Treatment of Uncertainties in ESH Assessments – New Approaches and Data Needs

Teleseminar

Task D3

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Outline

- Background
- Proposed ESH analysis methodology
- Construction of database for ESH assessment

Key Environmental Challenges and Needs

- More quantitative environmental metrics
- Systematical evaluation approach to environmental impacts
- Database that includes important chemical properties
- *Consideration of uncertainty in the environmental evaluation*
- Rapid environmental evaluation
- Life Cycle Assessment (LCA) beyond the factory
- Dynamic simulation of the processes
- Advanced process control, sensing and metrology
- Multi-objective optimization and decision support

Scope and Strategy

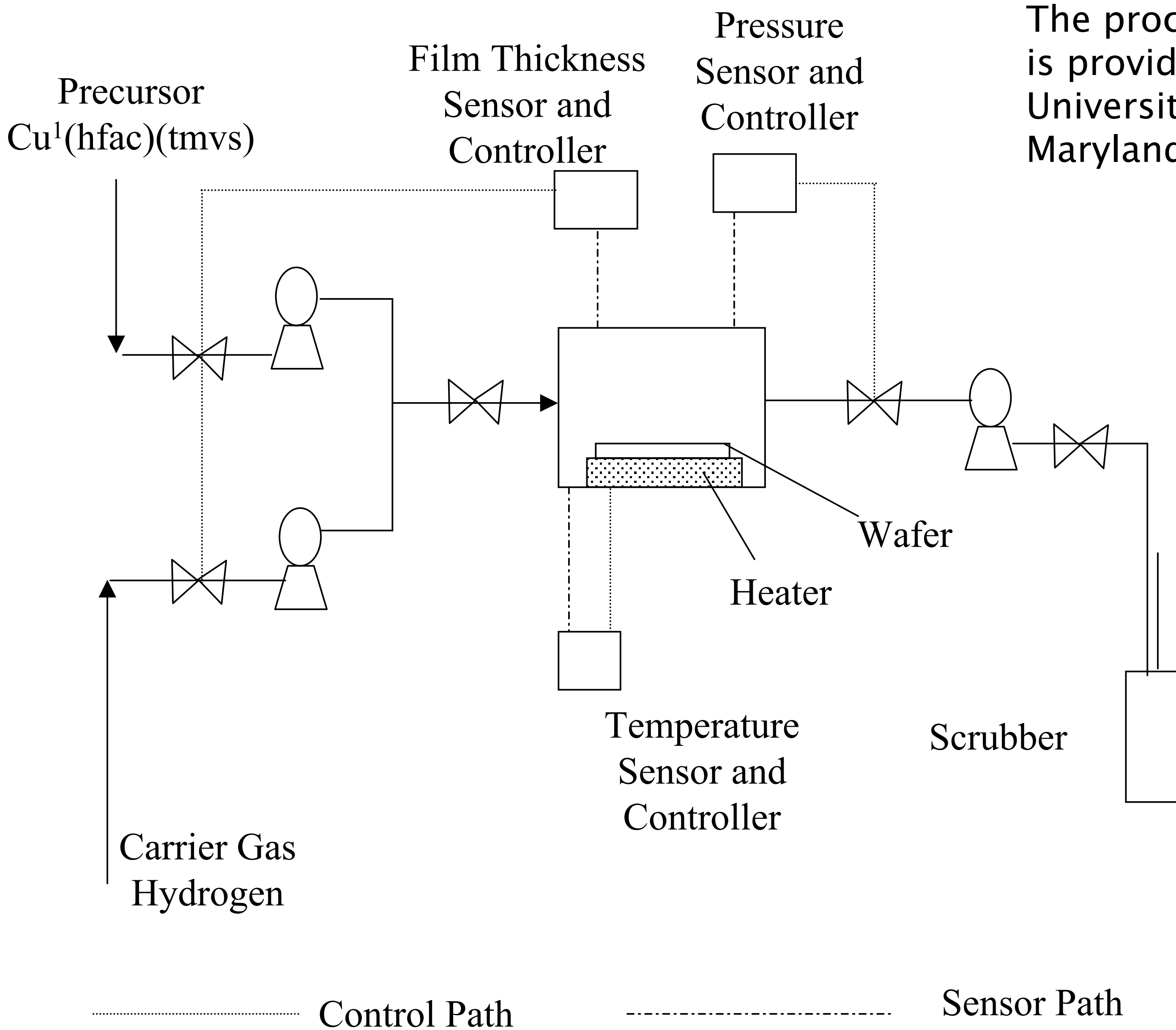
- Develop methodologies and metrics for *rapid economic and environmental evaluation*
- Integrate *the treatment of uncertainties* into decision making about alternative technologies
- Identify opportunities for creating 'win-win' situations
- Test procedures using case studies
- Collaboration with University of Maryland and UC Berkeley.

Proposed Analysis Methodology

1. Process model
2. Economic evaluation of technology choice (CoO Model)
3. Life cycle assessment model of environmental impacts
4. Treatment of uncertainties

Case Study—Cu CVD

The process model is provided by University of Maryland.



