Technology Choices in the Presence of Uncertainties

An Update on the Economic and Environmental Issues Influencing the Choice of NF₃ vs. F₂ as a Chamber Cleaning Gas

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Environmentally Benign Semiconductor Manufacturing
Tele-seminar 6th November 2003
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$_2$?)

<table>
<thead>
<tr>
<th>Decision Criteria</th>
<th>NF$_3$</th>
<th>F$_2$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluorine usage rate at the same etch rate (mole/min)</td>
<td>0.15</td>
<td>0.17</td>
<td>This work</td>
</tr>
<tr>
<td>Cost/mole of Fluorine</td>
<td>$6</td>
<td>$0.8</td>
<td>[1]</td>
</tr>
<tr>
<td>LCA Global Warming Effect (kg CO$_2$ equivalent/kg)</td>
<td>3.3</td>
<td>2.4</td>
<td>This work</td>
</tr>
<tr>
<td>Toxicity LC$_{50}$ (ppm)</td>
<td>6700</td>
<td>180</td>
<td>[2,3]</td>
</tr>
</tbody>
</table>

**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

Environmental Evaluation

- 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

- 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 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$_2$

**Comparison criteria**: cleaning performance, environmental impacts, cost
Including Downstream Treatment

SiF₄, F₂, N₂...

CH₄, Air

Burner

SiO₂ to Sewer

Packed-Bed Scrubber

CO₂, N₂, O₂, Ar, Low Concentration HF

Recycled Water

HF, CO₂...

HF(aq.) to Central Treatment

- Fuel Usage – Similar
- Water Usage – 548 gallon/yr for NF₃, 566 gallon/yr for F₂
  – Insignificant compared to 1 million gallon/day
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 Model Hierarchy

<table>
<thead>
<tr>
<th>Process Model Hierarchy</th>
<th>Distribution of Flows</th>
<th>Resources Needed</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Simple stoichiometric yield</td>
<td><img src="image1" alt="Graph" /></td>
<td>1</td>
</tr>
<tr>
<td>2 Lumped kinetics (3 reactions)</td>
<td><img src="image2" alt="Graph" /></td>
<td>10</td>
</tr>
<tr>
<td>3 Detailed kinetics (60 reactions)</td>
<td><img src="image3" alt="Graph" /></td>
<td>100</td>
</tr>
<tr>
<td>4 Model based experiments</td>
<td><img src="image4" alt="Graph" /></td>
<td>1000</td>
</tr>
</tbody>
</table>
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: $2\text{NH}_3 + 3\text{F}_2 \rightarrow 2\text{NF}_3 + 3\text{H}_2$

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

\[ E_{NF_3} = \frac{N_{SiO_2} E_{b-NF_3}}{F\%_{NF_3} \xi_{E-NF_3}} + tP_{plasma} \]
\[ E_{F_2} = \frac{N_{SiO_2} E_{b-F_2}}{F\%_{F_2} \xi_{E-NF_3}} + tP_{plasma} \]

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%, \( \xi_E \), and t

What to do

Use probability distribution functions to describe them
Bayes Theorem – Learning from Data/Models

Data/Model

Prior $p(\theta) \rightarrow$ Analysis System $\rightarrow$ Posterior $p(\theta | y)$

(Updated knowledge)

$\begin{align*}
p(\theta | y) &= \frac{p(y | \theta) p(\theta)}{p(y)}
\end{align*}$

T. Bayes (1702-1761)
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

… Both Bayesian and Frequentist views are useful in practice
Assumed Distributions of Efficiencies and Time

- **Fluorine Utilization Efficiency**
  - \( F\% \sim \text{uniform}(10^{-5}, 0.6) \)
  - \( f(F\%) = \frac{1}{0.6 - 10^{-5}} \)

- **Energy Utilization Efficiency**
  - \( \xi_E \sim \text{uniform}(10^{-10}, 0.6) \)
  - \( f(\xi_E) = \frac{1}{0.6 - 10^{-10}} \)

- **Cleaning Time**
  - \( t (s) \sim \text{uniform}(6 \times 10^{-4}, 1200) \)
  - \( f(t) = \frac{1}{1200 - 6 \times 10^{-4}} \)

