An Integrated Economic and ESH Framework for Making Technology Choices

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Key Message

ESH – Environment, Safety and Health

COO – Cost of Ownership

➡ **They must be seamlessly integrated for effective decision making**

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 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?

Why we need to solve this problem!!

Industry recognition of need

> **"…There is a critical need for an integrated way to evaluate and qualify environmental impact of process, chemicals, and process equipment…"**
>
> -- ITRS, 2001 Edition, Environmental, Safety, and Health

Emerging Driving forces for Change

> **"…The European Commission Integrated Product Policy (IPP) will look at <u>all</u> stages of a product's life cycle from cradle to grave…we are calling on industry to bring IPP to life"**
>
> -- M. Wallström, EU Environment Commissioner
>
> Press release 18th June 2003

Outline of Presentation

- **Review of Current Approaches**
  - CARRI, EnV-S, TEAM,…
- **Development of Decision criteria**
  - System boundary choice
  - Cost of Ownership (COO)
  - Environment, Health and Safety (EHS)
  - Integration of COO and EHS
- **Impact Assessment Models**
  - Process models for mass and energy balances
  - Hierarchical representations
  - Treatment of uncertainties
- **Example**
  - NF_3 vs. F_2 case study
- **Conclusions and Next Steps**

Comparison of Environmental Valuation Methods

	CARRI	S70	TEAM	EnV-S
Impact Categories Considered	Work space safety and health, broad characterization of environmental toxicity, regulatory, COO	Mass and energy consumed, transformed, and discharged	More than 50 categories such as global warming effect, human toxicity, aquatic/terrestrial eco-toxicity	COO, human health (cancer, acute toxicity, etc), regulatory
Applications	Relative risk of chemical usage	Determine the overall material and energy usage and waste products generated by the unit operations	Quantifying environmental impacts of the operations associated with products, processes, and activities	Tool design, choosing between alternative tools
System Boundary	Fab, downstream	Fab	Upstream, fab, downstream	Upstream, fab, downstream
Inputs based on database or model	Database	Static, averaged process model	Based on user input, databases	Process models
Site Specific	Yes	Yes	No	Yes
Linked to Cost	Yes	No	No	Yes
Include Uncertainty	Qualitative	No	User can set up limited probability distributions	PDFs, Monte Carlo simulations
Database availability	Inventories and impacts	Inventories	Inventories and impacts	Inventories

Key points from review of ESH models

- Widespread industry acceptance of SEMI COO model but it is not integrated into ESH methods
- Decision criteria are influenced by the choice of system boundaries but few methods look outside the plant boundaries
- No formalized treatment of uncertainties or means for identifying what controls decision outcomes
- Little consistency between databases used for analyses and there are many data gaps
- Little cross fertilization of good ideas from other industries

Operational Challenges

A new framework must:

- Be compatible with the short innovation cycle
- Show the value of treating environment as an objective in design and operations
- Handle different levels of understanding in the process and economic models
- Deal with the large EHS information uncertainties

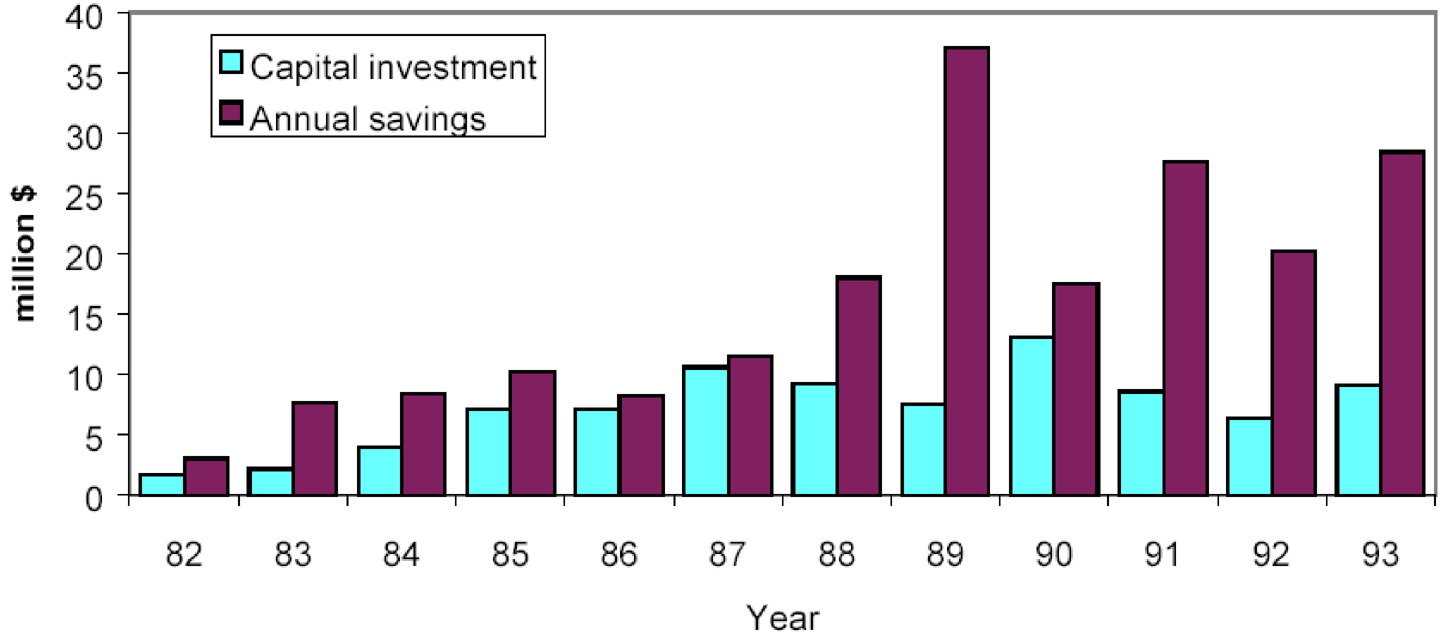
~1 orders of magnitude in air pollutant emission factors

2 ~ 3 orders of magnitude in cancer toxicity indicators

3 ~ 6 orders of magnitude in non-cancer toxicity indicators

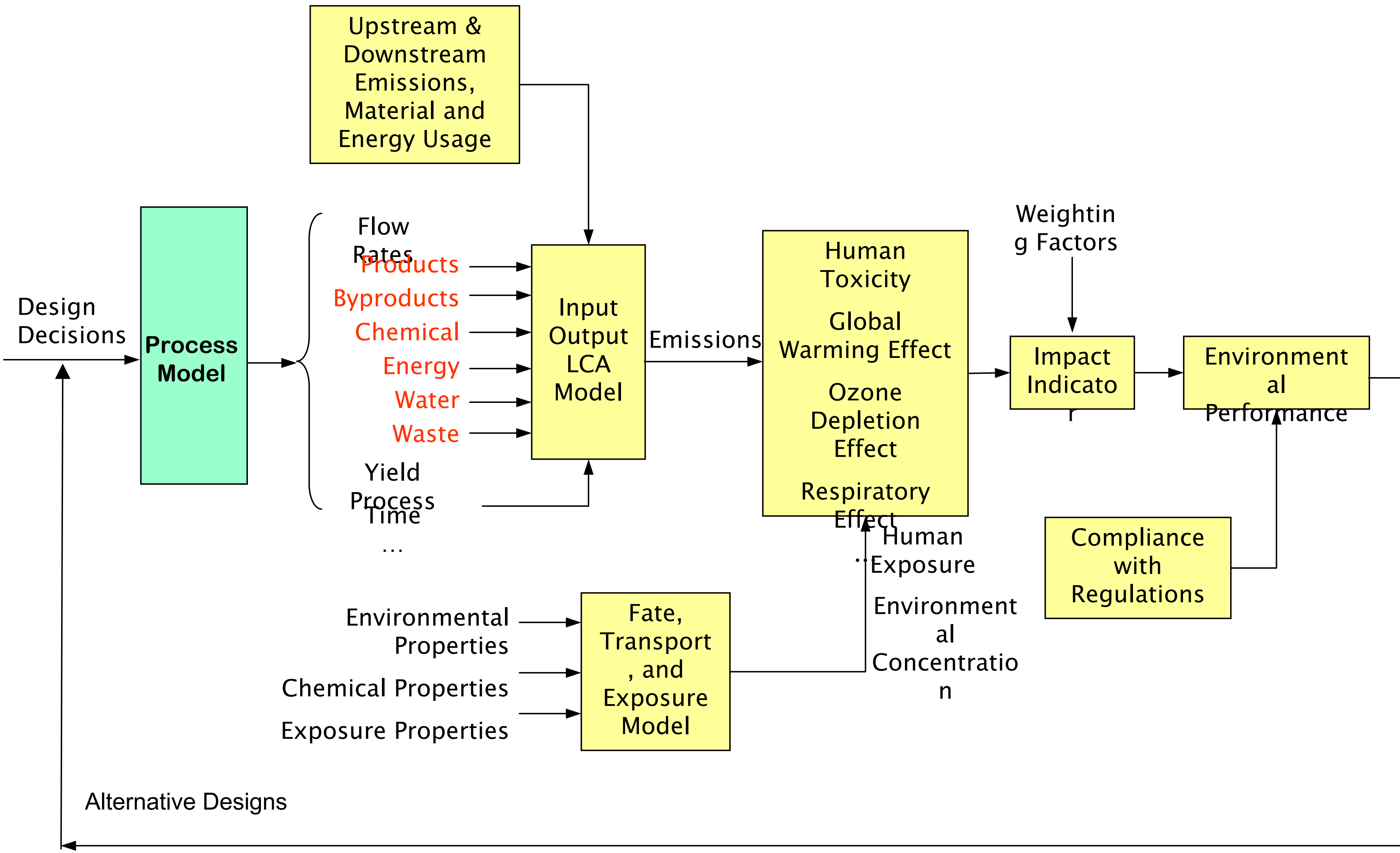
Value of Treating the Environment as an Objective