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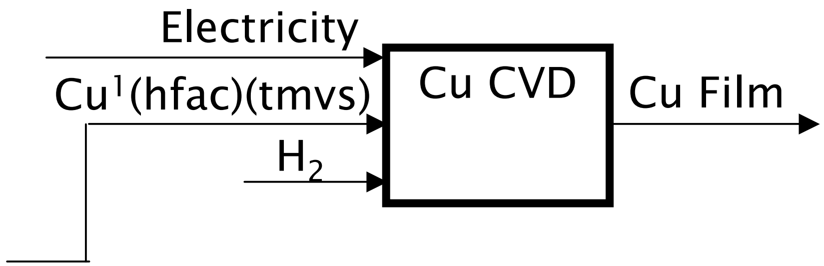
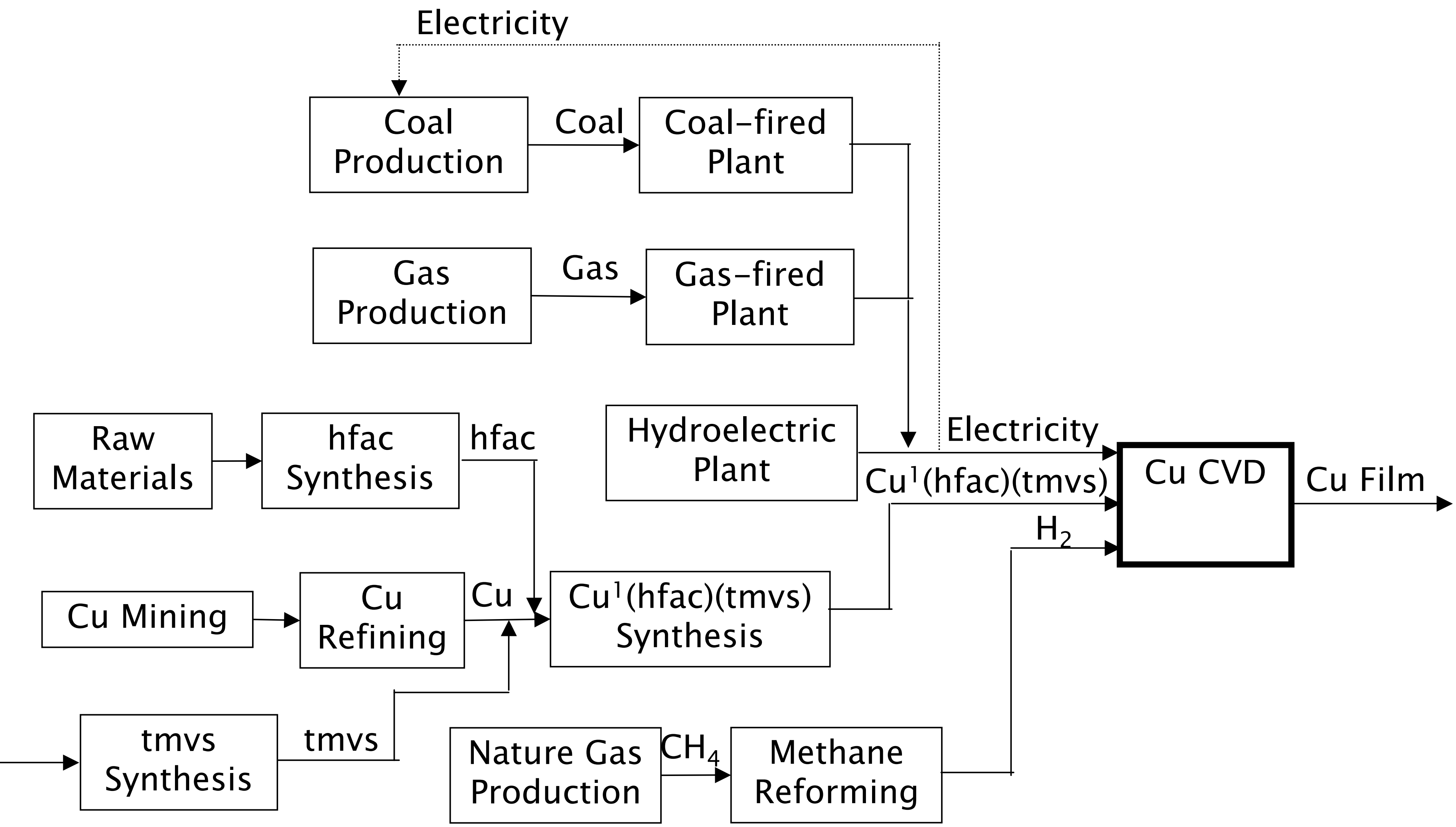
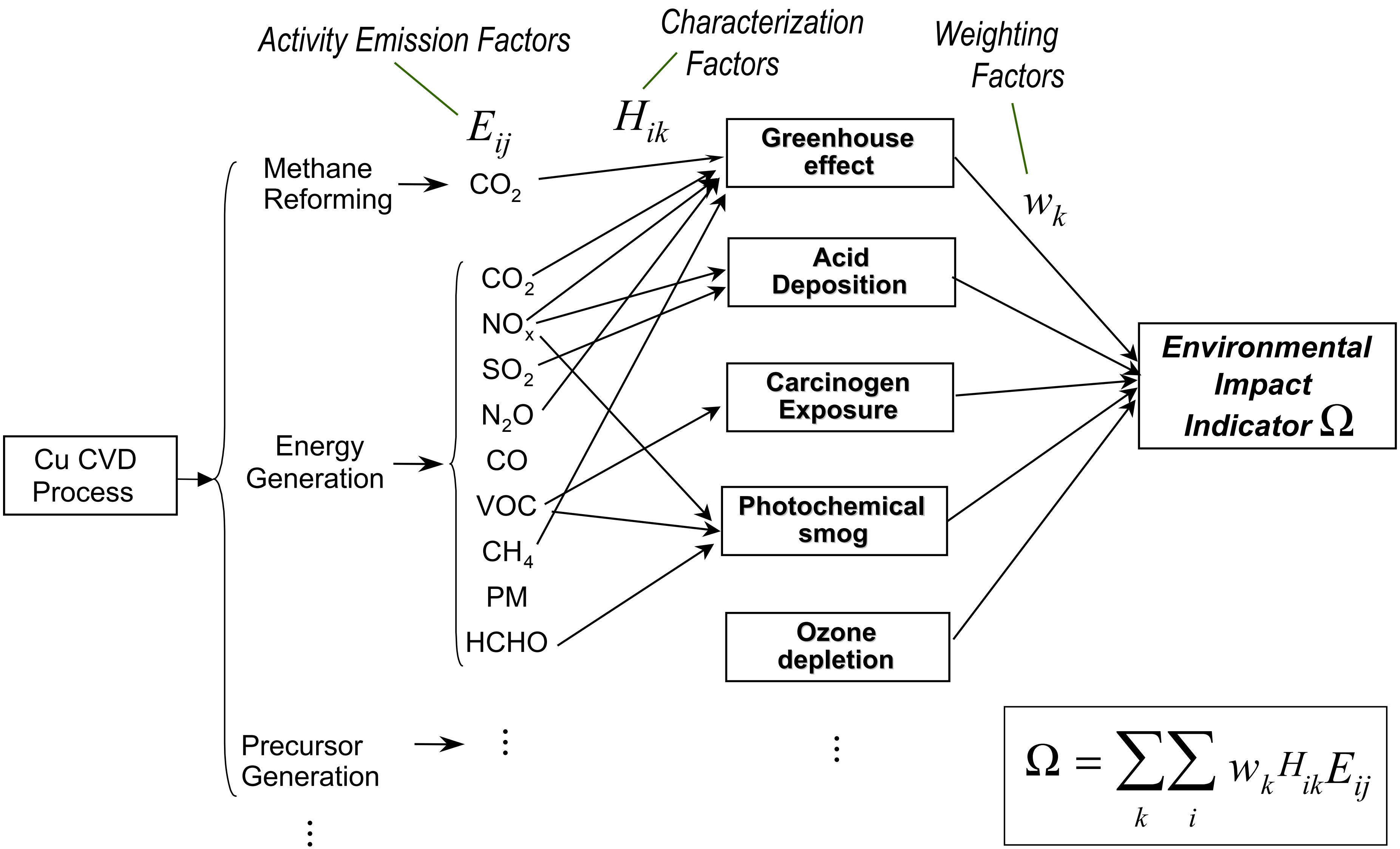
Cu CVD Process Model



Impacts beyond the Plant Boundaries (LCA)