- **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**

- **Process Model**
  - Design Decisions
  - Upstream & Downstream Emissions, Material and Energy Usage
  - Flow Rates
    - Products
    - Byproducts
    - Chemical Energy
    - Water
    - Waste
    - Yield
    - Process Time
    - ... Environmental Properties
    - Chemical Properties
    - Exposure Properties
  - Input Output LCA Model
  - Emissions
    - Human Toxicity
    - Global Warming Effect
    - Ozone Depletion Effect
    - Respiratory Effect
    - ... Human Exposure
    - Environmental Concentration
    - Fate, Transport, and Exposure Model
  - Impact Indicator
    - Weighting Factors
    - Compliance with Regulations
  - Environmental Performance

- Alternative Designs
Environmental Impacts from LCA

- Comparison of the global warming potential of the two processes
Where Shall We Go Next?

Uncertainty of 10% is too large for a confident decision?

Yes → Where to collect data and refine model?

No → Identify important parameters!

No need for further analysis

- Uncertainty can come from
  - Process model
  - Upstream and downstream data
  - LCA model/data
## Important Parameters of Affecting Relative GWP

### Table I

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Rank Correlation Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F%_{NF3}$</td>
<td>-0.64</td>
</tr>
<tr>
<td>$F%_{F2}$</td>
<td>0.46</td>
</tr>
<tr>
<td>Cleaning Time $t$ (s)</td>
<td>-0.28</td>
</tr>
<tr>
<td>$\xi_{E, NF3}$</td>
<td>-0.20</td>
</tr>
<tr>
<td>$\xi_{E, F2}$</td>
<td>0.12</td>
</tr>
<tr>
<td>NF3 Yield in NF3 Production from NH3 and HF</td>
<td>-0.11</td>
</tr>
<tr>
<td>H$_2$S Emission from Oil-Fired Power Plant (kg/ kW-h Energy)</td>
<td>-0.083</td>
</tr>
<tr>
<td>Electricity Used in Diesel Fuel Production (MJ/kg)</td>
<td>0.078</td>
</tr>
<tr>
<td>GWP of C$_2$H$_3$Cl$_3$ (kg CO$_2$ equivalent/kg)</td>
<td>0.067</td>
</tr>
<tr>
<td>GWP of CH$_2$Cl$_2$ (kg CO$_2$ equivalent/kg)</td>
<td>0.061</td>
</tr>
</tbody>
</table>

### 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 \( \text{Ar} + e \rightarrow \text{Ar}^+ + 2e \)
  - Electron loss and production are linear to electron concentration
  - Diffusion of electrons dominates the transport of electrons.

\[
\begin{align*}
NF_3 + e & \rightarrow NF_2 + F\cdot + e & k_3 = 2.06 \times 10^{-17} T_e^{1.7} \exp(-37274/T_e) \\
NF_2 + e & \rightarrow NF + F\cdot + e & k_2 = 1.57 \times 10^{-17} T_e^{1.8} \exp(-27565/T_e) \\
NF + e & \rightarrow N + F\cdot + e & k_1 = 1.57 \times 10^{-17} T_e^{1.8} \exp(-27565/T_e) \\
F_2 + e & \rightarrow F^- + F\cdot & k = 1.02 \times 10^{-5} T_e^{-0.9} \exp(1081.8/T_e)
\end{align*}
\]

\[
F\cdot + \text{SiO}_2 \rightarrow \text{SiF}_4
\]

\[
r = (8.97 \pm 0.82) \times 10^{-13} n_F T_s^{1/2} \exp\left(-\frac{0.163 eV}{kT_s}\right)
\]

\[
\begin{align*}
n_{F, NF_3} &= \frac{\beta_3 \tau n_{NF_3, in}}{1 + \beta_3 \tau} + \frac{\beta_2 \beta_3 \tau^2 n_{NF_3, in}}{(1 + \beta_2 \tau)(1 + \beta_3 \tau)} + \frac{\beta_1 \beta_2 \beta_3 \tau^3 n_{NF_3, in}}{(1 + \beta_1 \tau)(1 + \beta_2 \tau)(1 + \beta_3 \tau)} \\
n_{F, F_2} &= \frac{\beta_{F_2} \tau n_{F_2, in}}{1 + \beta_{F_2} \tau} \\
\beta_i &\equiv k_i n_e
\end{align*}
\]
Process Modeling Results