- The Energy and Waste Reduction Contests at Dow Chemical



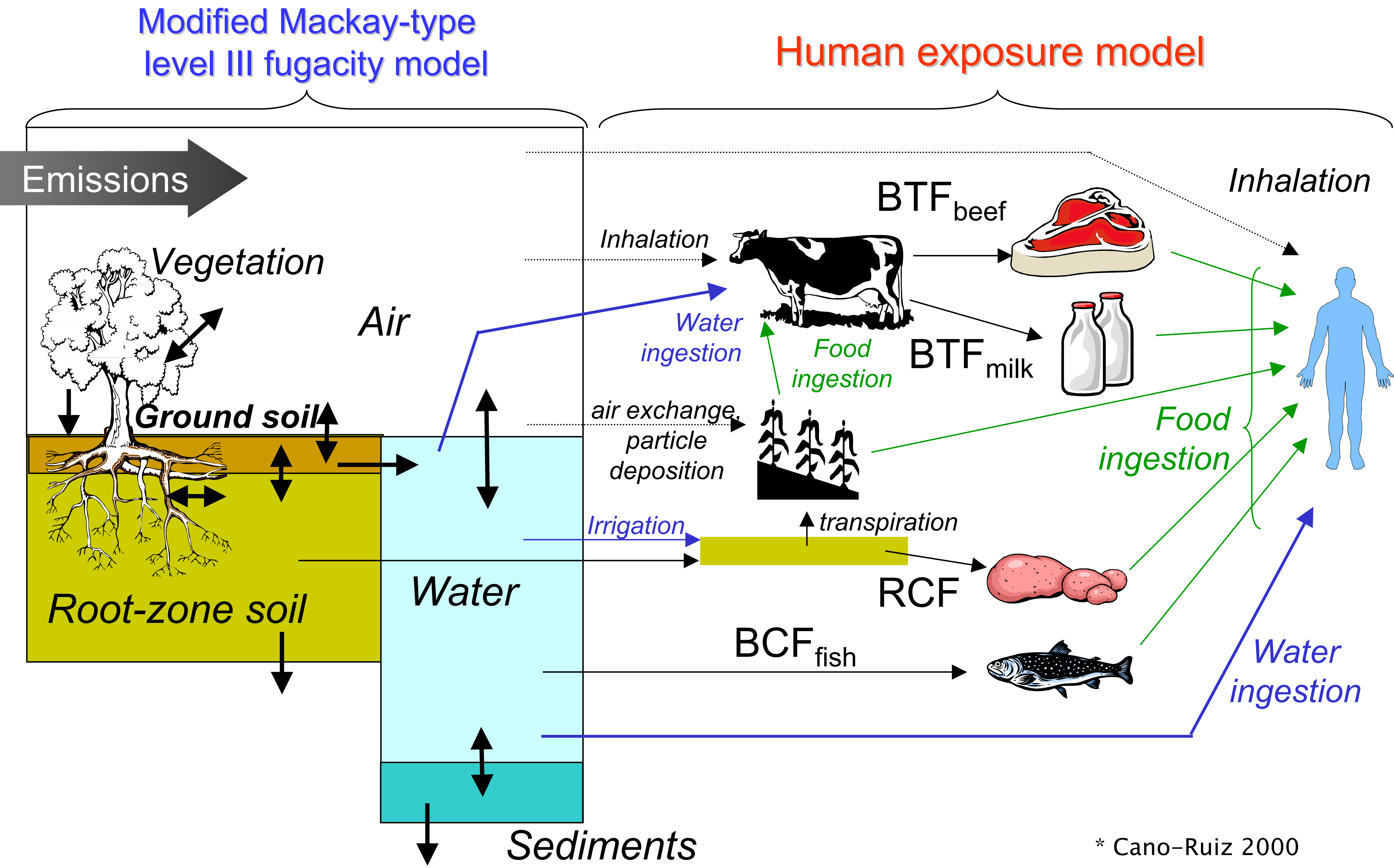
- A 180% annual return on $3 million invested in projects to reduce toxic waste generation and emissions (Midland site, Dow Chemical).

An Environmental Evaluation Model



Human Exposure Modeling: Complex Interactions*

Very complicated system, large number of parameters



* Cano-Ruiz 2000

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)

$$e = Ex$$

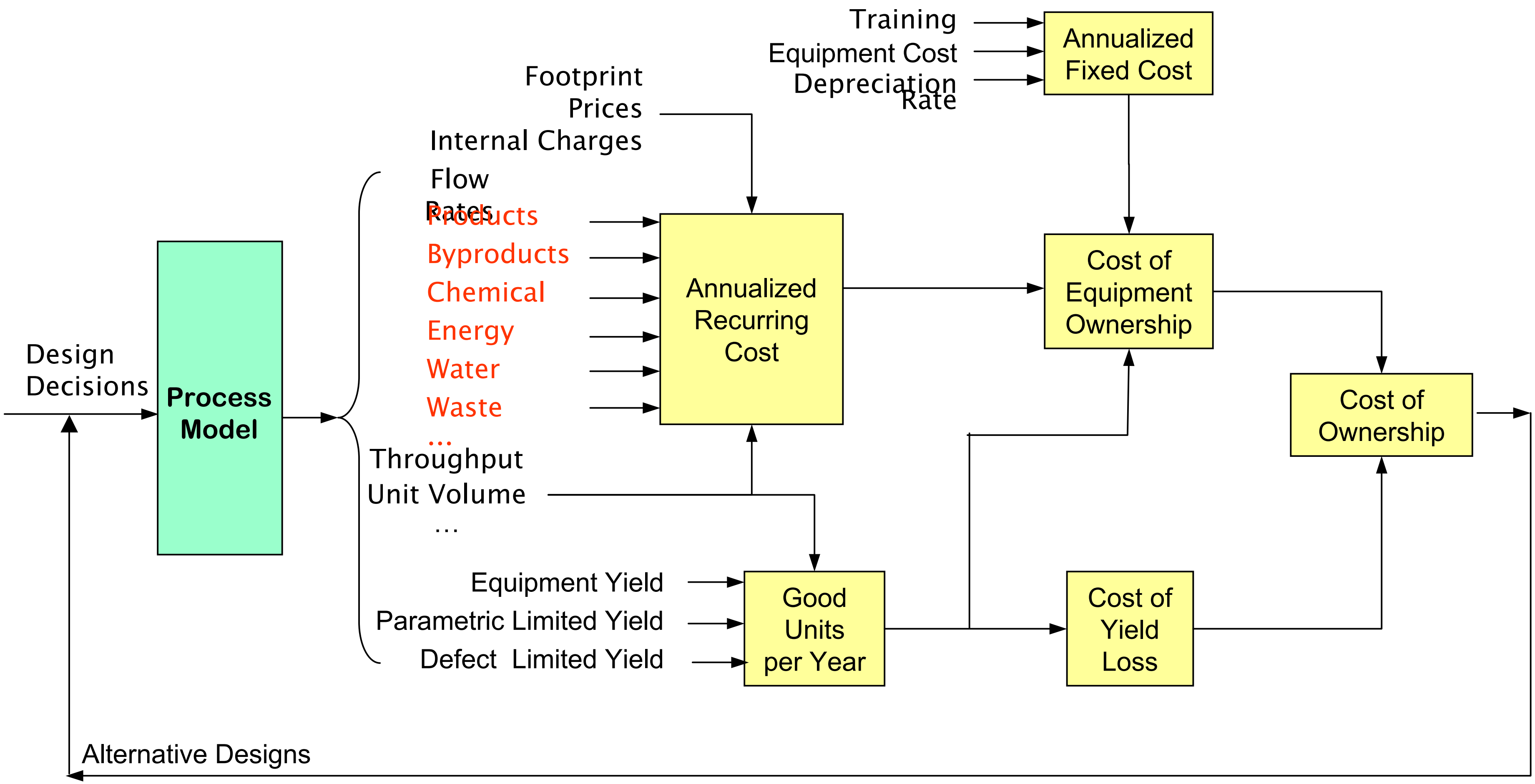
- Impact valuation by process ($\Omega_{process}$)