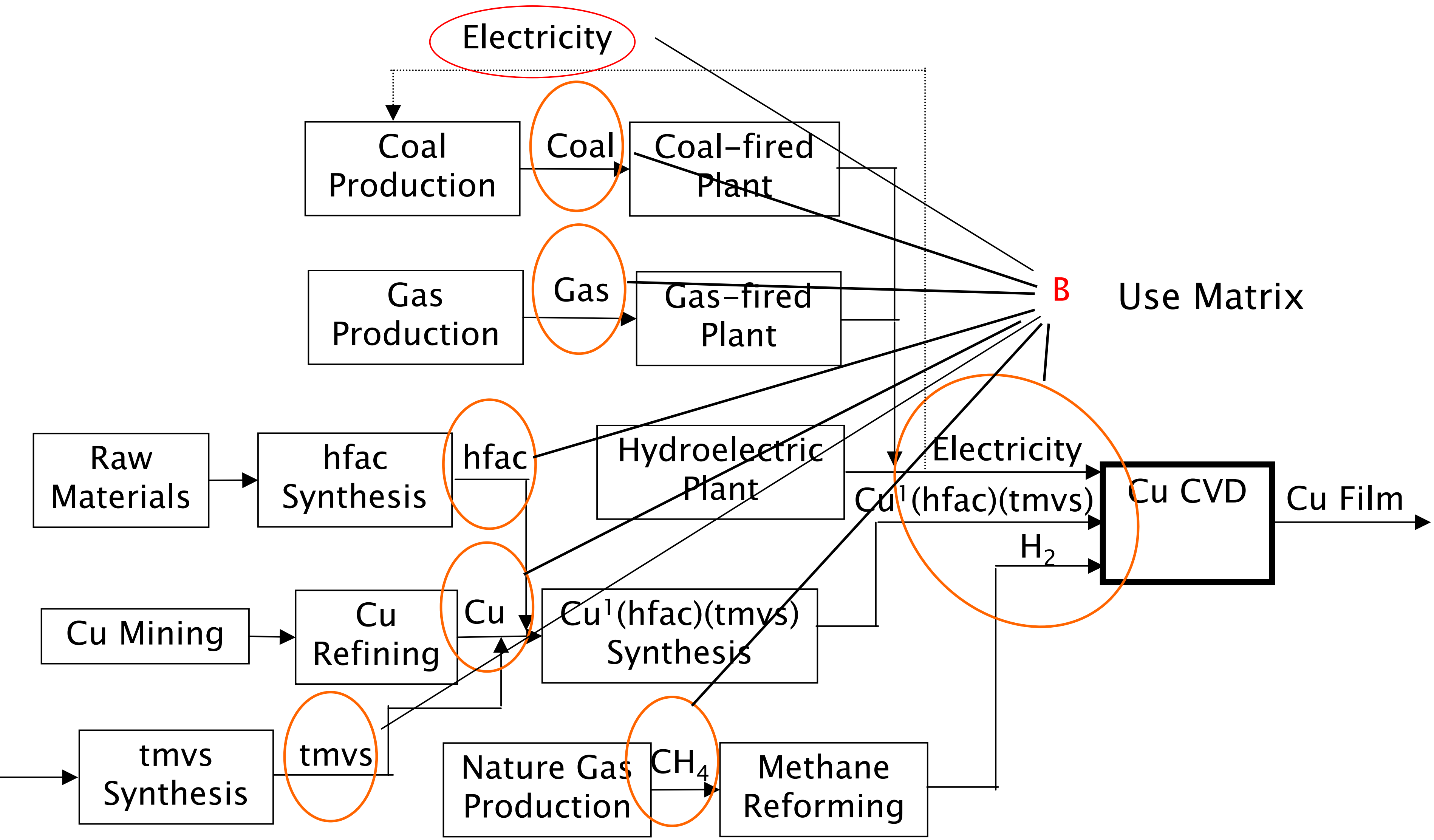
Components of an Environmental Valuation Model*



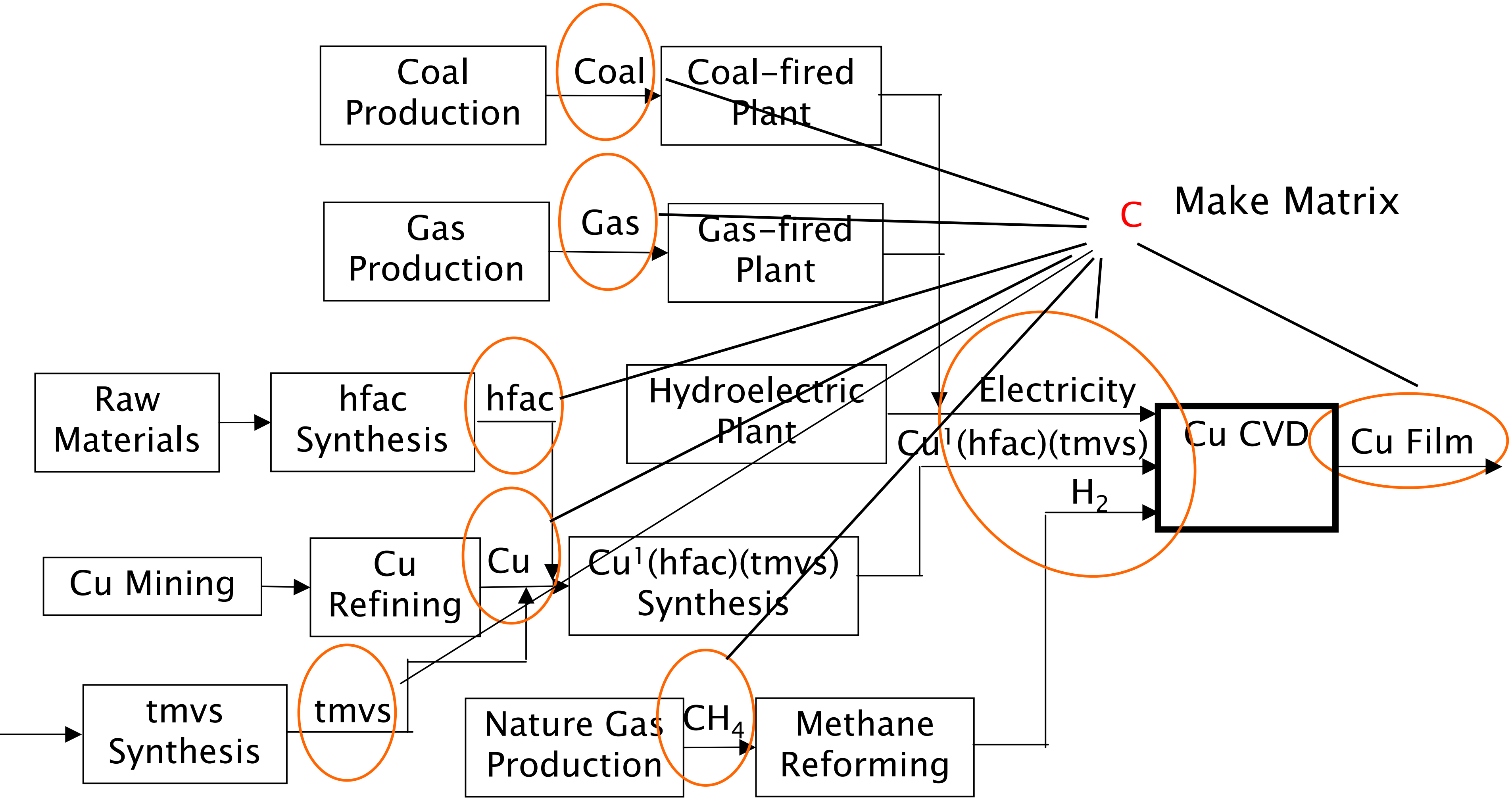
$$\Omega = \sum_k \sum_i w_k H_{ik} E_{ij}$$

