A New Inventory Data Model and Method for Uncertainty Evaluation in Life Cycle Assessment

Hirokazu Sugiyama
The University of Tokyo
Swiss Federal Institute of Technology
Introduction

Inventory analysis with industry

Market share

Input → Output

e.g. kWh-electricity per kg-product

Source of uncertainty in LCI phase

More informed decision making

Differences in emission between factories which produce same product

Huijbregts, Int. J. LCA (1998)

Option A

Option B

Environmental impacts

International Workshop on Quality of LCI Data
21.10.03 Karlsruhe, Germany
Introduction

Inventory analysis with industry

"Please don’t publish individual data"

Input  Output

Market share

e.g. kWh-electricity per kg-product

Source of uncertainty in LCI phase

... Differences in emission between factories which produce same product

Huijbregts, Int. J. LCA (1998)

More informed decision making

Option A

Option B

Environmental impacts
Objectives

Inventory analysis with industry.

"Please don’t publish individual data."

Option A

Option B

Environment impacts

More informed decision making

Decision making procedure

Source of uncertainty in LCI phase:

Differences in emission between factories which produce same product

Huijbregts, Int. J. LCA (1998)

Data Model

σ²

Market share

e.g. kWh-electricity per kg-product
Inventory data model: conventional

Raw material $X_i$

Utility $Y_i$

Product $Z_i$

Market share $w_i$

Production process

Difference in Input/Output per unit amount of production $w_i$
Inventory data model: conventional

\[ \sum w_i X_i \]

Factory i

Factory j

Factory k

Production process

\[ \sum w_i Y_i \]

\[ \sum w_i Z_i \]

Difference in Input/Output per unit amount of production

\[ \sum w_i X_i \]

\[ w \]

Weighted average

- Information of scattering are lost
- LCA result is obtained as deterministic value
Inventory data model: proposed

1) Probability distribution
2) Correlation coefficient

LCA result is obtained as probability distribution by Monte Carlo simulation.

Difference in Input/Output per unit amount of production

Fitted probability distribution
- Scattering can be preserved
- Individual datapoints are masked
1) Distribution fitting

Original data from industry \((X_i, w_i)\)  

- \(X_i\) raw material/product in factory \(i (i=1\sim n)\)
- \(w_i\) marketing share of factory \(i (i=1\sim n)\)

Fit distribution for \(X\)

- Property of original data, Goodness-of-Fit statistics

\[ X = \text{Distribution} \quad \text{(parameter)} \quad \text{Lognormal (mean, standard dev.)} \]

Maximum Likelihood Estimators \(\alpha\) which maximize

\[
L(\alpha) = \prod_{i=1}^{n} (f(X_i, \alpha))^{Nw_i}
\]

\(\alpha\) is given by

\[
\frac{\delta L(\alpha)}{\delta \alpha} = 0
\]
2) Correlation modeling

Rank order correlation coefficient

\[ r_{X-Y} = \frac{\sum_{i=1}^{n} \left( rank(X_i) - \frac{n+1}{2} \right) \left( rank(Y_i) - \frac{n+1}{2} \right)}{n(n+1)(n-1)/2} \]

- Calculating correlation of rank order between parameters
- Suitable for correlated sampling in Monte Carlo simulation rather than regression coefficient

Correlated sampling

Fitted distribution
Decision making procedure

1. Collect data from industry
   - Input/Output data
   - Market share

2. Model inventory data
   - 1) Probability distribution
   - 2) Correlation coefficient

LCA by Monte Carlo simulation
   - Result as probability distribution

3. Compare distributions

Sensitivity analysis
   - Prioritizing data to be refined

Decision considering uncertainty

Option A

Option B

Environmetal impacts
Case Study

The Life cycle of PET products

Reaction selection

Secondary monomer

Option 1
- Hydrolysis
- Methanolysis
- Polymerization

Option 2
- Hydrolysis (Super Critical)
- Glycolysis
- Methanolysis

Option 3
- Secondary monomer
- Glycolysis
- Methanolysis

Oil Refinery

PET

EG
PTA

BHET

Esterification

Trans Esterification

s-phase Polycondensation

B-PET

Bottle Manufacturing

Consumption

Incineration

Used Bottles

Flaking + Washing

Reaction selection

The Life cycle of PET products

Reaction selection

Secondary monomer
Case Study

Process Simulator

Function unit at 1,000 t/yr PET input

Oil Drilling & Oil Refinery

EG
PTA

Esterification

BHET

Trans Esterification

s-phase Polycondensation

B-PET

Bottle Manufacturing

Consumption

Incineration

Used Bottles

Flaking + Washing

Electro.