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

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

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

Cost of Ownership (CoO) Model



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

Matrix Presentation of Cost-of-Ownership

- COO = Cost of Equipment Ownership (CEO) + Cost of Yield Loss (CYL)

- CEO = Fixed Cost + Recurring Cost

- $$\text{Recurring Cost} = \begin{bmatrix} P_{NF_3} & P_{N_2} & P_{Ar} & P_{Energy} & P_{Water} & P_{WasteDisposal} & P_{Lbm} & \cdots & P_{Sp} & P_{Sc} \end{bmatrix} \times \begin{bmatrix} U_{NF_3} & U_{N_2} & U_{Ar} & U_{Energy} & U_{Water} & U_{WasteDisposal} & U_{Lbm} & \cdots & U_{Sp} & U_{Sc} \end{bmatrix}^{-1}$$

- $$CYL = \begin{pmatrix} \text{annualized cost} & & \text{annualized attributed} \\ \text{of wafers lost due} & + & \text{cost of wafers lost due to} \\ \text{to equipment yield} & & \text{defect \& parametric yield} \end{pmatrix} \cdot \frac{1}{\text{good units per year}}$$

Excerpt from an Life Cycle Assessment Calculation

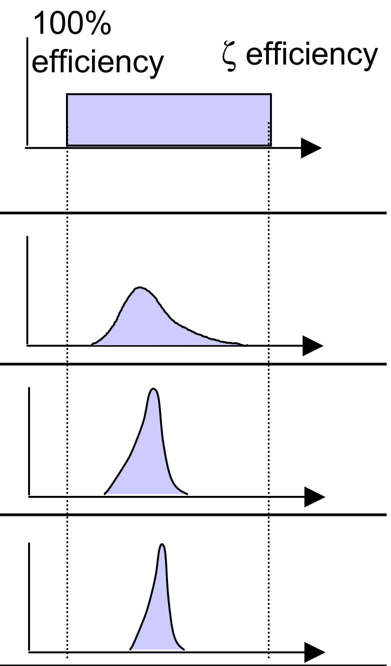
Usage Matrix

PRODUCT INPUTS	UNITS \ PROCESS	Coal furnace	Coal production	Coal-fired power plan	F2 chamber cleaning-	F2 production	Industrial gas furnace	Natural gas productio	NF3 chamber cleanin	NF3 production	Oil furnace	Oil production	Oil-fired power plant	⋮
Ar	kg	0	0	0	0.03	0	0	0	0.03	0	0	0	0	
clean chamber		0	0	0	0	0	0	0	0	0	0	0	0	
Coal	kg	1	0	0	0	0	0	0	0	0	0	0	0	
Diesel fuel	kg	0	0	0	0	0	0	0	0	0	0	0	0	
Electricity	MJ	0	0.05	0	6.55	8	0	0.1	6.55	18	0	0	0	
F2	kg	0	0	0	0.06	0	0	0	0	3.3	0	0	0	
Fluorine from Chamber Cleaning	kg	0	0	0	0	0	0	0	0	0	0	0	0	
HF	kg	0	0	0	0	2.5	0	0	0	0	0	0	0	
KF	kg	0	0	0	0	0.1	0	0	0	0	0	0	0	
N2	kg	0	0	0	0.05	0.1	0	0	0.05	0	0	0	0	
Natural gas	kg	0	0	0	0	0	20	0	0	0	0	0	0	
NF3	kg	0	0	0	0	0	0	0	0.07	0	0	0	0	
Oil	kg	0	0	0	0	0	0	0	0	0	23	0	0	
SiF4	kg	0	0	0	0	0	0	0	0	0	0	0	0	
Thermal energy from coal furnace	MJ	0	0.01	10	0	0	0	0	0	0	0	0	0	
Thermal energy from industrial gas furnace	MJ	0	0	0	0	0	0	1.3	0	0	0	1	0	
Thermal energy from oil furnace	MJ	0	0	0	0	0	0	0	0	0	0	0	10	
Thermal energy from utility gas furnace	MJ	0	0	0	0	0	0	0	0	0	0	0	0	
…														

Hierarchical Modeling

Time and cost ncrease

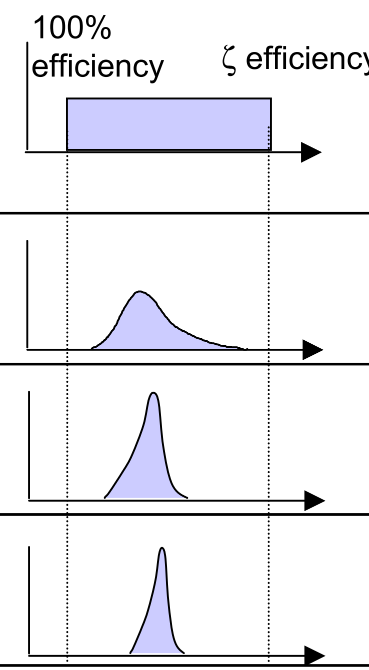
	Pro	Assumption	Likely distributions for gas usage
1	Tolerable efficiency	Yield of = ζ (ζ is a very small number)	
	Stoichiometric	100% efficiency, extremely quick etching	
2	Simple kinetics	Only a few key reactions	
3	Detailed kinetics	First principles	
4	Experiments		



Hierarchical Modeling

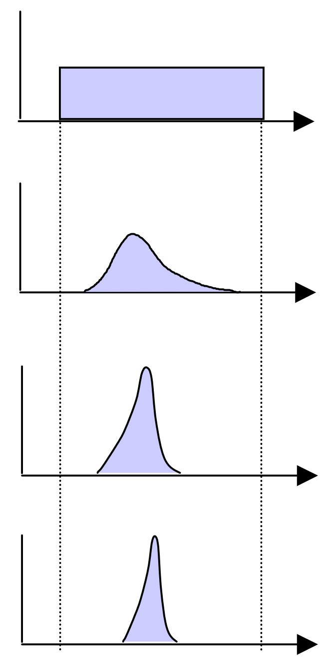
Time and cost increase

	Process Model		Likely distributions for gas usage
2	Simple kinetics	Only a few key reactions	
3	Detailed kinetics	First principles	
4	Experiments		



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



Simple Stoichiometic Yield Model

Gas	Model	gm of gas / mole SiO_2 η = 5%	η = 100%
NF_3	$\frac{1}{\eta} \cdot \frac{4SiF_4 + HF}{3}$	**1900**	**95**
F_2	$\frac{1}{\eta} \cdot \frac{4SiF_4 + HF}{2}$	**1520**	**76**

Lumped Kinetics and CSTR Model

Key Assumptions

- Free electrons are generated mainly by ionization $X_2 + e \rightarrow X_2^+ + 2e$
- Electron loss and production are linear to electron concentration
- Diffusion of electrons dominates the transport of electrons.

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

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

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

$$\beta_i \equiv k_i n_e$$

Uncertainty Analysis for NF_3 Etch Rate

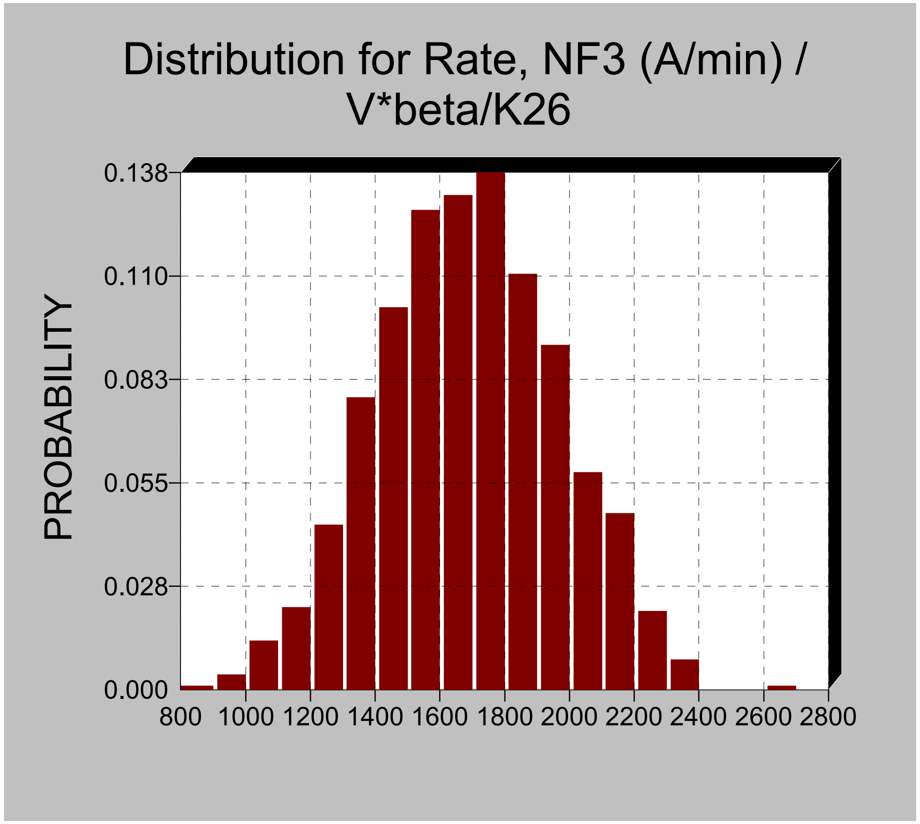
Assume 10% uncertainty in A_i and E_{ai}, no uncertainty in β_i.