* Cano-Ruiz 2000

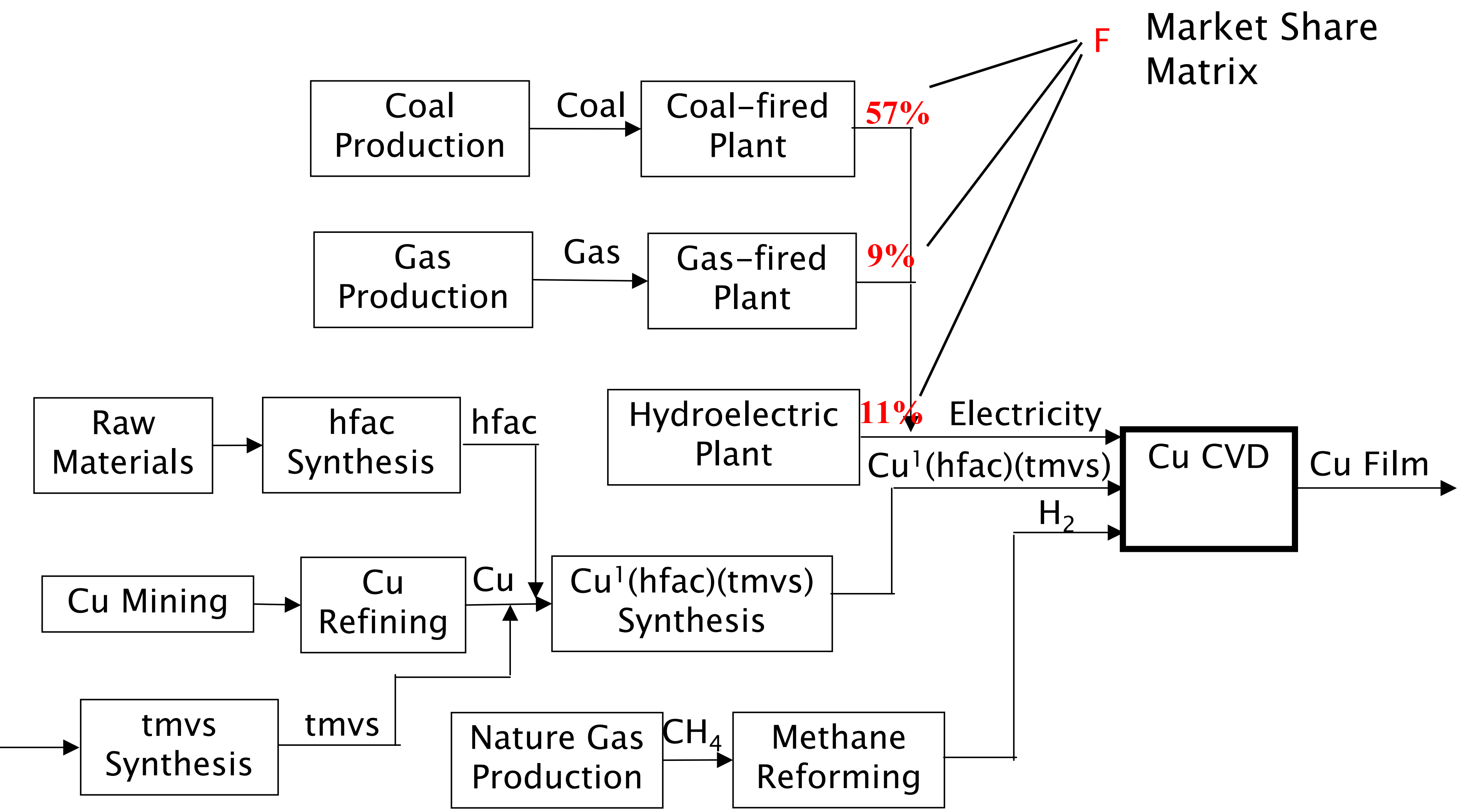
Model Input One: Use Matrix (B)



Model Input Two: Make Matrix (C)



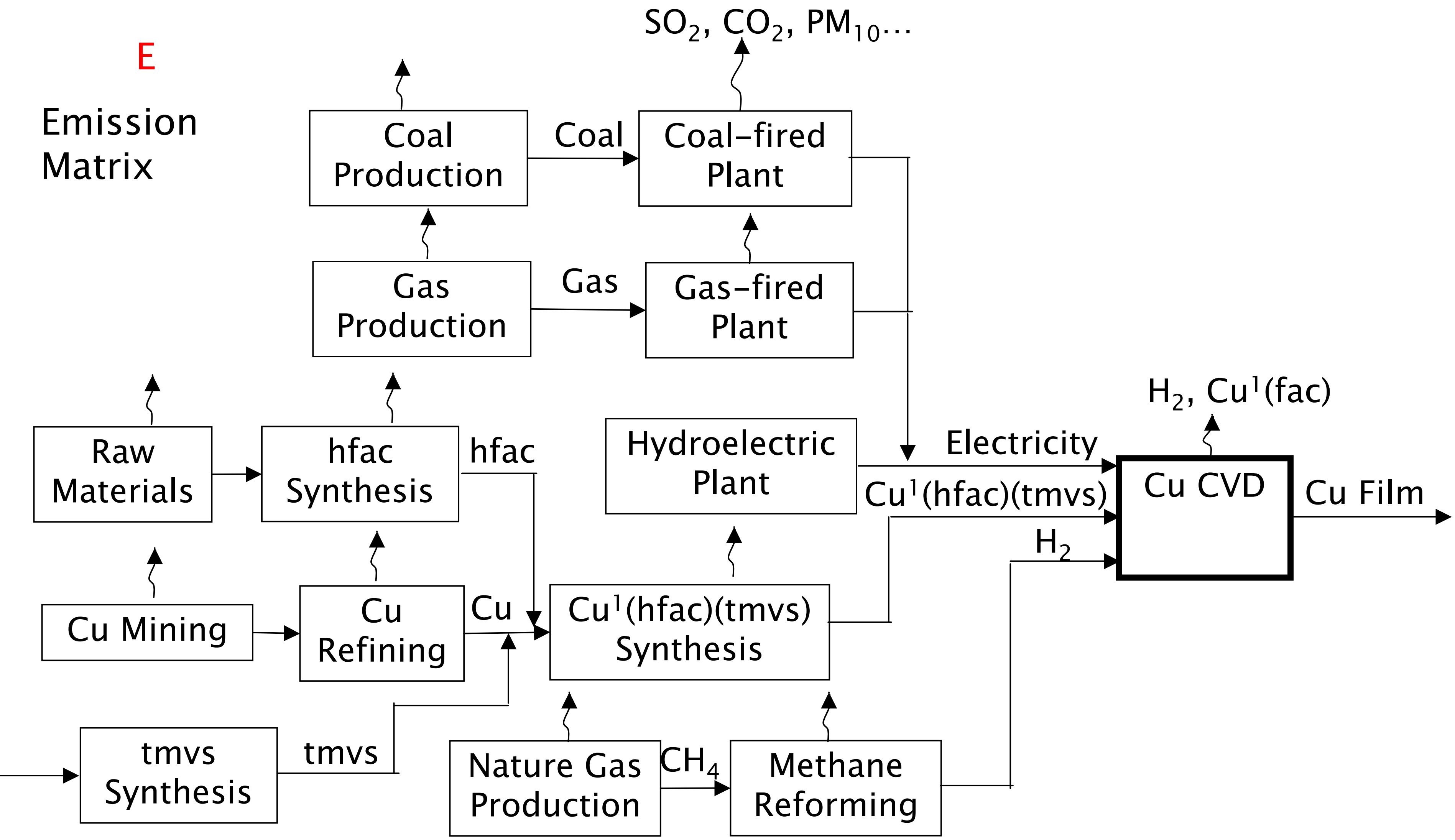
Model Input Three: Market Share Matrix (F)



Model Input Four: Emission Matrix (E)