Etch Rate – Falls into industrial experience

Table II

<table>
<thead>
<tr>
<th>Important Parameters that Affect Etch Rate</th>
<th>Rank Correlation Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Film surface temperature (K)</td>
<td>0.545</td>
</tr>
<tr>
<td>Activation energy in the SiO₂ etch rate equation (J)</td>
<td>-0.403</td>
</tr>
<tr>
<td>Power of the electron temperature of NF₃ disassociation reaction in plasma</td>
<td>0.416</td>
</tr>
<tr>
<td>Chamber temperature (K)</td>
<td>-0.371</td>
</tr>
<tr>
<td>Electron temperature (eV)</td>
<td>0.243</td>
</tr>
</tbody>
</table>
Fluorine Utilization Efficiency Results

- The F₂ 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

• 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.

First Process Modeling Level

Second Process Modeling Level
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

Boundary I
- SiF$_4$, F$_2$, N$_2$…
- Ar, N$_2$
- H$_2$ Production
- F$_2$ Production
- NF$_3$ Production
- NH$_3$ Production
- H$_2$ Production
- N$_2$ Production
- Coal-fired Plant
- Gas-fired Plant
- Nature Gas Production
- Coal Production

Boundary II
- Burner
- Scrubber
- Central Treatment
- Plasma Generator
- CVD Chamber
- Cleaning Process
- SiO$_2$ to Sewer
- CO$_2$, HF…
- HF(aq.)
- Ca(OH)$_2$
- CaF$_2$, HF(aq.)

Boundary III
- Hydroelectric Plant
- Upstream
- Downstream

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### Again, Where Shall We Go Next?

#### Table III

<table>
<thead>
<tr>
<th>Important Parameter of Relative GWP at Second Process Modeling Level</th>
<th>Rank Correlation Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power Used in Plasma Generator (W)</td>
<td>0.69</td>
</tr>
<tr>
<td>Power to the Electron Temperature in NF&lt;sub&gt;3&lt;/sub&gt; Disassociation Reaction</td>
<td>-0.37</td>
</tr>
<tr>
<td>NF&lt;sub&gt;3&lt;/sub&gt; Yield in NF&lt;sub&gt;3&lt;/sub&gt; Production from NH&lt;sub&gt;3&lt;/sub&gt; and HF</td>
<td>-0.33</td>
</tr>
<tr>
<td>Energy Used in F&lt;sub&gt;2&lt;/sub&gt; Production (J)</td>
<td>0.21</td>
</tr>
<tr>
<td>Power to the Electron Temperature in NF&lt;sub&gt;2&lt;/sub&gt; Disassociation Reaction</td>
<td>-0.19</td>
</tr>
<tr>
<td>Electron Temperature in the Plasma Source (eV)</td>
<td>-0.13</td>
</tr>
<tr>
<td>Temperature of Surface to be Cleaned (K)</td>
<td>-0.087</td>
</tr>
<tr>
<td>NH&lt;sub&gt;3&lt;/sub&gt; Flow Rate in NF&lt;sub&gt;3&lt;/sub&gt; Production (sccm)</td>
<td>-0.085</td>
</tr>
<tr>
<td>Pre-exponential Term of F&lt;sub&gt;2&lt;/sub&gt; disassociation Reaction in the Plasma</td>
<td>-0.066</td>
</tr>
<tr>
<td>Stir Rate in NF&lt;sub&gt;3&lt;/sub&gt; Production (W/m&lt;sup&gt;3&lt;/sup&gt;)</td>
<td>0.058</td>
</tr>
</tbody>
</table>
Framework of Decision-Making Process

Generate new alternatives

Refine model, collect more data, increase data accuracy...

Ranking and Sensitivity Analysis

No

Info is enough for decision?