NF_3 + e -- > NF_2 + F· + e
NF_2 + e -- > NF + F · + e
NF + e -- > N + F · + e

$$k_i = A_i \cdot T_e^{\beta_i} \cdot e^{-E_{ai}/T_e}$$

F· + SiO2 -- > SiF4

$$r = k \times n_{F\cdot} \times T_s^{1/2} \times \exp\left(-0.163 \times eV / k_B T_s\right)$$

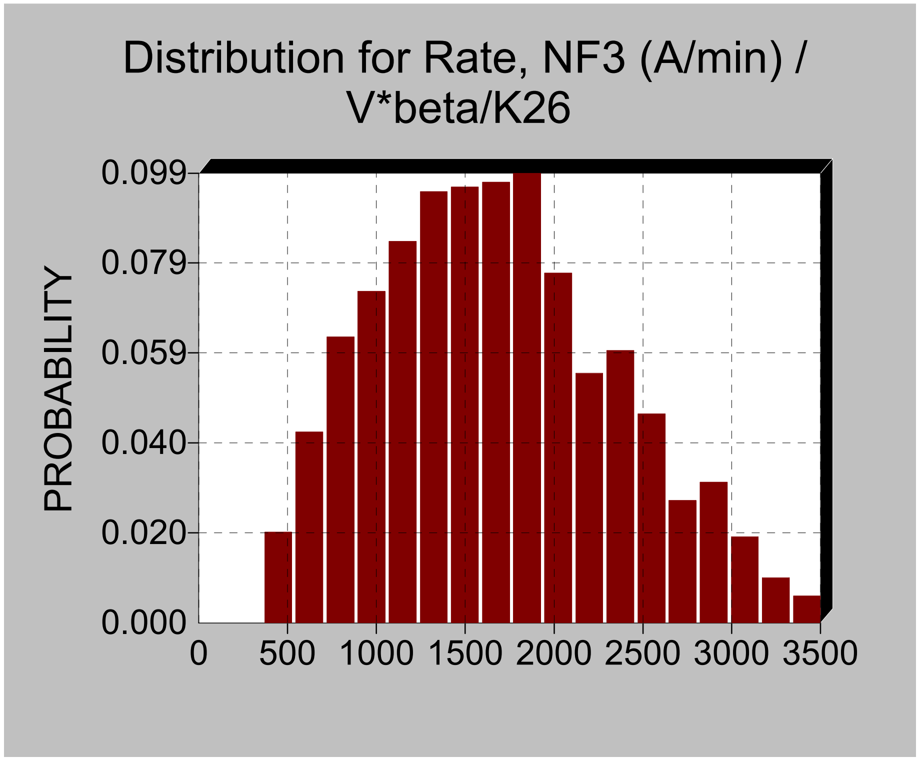


Parameters	Rank Correlation Coefficient
Intercept for k_B*T_e~E_e/p	0.659466
Activation energy E_{a3} for NF_3 decomposition	-0.65332
Rate constant *k* for etch reaction	0.227614
Activation energy E_{a2} for NF_2 decomposition	-0.10335
Pre-exponential coefficient A_3 for NF_3 decomposition	0.093827

Identifying Important Parameters to GWP

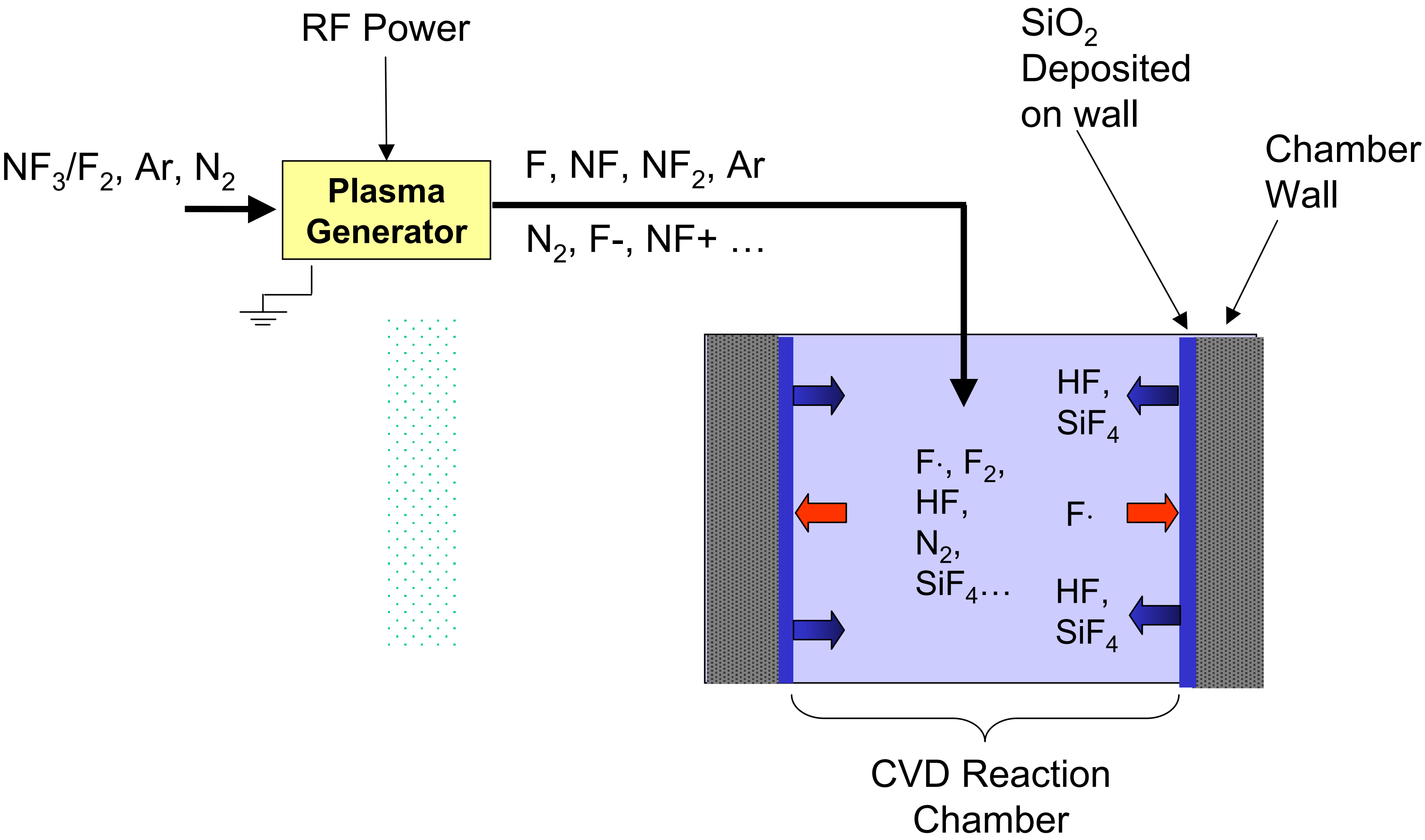
Parameters	Rank Correlation Coefficient
NF_3 Yield in NF_3 Production	-0.71
Energy Usage in F_2 production	0.42
Intercept for k_B*T_e~E=/p	-0.39
Activation Energy E_{a3} for NF_3 decomposition	0.34
Energy Usage in NH_3 production	0.13

Assume 10% uncertainty in A_i, E_{ai}, and β_i.