E

Emission Matrix



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 → Valuation Factor

- Large uncertainties imbedded in the values

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)

$$e = Ex$$

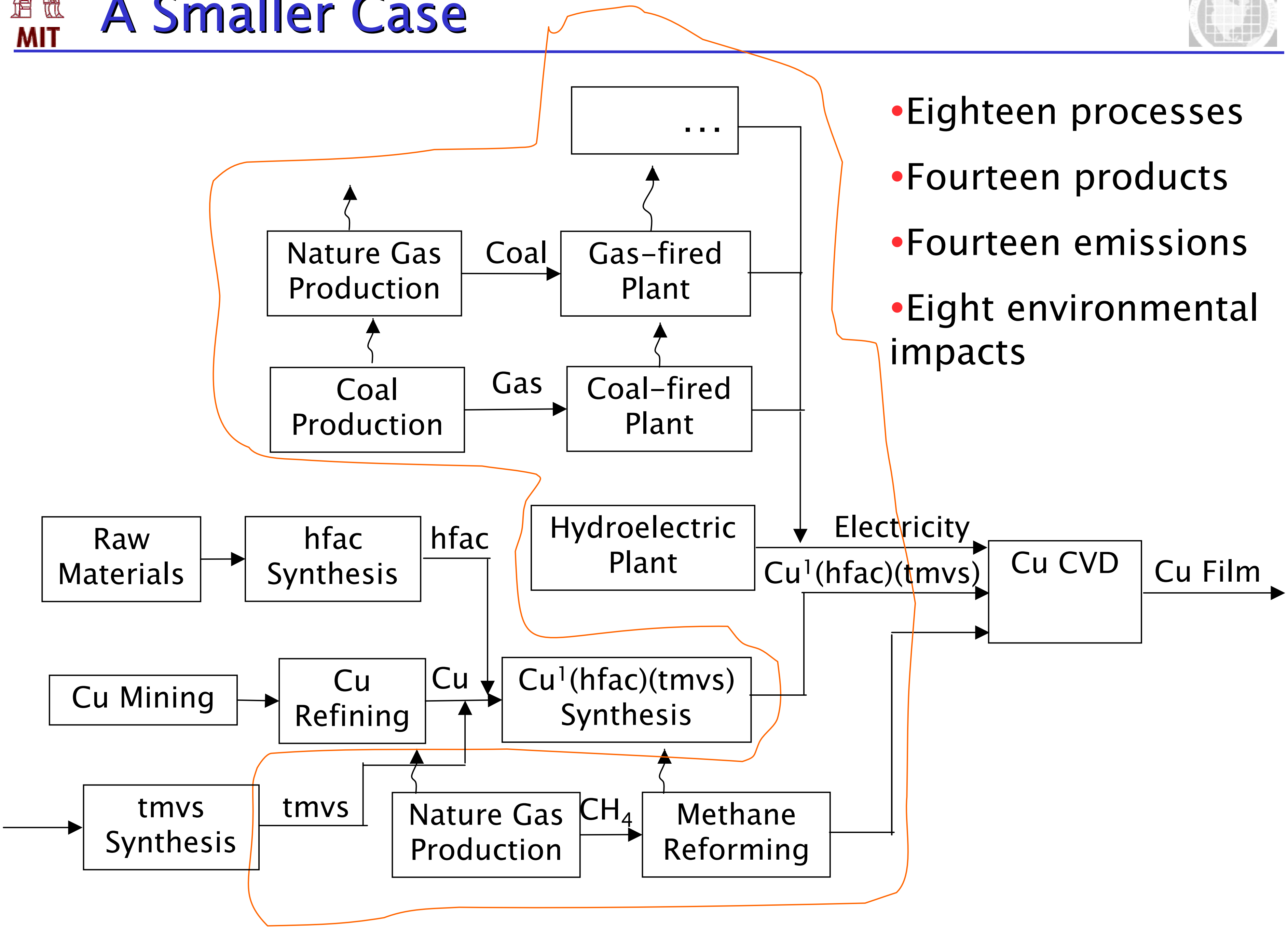
- Impact valuation by process ($\Omega_{process}$)

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

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

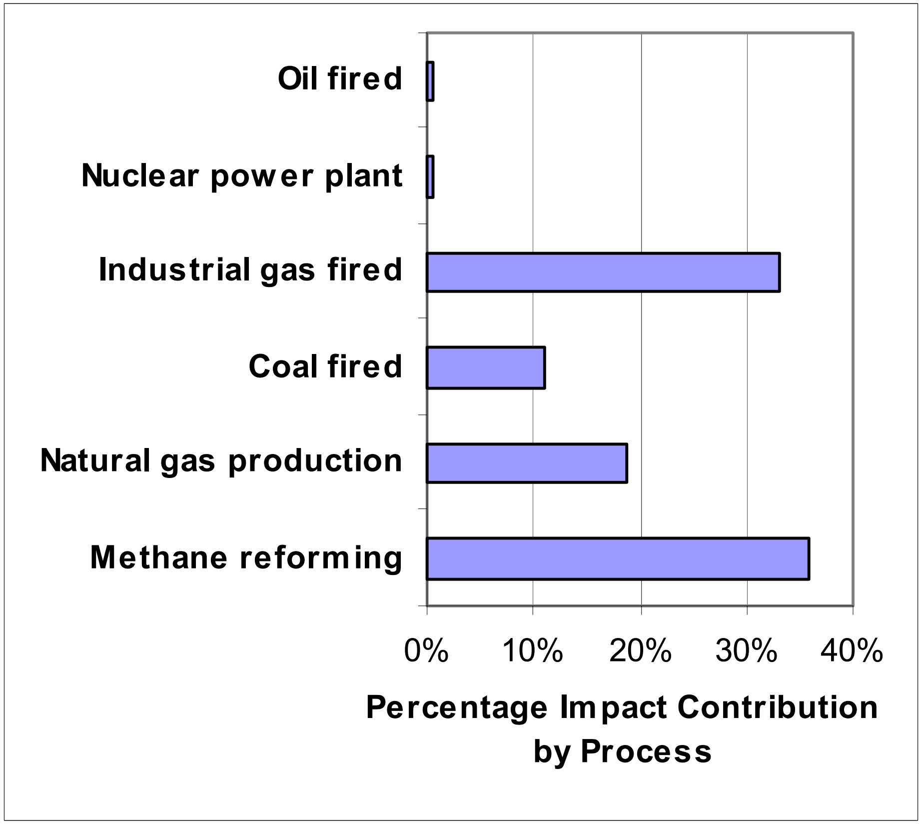
$$\Omega_{emission} = \mathrm{Diag}(e)\, H\, w$$