Polymerization

EG
PTA

Hydrolysis

DMT

Polymerization

EG
DMT

PET resin

Fibering

Manufacturing

Consumption

Incineration
Case Study

Decision problem

Under uncertainty in inventory data

Select recycling option reducing CO₂ most

Existing process

Polymerization

Process Simulator

Function unit at 1,000 t/yr PET input

Hydrolysis (Super Critical)

PET

EG

DMT

Polymerization

EG

DMT

Esterification

BHET

Trans Esterification

s-phase Polycondensation

B-PET

Bottle Manufacturing

Consumption

Incineration

Flaking+

Washing

Used Bottles

Option 1

Option 2

Option 3

Existing process

Oil Refinery

Esterification

BHET

Trans Esterification

s-phase Polycondensation

B-PET

Bottle Manufacturing

Consumption

Incineration

Flaking+

Washing

Used Bottles

Option 1

Option 2

Option 3

Existing process

Oil Refinery

Esterification

BHET

Trans Esterification

s-phase Polycondensation

B-PET

Bottle Manufacturing

Consumption

Incineration

Flaking+

Washing

Used Bottles

Option 1

Option 2

Option 3

Existing process

Oil Refinery

Esterification

BHET

Trans Esterification

s-phase Polycondensation

B-PET

Bottle Manufacturing

Consumption

Incineration

Flaking+

Washing

Used Bottles

Option 1

Option 2

Option 3
Objectives in case study

1) Probability distribution
2) Correlation coefficient

Collect data from industry
- Input/Output data
- Market share

Model inventory data
- 1) Probability distribution
- 2) Correlation coefficient

LCA by Monte Carlo simulation

Compare distributions

Sensitivity analysis

Decision considering uncertainty

Assumed data

Show the importance to collect & model uncertainty information

Demonstrate the procedure
LCA result: deterministic values

Changes of CO₂ emissions after installation of plant [t-CO₂]

Option 1 (PET → PTA → PET bottle by super critical water) seems the best option

Option1 option2 option3

Production Use Incineration

ΔCO₂ = Option 1~3 - Incineration

Balance
LCA result: considering uncertainty

\[ \Delta CO_2 = \text{Option1} \sim \text{Option3} (p_{\text{Opt,}i}) - \text{Incineration}(p_{\text{Inc}}) \]

Inventory as probability distribution

Utility
- kg-steam/kg-PET resin
- \( \sigma/\mu = 0.5 \)

Transportation
- km/kg-beverage
- \( \pm 50\% \)

\( CO_2 \) emission factor
- kg\( CO_2 \)/kWh
- kg\( CO_2 \)/steam
- kg\( CO_2 \)/PET resin
- km\( CO_2 \)/beverage

International Workshop on Quality of LCI Data
21.10.03 Karlsruhe, Germany
LCA result: considering uncertainty

Option 1, 3 result in the reduction of CO$_2$ by 99% confidence.

Option 2 does not necessarily lead to overall reduction.
Comparison: relative measurements

Inventory as probability distribution

\[ \Delta CO_2 = Option2,3(p_{Opt.2,3}) - Option1(p_{Opt.1}) \]

Integration over 0 = confidence that Option 1 superior to Option3: 62%

Sensitivity analysis
Sensitivity analysis: regression model

LCA Model
\[ \Delta CO_2 = Option 2,3(p_{Opt.2,3}) - Option 1(p_{Opt.1}) \]

Regression model
\[ \sum_{k} a_k x_k + b \]

Standardized partial regression coefficient

- CO₂ emission factor for electricity
- Electricity for PET polymerization
- Low pressure steam for PET polymerization
- Middle pressure steam for PET polymerization
- Low pressure steam for PTA production

Priority for the further data collection
Conclusions

- **Data Model**
  - Probability distribution for incorporation of uncertainty and for masking individual data
  - Rank order correlation coefficient for correlated sampling in Monte Carlo simulation

- **Decision Making Procedure**
  - LCA result in probability distribution
  - Relative measurement + Sensitivity analysis
  - Case study: Assumption needed

Even obtaining the mean value is still difficult.
Conclusions

- *To help industry open more data for LCA practitioner...*
  - Clarification of data development procedure as data model is effective.
  - Even if assumed data is used, case studies illustrating the effectiveness of uncertainty evaluation are important.
I would like to acknowledge

Prof. Dr. M. Hirao in The University of Tokyo
Prof. Dr. K. Hungerbühler in Swiss Federal Institute of Technology

for the supervision of the work and fruitful discussions.