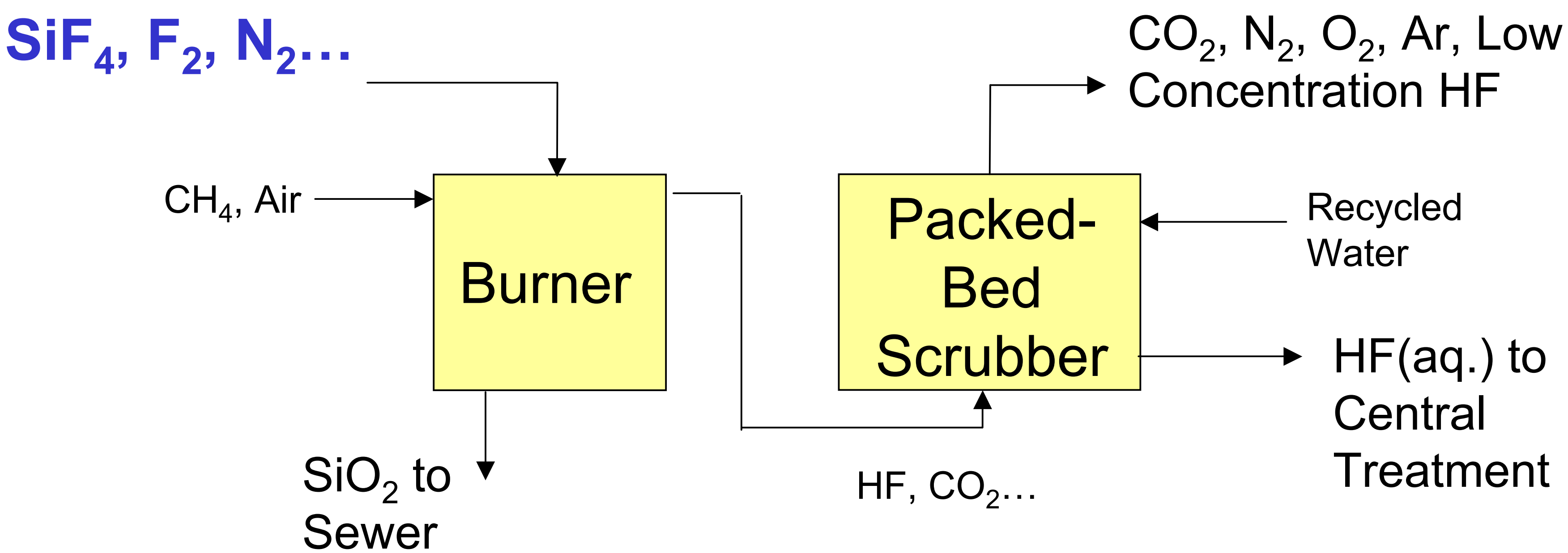


Parameters	Rank Correlation Coefficient
Power β_3 to the electron temperature for NF_3 decomposition	0.87
Activation Energy E_{a3} for NF3 decomposition	-0.27
Power β_2 to the electron temperature for NF2 decomposition	0.267
Intercept for $k_B*T_e \sim E_e/p$	0.24
Power β_1 to the electron temperature for NF decomposition	0.13

Chamber Cleaning with NF_3/F_2



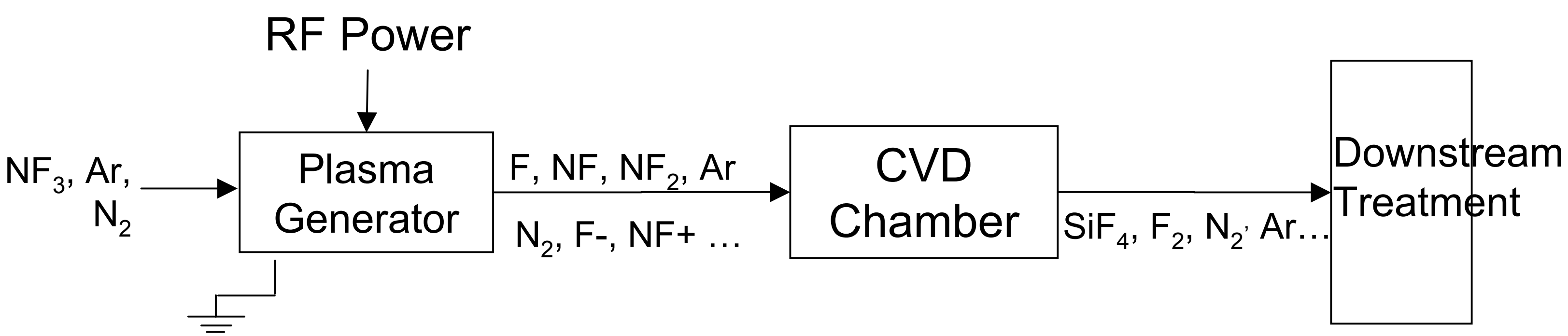
Including Downstream Treatment



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

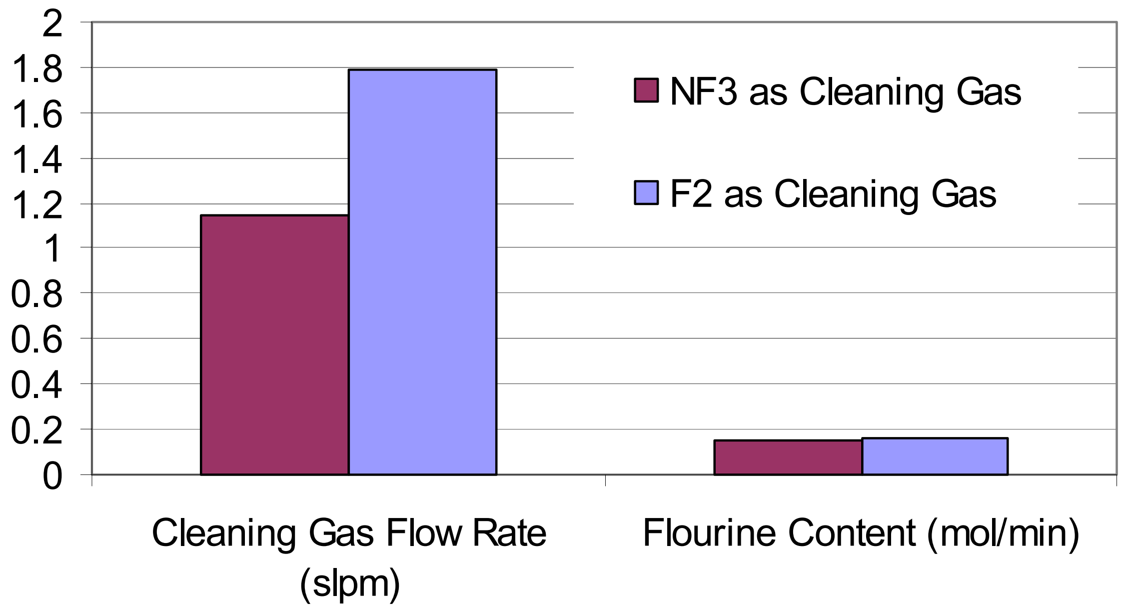
Case Study: NF_3 vs. F_2 as Chamber Cleaning Gas

- Merits of NF_3
  - High disassociation rate
  - High removal rate
  - High etch rate
- Drawback of NF_3
  - High cost
- Merits of F_2
  - Low cost
- Drawbacks of F_2
  - High toxicity
  - High reactivity
  - POU generation creates explosive H_2
- NF_3 Cleaning Process in the Fab