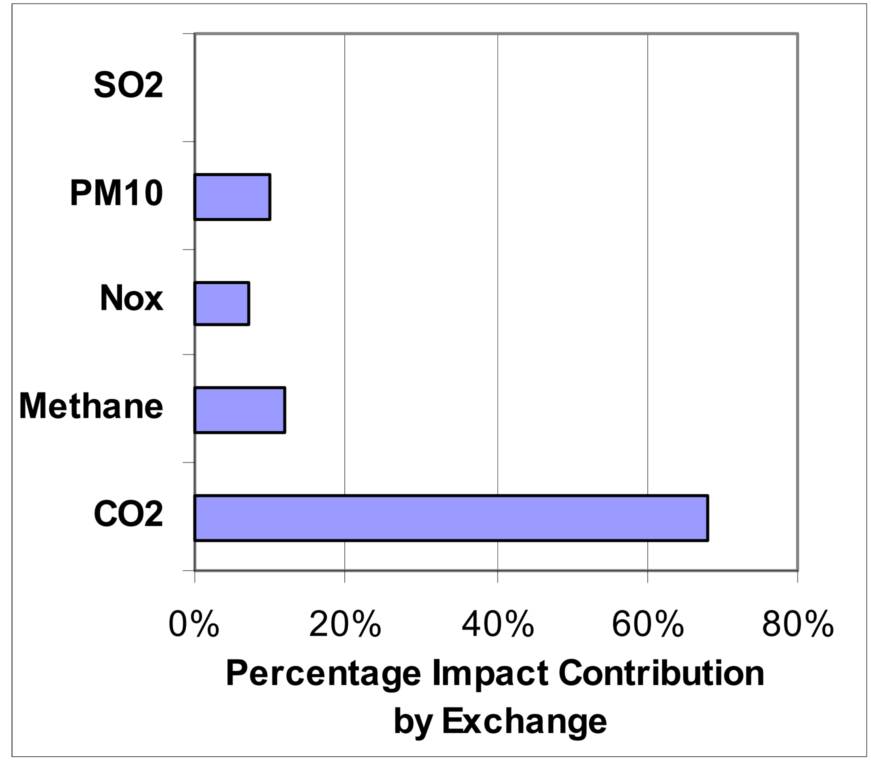
A Smaller Case



- Eighteen processes
- Fourteen products
- Fourteen emissions
- Eight environmental impacts

Evaluation Results





- Large impact is also from methane reforming to produce H_2 in contrast to common perception that power generation has the dominant impact
- Changing carrier gas may reduce environmental impact

Data Needed for Complete Evaluation

- Production methods of hfac, tmvs, and Cu^{1}(hfac)(tmvs)
- ESH information of hfac, tmvs, and Cu^{1}(fac)

Proposed Analysis Methodology

1. Process model
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Motivation for Uncertainty Analysis

- To better identify important parameters
- To decrease decision uncertainty in choosing alternative technologies

- Large uncertainties are imbedded in environmental evaluation

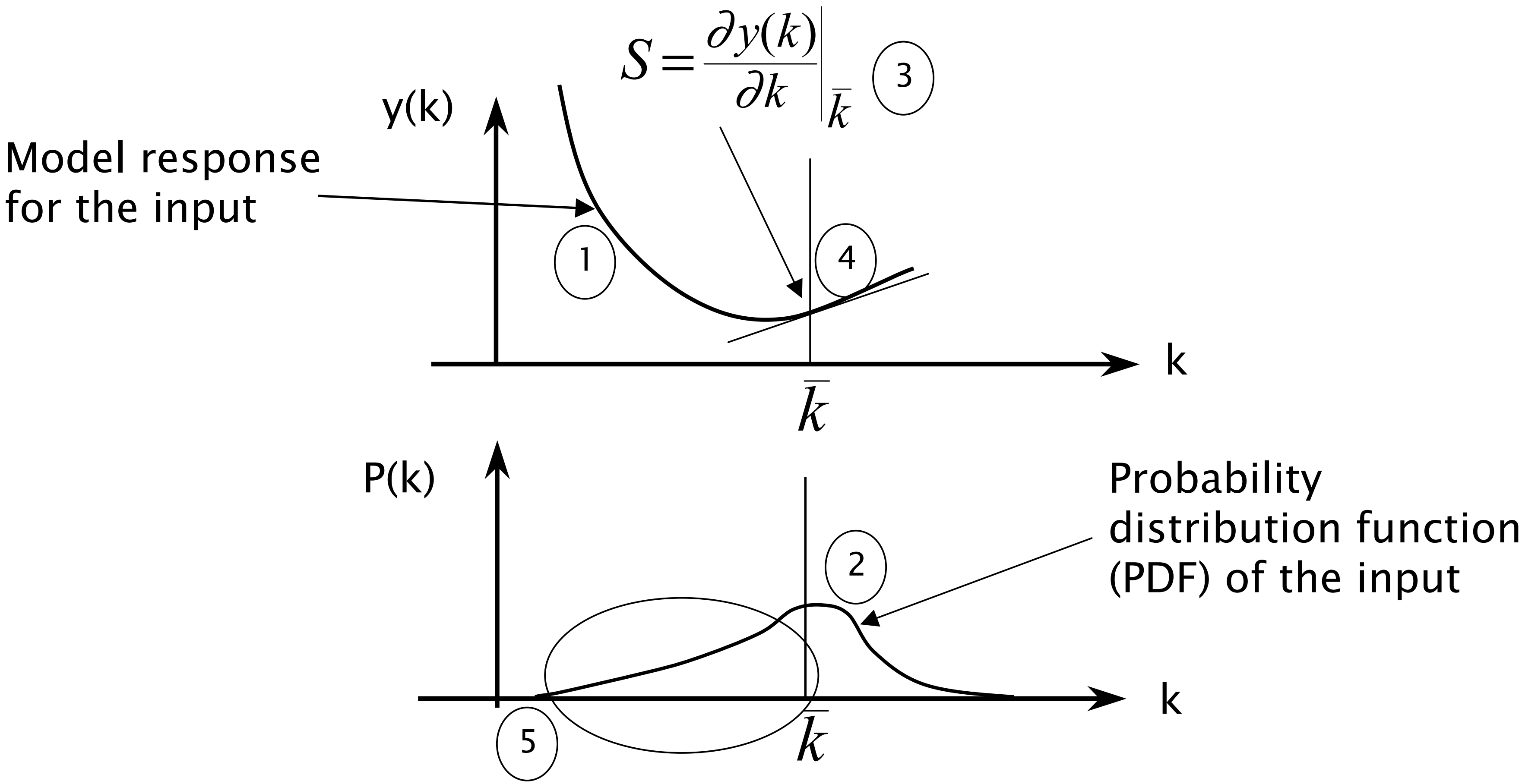
Example: ~1 order of magnitude in air pollutant emission factors