Yes

Do nothing, or change to alternative

Uncertainty Analysis

Cost of Ownership

Process Model

Environ. Impacts

Alternative Technologies:

NF$_3$ vs. F$_2$

Cu CVD vs. Cu plating

…
SEMI Cost of Ownership (CoO) Model

**Design Decisions**

- Process Model
  - Flow Rates
    - Products
    - Byproducts
    - Chemical
    - Energy
    - Water
    - Waste
    - Throughput
    - Unit Volume
  - Equipment Yield
    - Parametric Limited Yield
    - Defect Limited Yield

**Annualized Recurring Cost**

- Footprint Prices
- Internal Charges
- Training
- Equipment Cost
- Depreciation Rate

**Annualized Fixed Cost**

**Cost of Equipment Ownership**

**Cost of Yield Loss**

**Good Units per Year**

**Alternative Designs**
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

\[
\begin{align*}
  f(x) &= \frac{2[x-(1-\alpha)m]}{2\alpha^2 m^2} \quad \text{if } (1-\alpha)m < x < m \\
  f(x) &= \frac{2[(1+\alpha)m-x]}{2\alpha^2 m^2} \quad \text{if } m < x < (1+\alpha)m
\end{align*}
\]

- Example:
  Assume nominal value of NF3 price is $0.26/g. Then when \( \alpha = 50\% \), the price of the NF3 gas can change between $0.13/g and $0.39/g.

\( x \) – random variable;
\( \alpha \) – the percentage of change in the nominal value. \( \alpha \sim \text{uniform}(10\%, 90\%); \)
\( m \) – nominal value of the variable.
Distributions of Parameters of the $F_2$ Process

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

\[
\begin{align*}
  f(x) &= \begin{cases} 
  \frac{2[x-(1-\alpha)m]}{\alpha m[\beta m-(1-\alpha)m]} & \text{if } (1-\alpha)m < x < m \\
  \frac{2[1+\alpha)m-x]}{(\beta m-m)[\beta m-(1-\alpha)m]} & \text{if } m < x < \beta m
  \end{cases}
\end{align*}
\]

$\beta$ – Percentage of increase in the nominal value. $\beta \sim \text{uniform}(200\%, 1800\%)$.

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

- By setting the coefficients $\alpha$ and $\beta$ to be random variables, the uncertainty introduced by how these variables are modeled can be studied.
• There is less than 5% that F\textsubscript{2} cleaning will be more costly than NF\textsubscript{3} cleaning

- Where do the large uncertainty of the NF\textsubscript{3} COO come from?
## Identifying Important Parameters of NF$_3$ COO

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Rank Correlation Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power to the Electron Temperature in NF$_3$ Disassociation Reaction</td>
<td>-0.61</td>
</tr>
<tr>
<td>Price of NF3 Gas ($/g)</td>
<td>0.34</td>
</tr>
<tr>
<td>Temperature of Surface to be Cleaned (K)</td>
<td>-0.27</td>
</tr>
<tr>
<td>Power to the Electron Temperature in NF$_2$ Disassociation Reaction</td>
<td>-0.24</td>
</tr>
<tr>
<td>Activation Energy of Etch Reaction (J)</td>
<td>0.23</td>
</tr>
<tr>
<td>Chamber Temperature (K)</td>
<td>0.20</td>
</tr>
<tr>
<td>Electron Temperature in the Plasma Source (eV)</td>
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</tr>
<tr>
<td>Pre-Exponential Term of Etch Reaction</td>
<td>-0.13</td>
</tr>
<tr>
<td>Power to the Electron Temperature in NF$_2$ Disassociation Reaction</td>
<td>-0.12</td>
</tr>
<tr>
<td>Price of Argon Gas ($/g)</td>
<td>0.092</td>
</tr>
</tbody>
</table>

- 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
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  - Weight for Human Toxicity

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

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**
Acknowledgements

- Laura Losey, David Bouldin, Mike Kasner, Tim Yeakley, Larry Novak, Daren Dance, Tina Gilliland – Texas Instruments
- Alejandro Cano-Ruiz and Pauline Ho – Reaction Design
- Joe Van Gompel – BOC Edwards
- Karen Gleason, Herb Sawin and Joel Clark – MIT
- Holly Ho – SEMATECH International
- Engineering Research Center for Environmentally Benign Semiconductor Manufacturing – NSF/SRC.
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