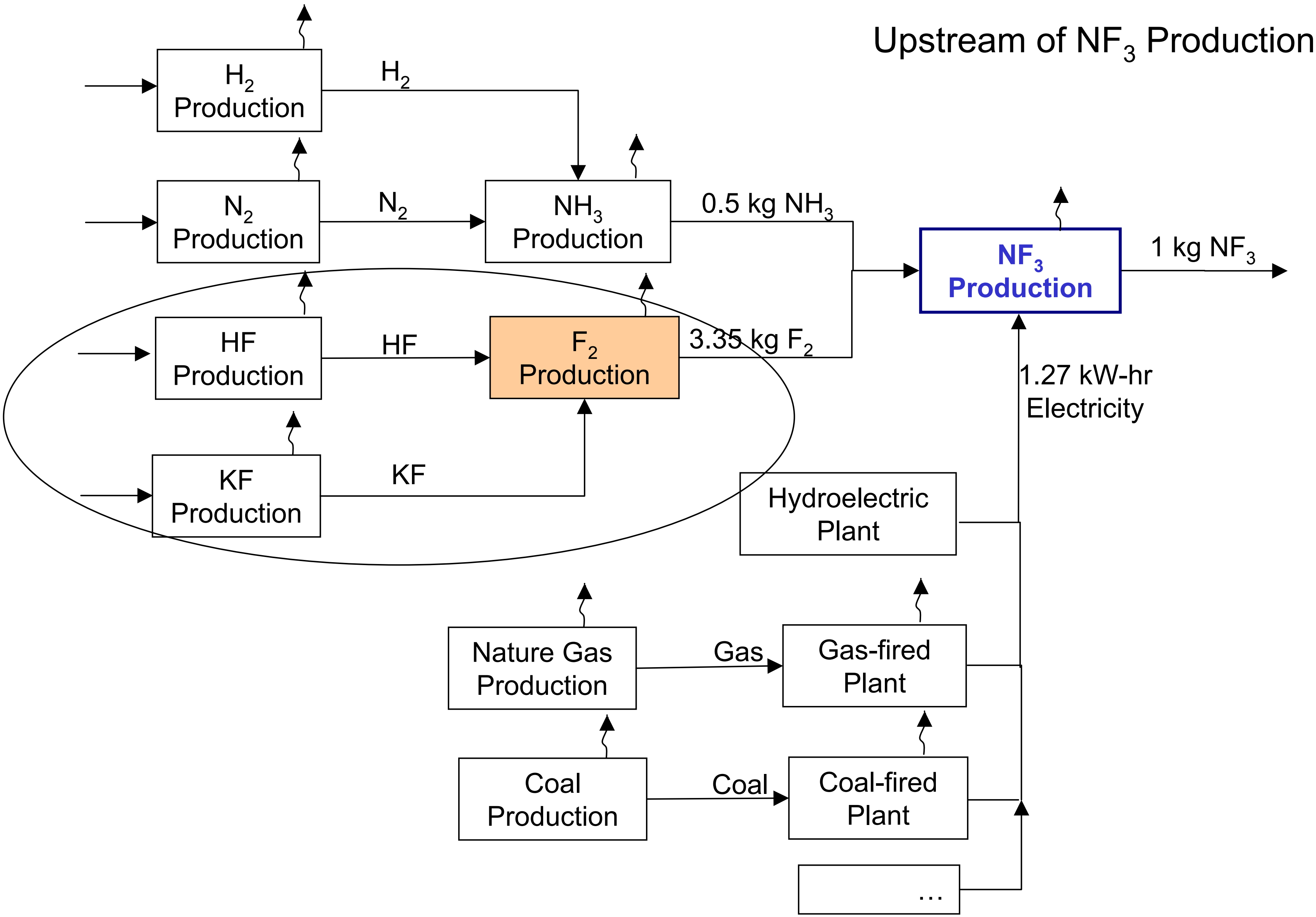
- Basis for Comparison – Same etch Rate r_e for both processes
- Strategy – Same process parameters except $F_{cleaning\ gas,\ in}$
  – Vary $F_{cleaning\ gas,\ in}$ to achieve same r_e

Comparison Boundary – Unit Process



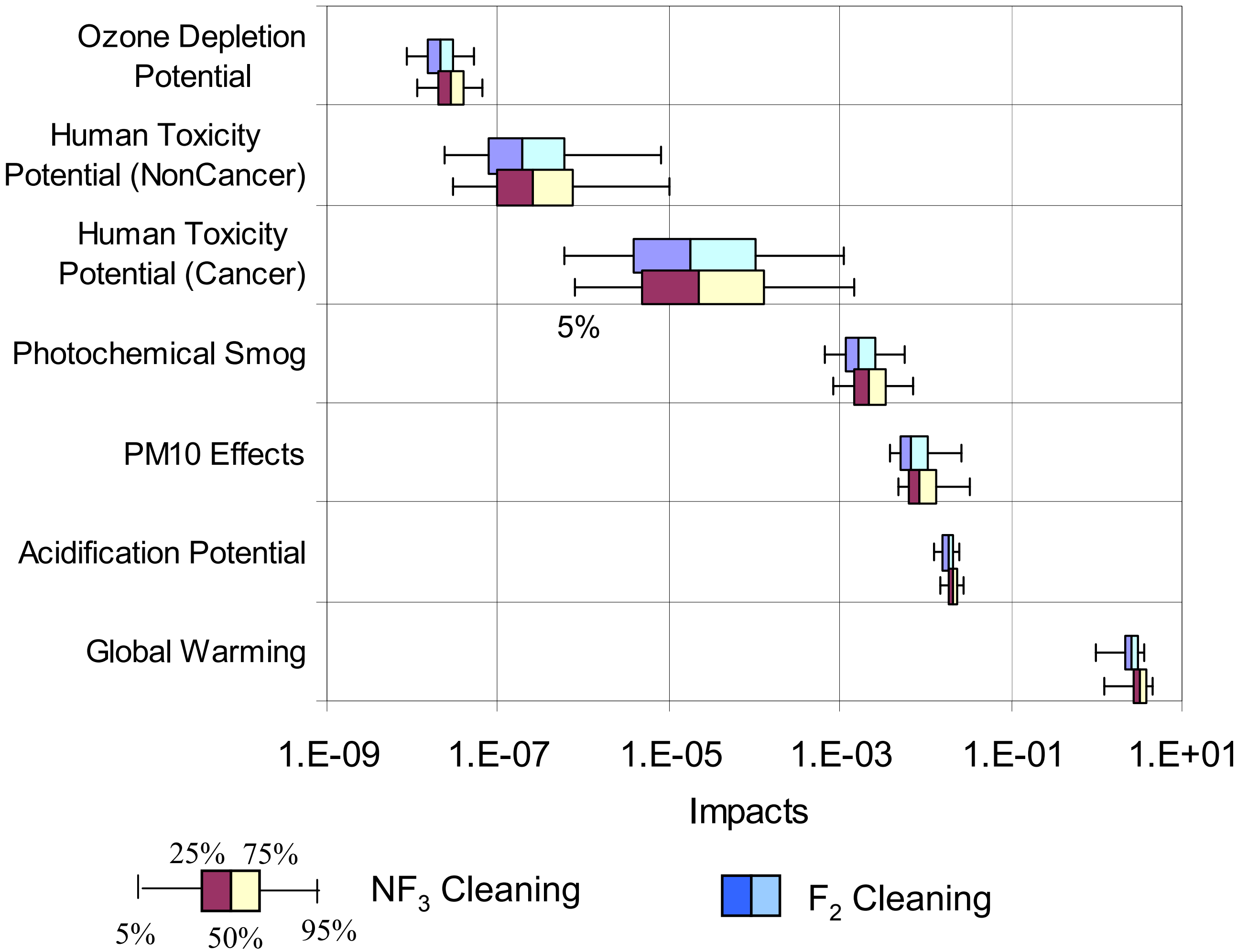
- Similar in Environmental Impacts due to the Same Power, Cleaning Time, and Chamber Temperature
- Similar in Cost of Running the Process

Including Upstream Processes



Comparison in the Life Cycle Boundary

- NF_3 cleaning has higher impacts in all the areas than F_2
- Higher impacts due to energy generation for producing NF_3

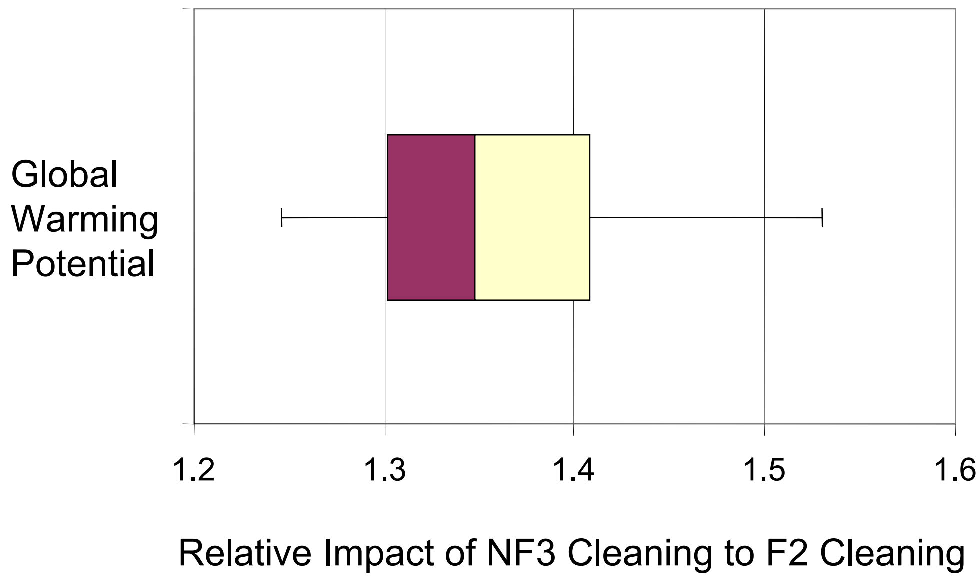


- Ozone Depletion Potential (kg CFC-11 equivalent/kg)
- Human Toxicity Potential-NonCancer (DALYs/kg)
- Human Toxicity Potential-Cancer (DALYs/kg)
- Photochemical Smog (kg Ethylene equivalent/kg)
- PM10 Effects (kg PM10 equivalent/kg)
- Acidification Potential (kg SO2 equivalent/kg)
- Global Warming (kg CO2 equivalent/kg)