2 ~ 3 orders of magnitude in cancer indicators

3 ~ 6 orders of magnitude in non-cancer indicators

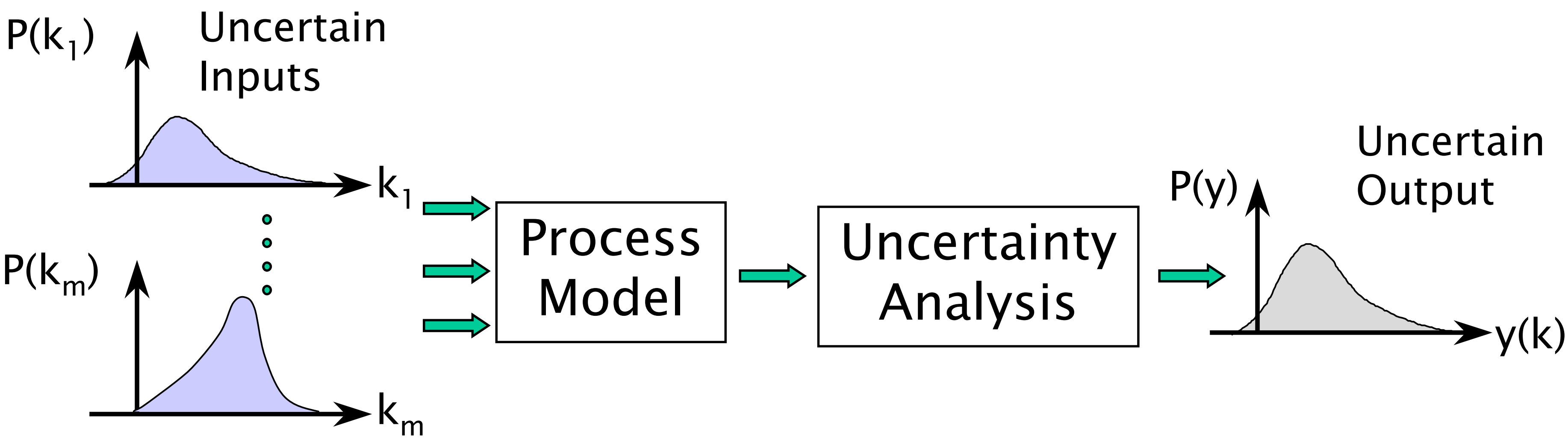
Limitation of Sensitivity Analysis

- Insufficient when inputs vary over a wide range



Uncertainty Analysis

- Combine model response with parameter variability to better present the reality



Parametric Uncertainty Analysis of Cu CVD

- Analyzed the uncertainty of which parameter has larger effect on the uncertainty of the outputs
- Compared uncertainty analysis with sensitivity analysis and analysis of variance (ANOVA)
- System specification
  - Precursor flow rate F: 0.1 - 2.5 ± 10% ccm
  - Temperature T : 150–250 ± 2 °C
- Nominal values

$$F_0 = 2 \text{ ccm}, T_0 = 190 \text{ °C}$$

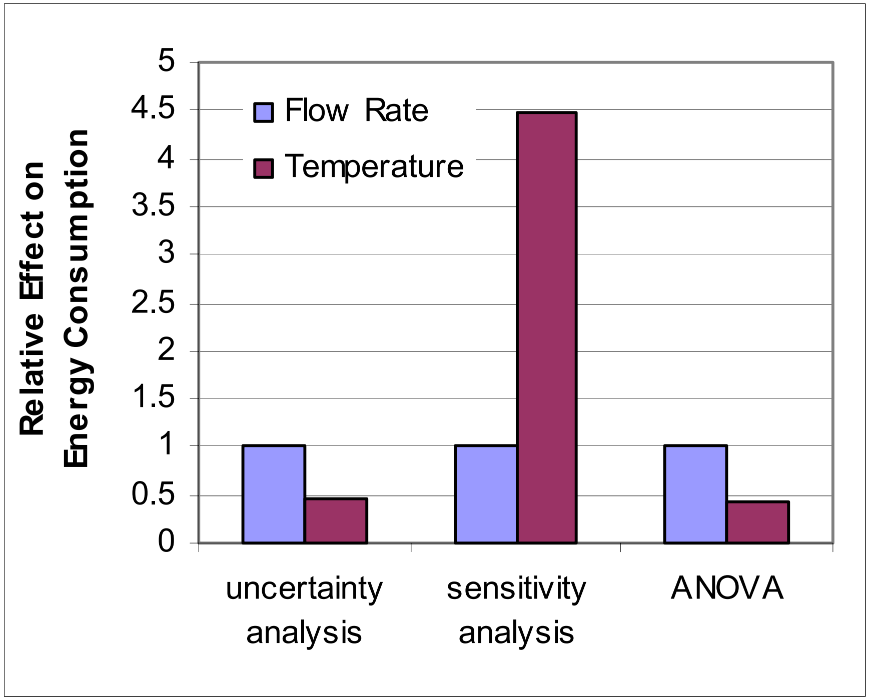
- PDFs of parameters

$$F \sim \text{Normal Distributed, } N(2, 0.04)$$
$$T \sim \text{Normal Distributed, } N(190, 4)$$

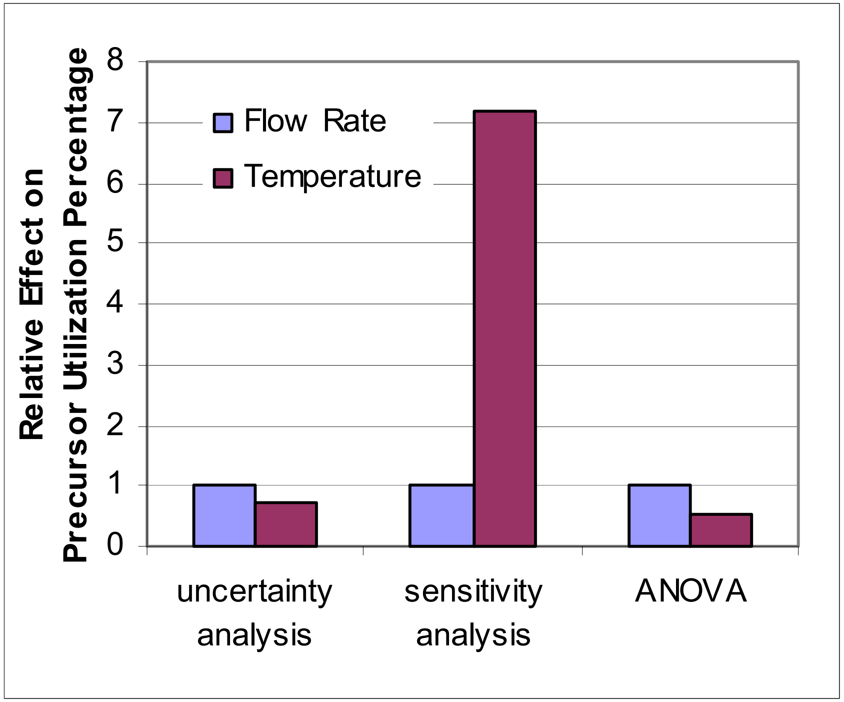
- Sensitivity analysis perturb ± 0.2% around nominal values

Results

- Uncertainty analysis tells the relative importance of parameters.



