  - Added value due to lower down time of chamber system was not considered

Distributions of Parameters in COO

- Wide triangle distributions were used to describe parameters

$$\begin{cases} f(x) = \dfrac{2[x-(1-\alpha)m]}{2\alpha^2 m^2} & \text{if } (1-\alpha)m < x < m \\ f(x) = \dfrac{2[(1+\alpha)m-x]}{2\alpha^2 m^2} & \text{if } m < x < (1+\alpha)m \end{cases}$$

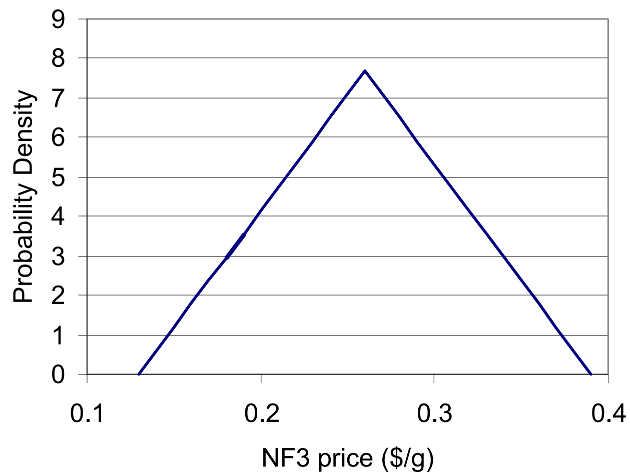
x – random variable;

α – the percentage of change in the nominal value. α ~ uniform(10%, 90%);

m – nominal value of the variable.

- Example:

  Assume nominal value of NF3 price is \$0.26/g. Then when α = 50%, the price of the NF3 gas can change between \$0.13/g and \$0.39/g.



Distributions of Parameters of the F_2 Process

- Variables of the F_2 process have larger upper limits to incorporate its less certainty.

$$
\begin{cases}
f(x) = \dfrac{2\left[x-(1-\alpha)m\right]}{\alpha m\left[\beta m-(1-\alpha)m\right]} & \text{if } (1-\alpha)m < x < m \\
f(x) = \dfrac{2\left[(1+\alpha)m-x\right]}{(\beta m-m)\left[\beta m-(1-\alpha)m\right]} & \text{if } m < x < \beta m
\end{cases}
$$

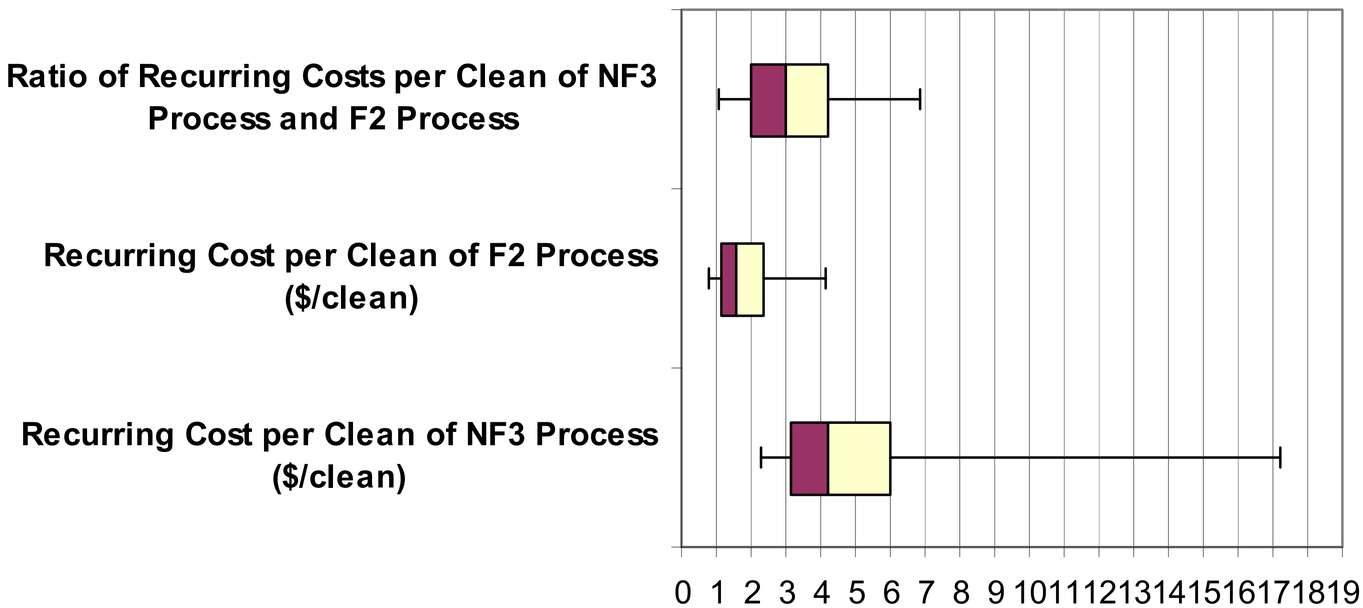
β – Percentage of increase in the nominal value. β ~ uniform(200%, 1800%).

- Miscellaneous cost of training per system ranges from \$3200 to \$400,000 with the nominal value of \$4000.

- By setting the coefficients α and β to be random variables, the uncertainty introduced by how these variables are modeled can be studied.

Results of COO Analysis

- There is less than 5% that F_2 cleaning will be more costly than NF_3 cleaning



- Where do the large uncertainty of the NF_3 COO come from?

Identifying Important Parameters of NF_3 COO

Parameter	Rank Correlation Coefficient
Power to the Electron Temperature in NF_3 Disassociation Reaction	-0.61
Price of NF3 Gas ($/g)	0.34
Temperature of Surface to be Cleaned (K)	-0.27
Power to the Electron Temperature in NF_2 Disassociation Reaction	-0.24
Activation Energy of Etch Reaction (J)	0.23
Chamber Temperature (K)	0.20
Electron Temperature in the Plasma Source (eV)	-0.19
Pre-Exponential Term of Etch Reaction	-0.13
Power to the Electron Temperature in NF_2 Disassociation Reaction	-0.12
Price of Argon Gas ($/g)	0.092

- Most of the parameters are still from the process model!
- These are the same parameters that affect environmental impacts.

Overlapping Data Requirements

Cost of Ownership

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 Evaluation

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

Conclusions and Key Points

- The integration of process models, COO, and environmental evaluations is critical and feasible.
- Large uncertainty in the inputs does not necessarily lead to low confidence in decisions.
- Hierarchical modeling in combination with uncertainty analysis are efficient way to support the decision making and resource allocation process.
- The next step is to develop an integrated software environment

UNCERTAINTY ≠ IGNORANCE

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End of Presentation