Relative Impact of Two Cleaning Processes

- Strong correlation between results of NF_3 case and F_2 case
- Reduce correlation effect by using relative values

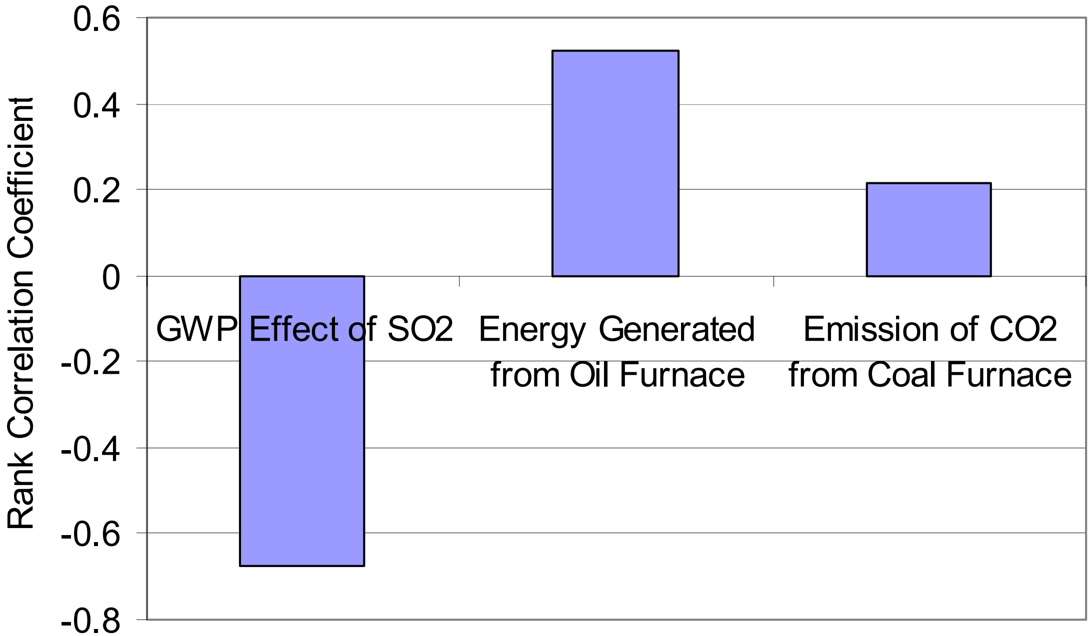
$$\frac{\left(\sum_i H_{i,GWP} E_i\right)_{NF_3}}{\left(\sum_i H_{i,GWP} E_i\right)_{F_2}} \Rightarrow$$



- Uncertainty of relative impact is much smaller than inputs

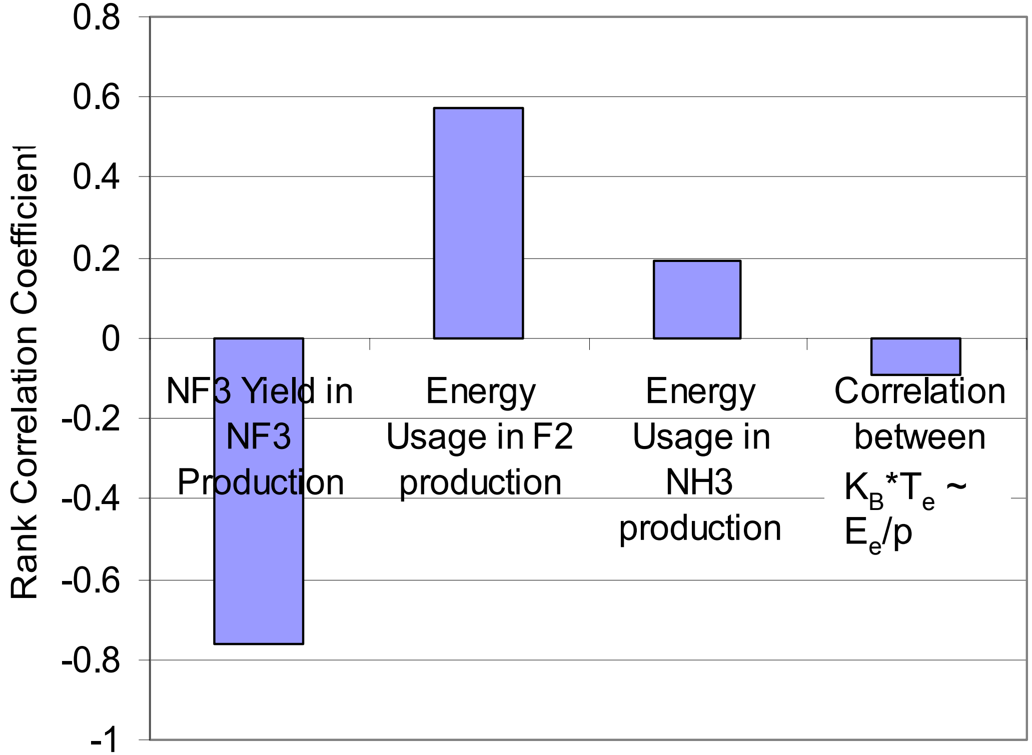
Identifying Important Parameters

- Which parameters are important is also influenced by the goals of the analysis



Top three parameters that contribute the most to the uncertainty of GWP of F_2 cleaning

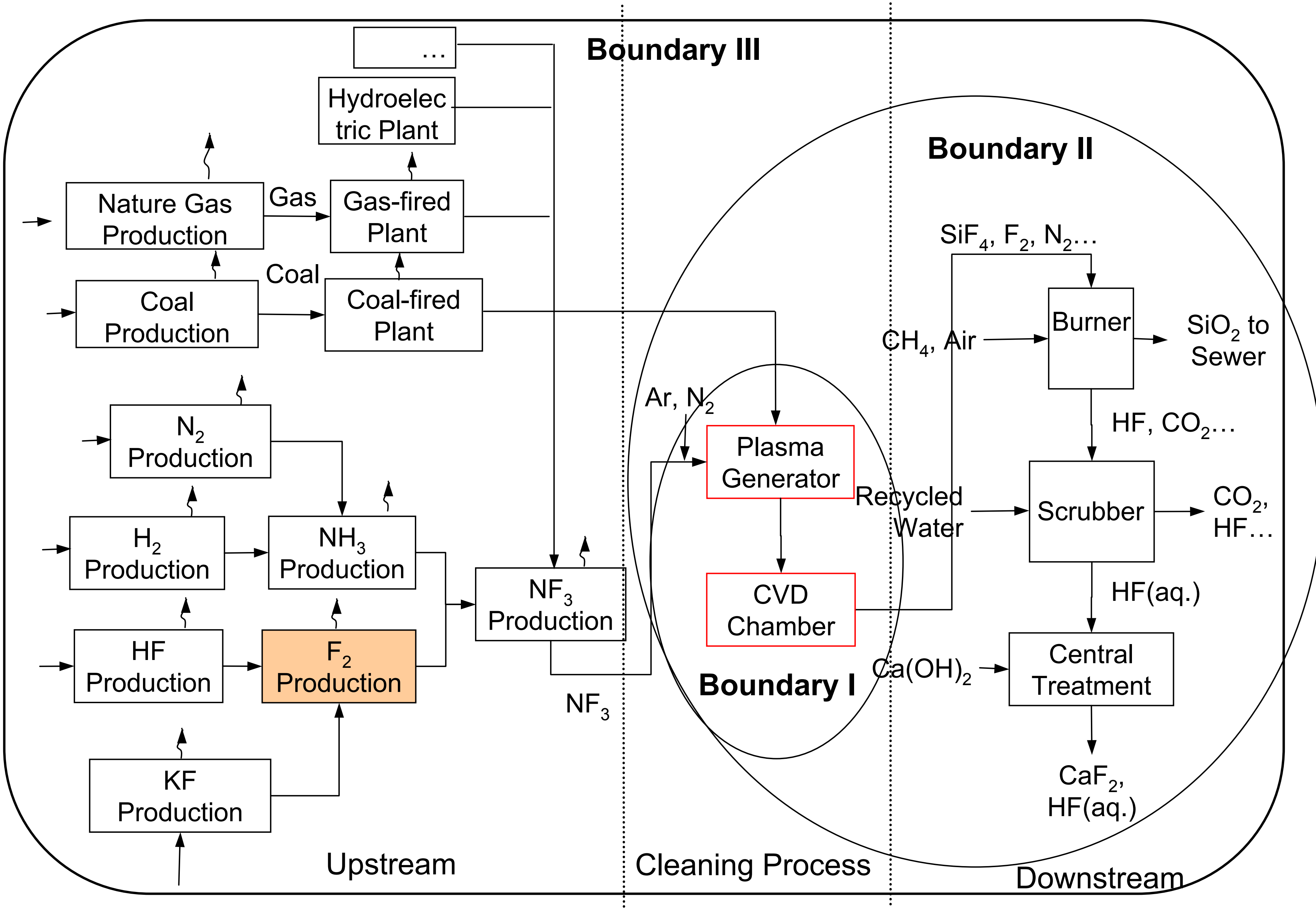
Identifying Important Parameters



Top four parameters that contribute the most to the uncertainty of the relative impact of GWP