Energy Consumption

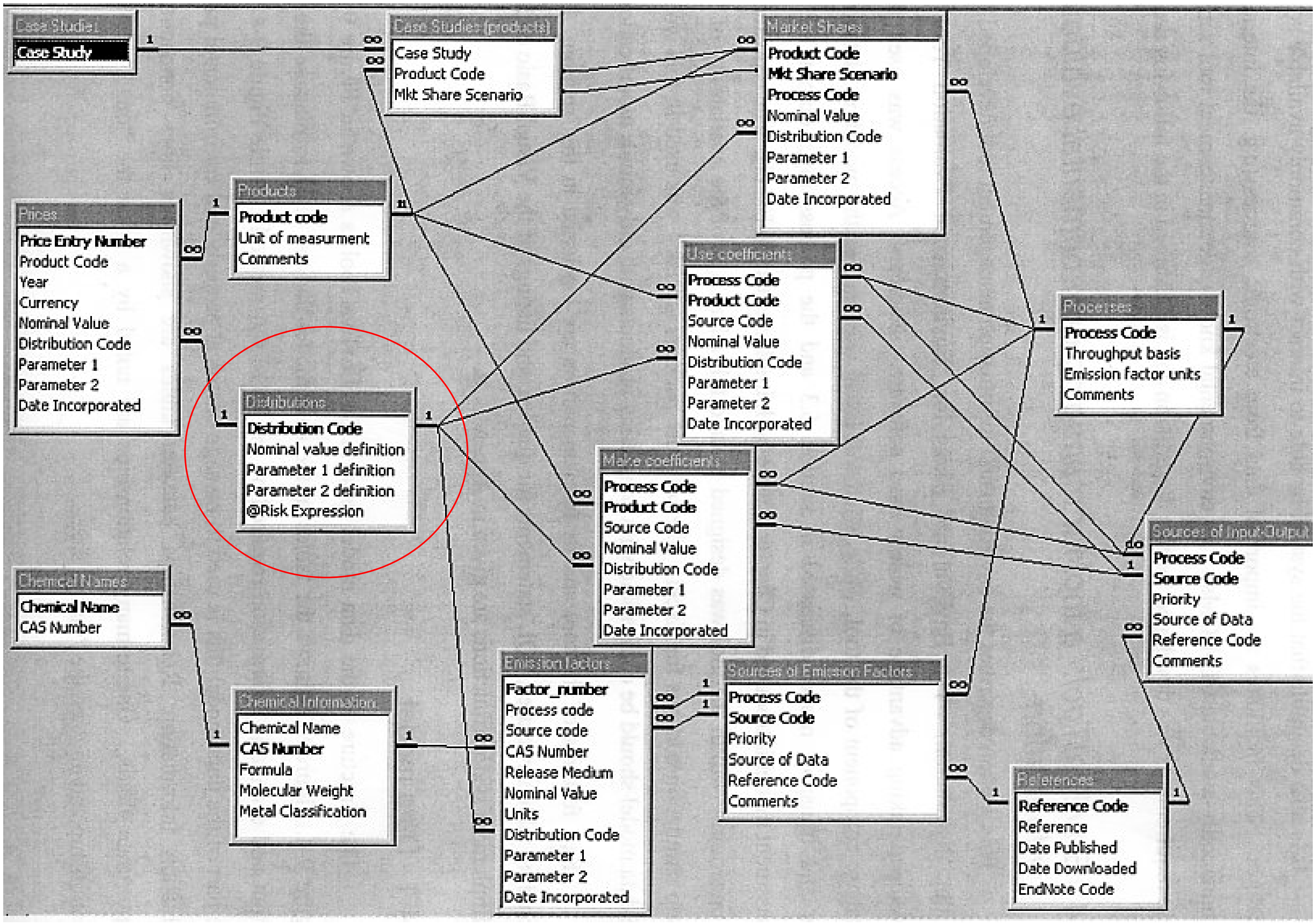


Precursor Utilization

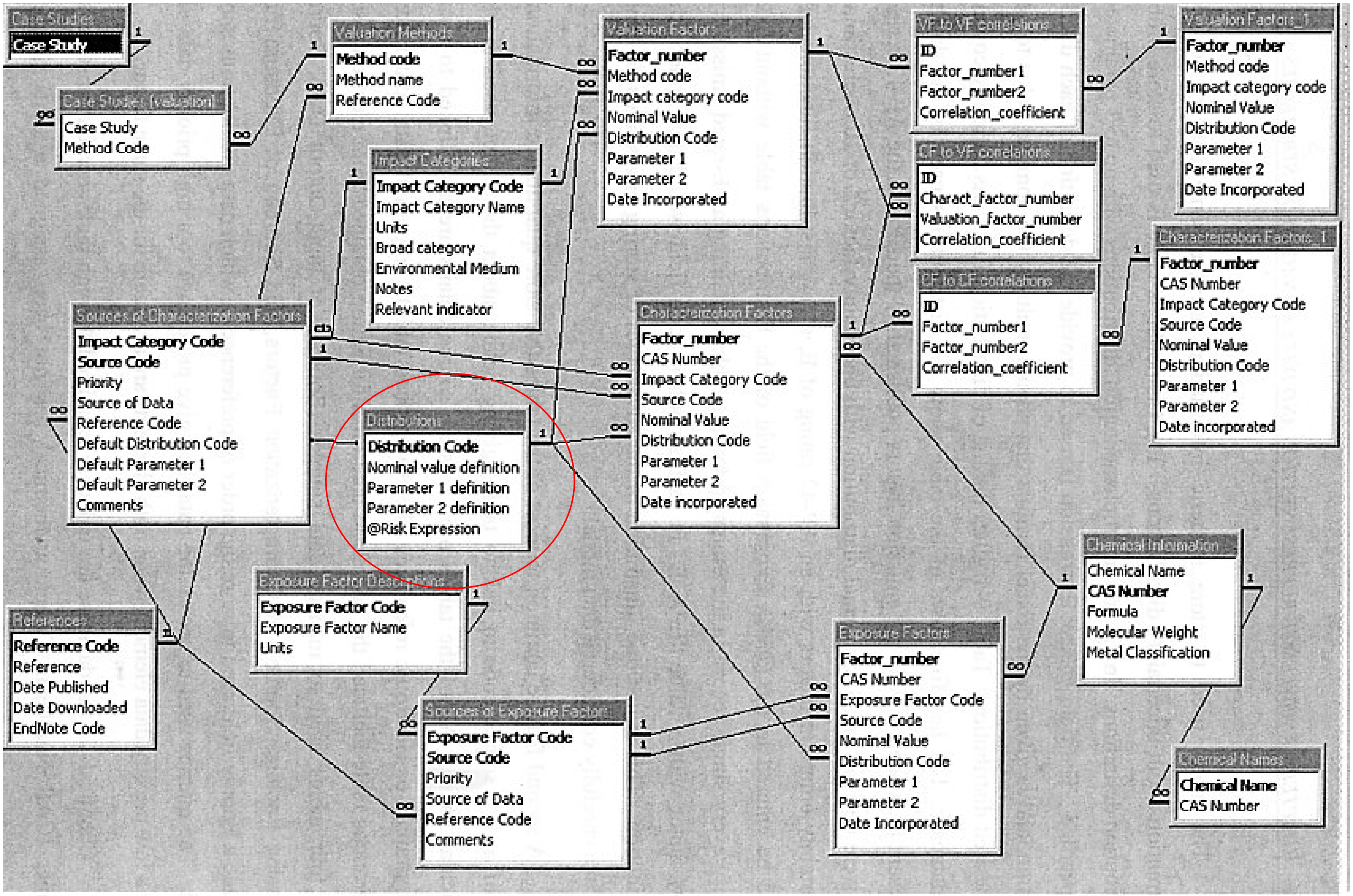
- Important parameter: Flow Rate
- To reduce process fluctuation, reduce the fluctuation of flow rate first

Data Storage: Database Structure*

Input-output data and economic information



Chemical Properties and Valuation Factors



Next Steps

1. Complete uncertainty analysis on environmental evaluation of Cu CVD
2. Determine the important parameters through uncertainty analysis
3. Based on the Cu CVD case, evaluate existing metrics according to:
    1. Relevance to semiconductor industry
    2. Time length needed for data collection
    3. Accuracy of available data
4. Reevaluate Cu CVD case based on the chosen metrics

- Establish collaboration with interested companies/organizations, such as SEMATECH (the chemical data acquisition project)

Summary

- Performed life cycle analysis on Cu CVD process
  - Large impact from methane reforming
  - Changing carrier gas may reduce environmental impact
- Performed uncertainty analysis on Cu CVD process model
  - Flow rate is the important parameter
  - To reduce process fluctuation, reduce the fluctuation of flow rate first
- Proposed standardized database structure and including probability distribution in data collection
- Future steps