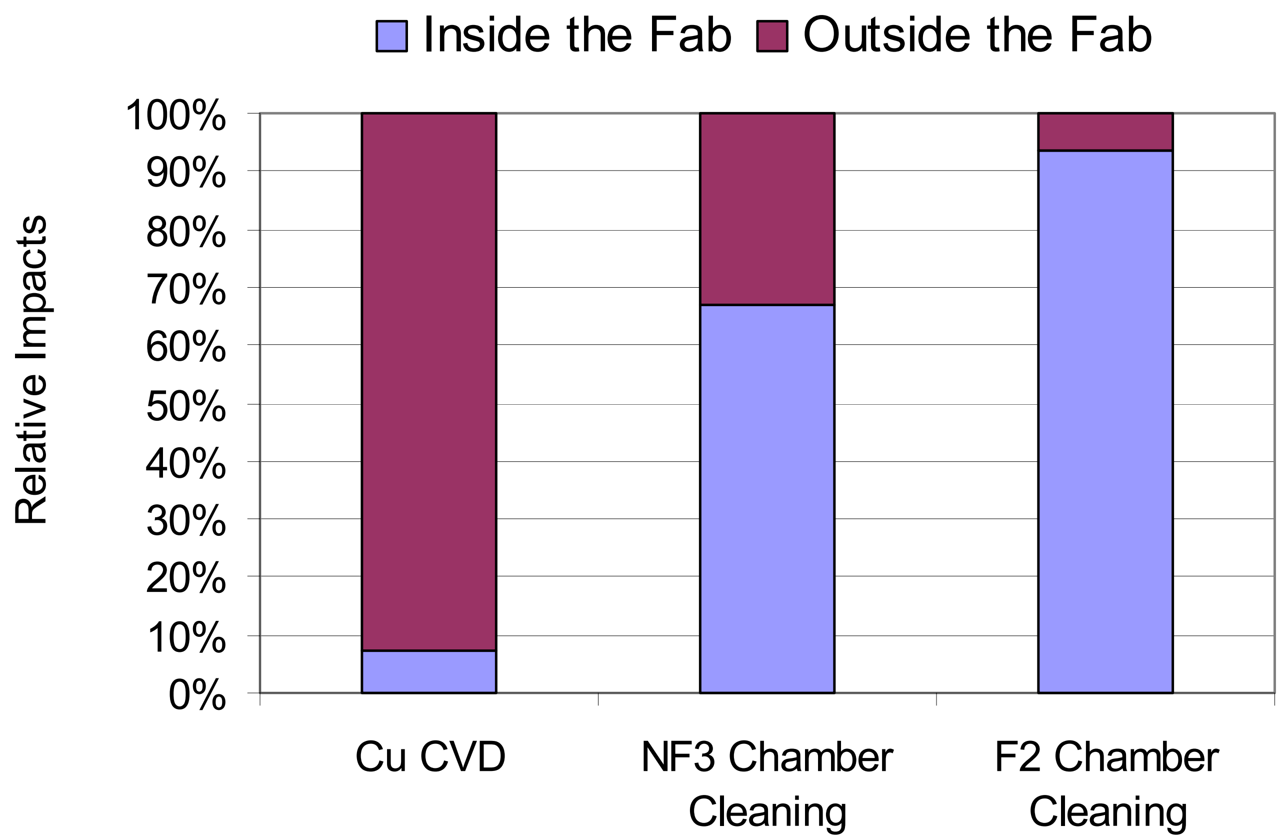
- Top three parameters are related to upstream production
- Identification of important parameters enables efficient allocation of data collection effort – spend money and time in the most valuable place!

Importance of Considering Multi-Boundaries

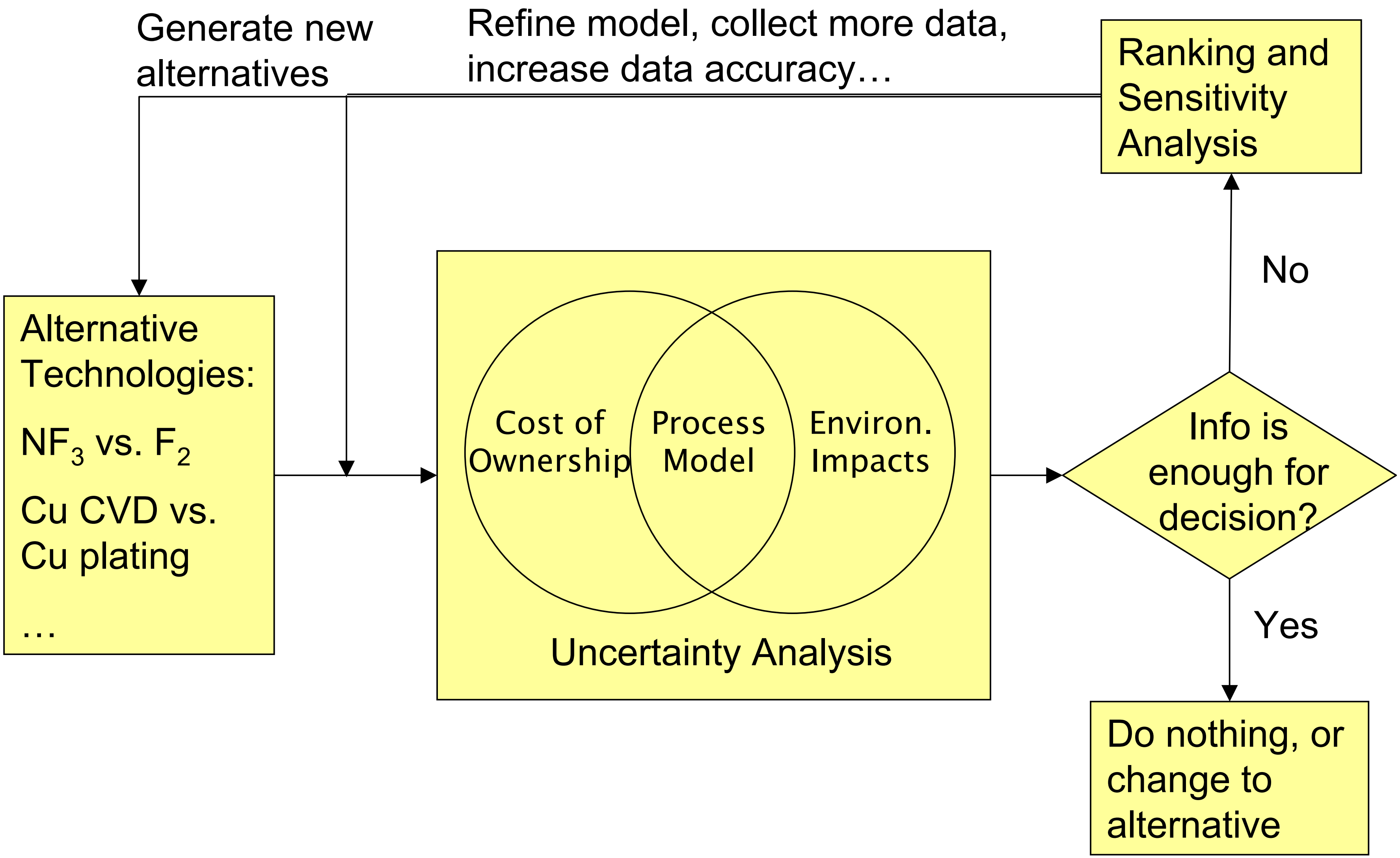


Boundary of Environmental Analysis

- Boundary of the environmental analysis directly affects the results



Framework of Decision-Making Process



Conclusions and Key Points

- The integration of process models, COO, and environmental evaluations is critical and doable.
- Large uncertainty in the inputs does not necessarily lead to low confidence in decisions.
- System boundaries strongly affect the outcomes of the evaluations.

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End of Presentation