Sustainability Analysis for Products and Processes

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SNO Conference, November, 2012
Nanotech Product Categories

- **Appliances**
  - Batteries
  - Heating, cooling and air conditioning
  - Kitchen appliances
  - Laundry and clothing care

- **Automotive**
  - Exterior
  - Maintenance & accessories
  - Watercraft

- **Crosscutting**
  - Coatings

- **Electronics & computers**
  - Audio/video/display
  - Cameras & film
  - Computer hardware/mobile devices/communication equipment

- **Health & fitness**
  - Clothing
  - Personal care/cosmetics/sunscreen
  - Sporting goods

- **Children’s goods**
  - Toys and games

- **Home & Garden**
  - Cleaning
  - Construction materials
  - Home furnishing
  - Luggage
  - Luxury
  - Paints
  - Pet products
Extensive use of elements from the Periodic Table in the Semiconductor Industry

Courtesy of Prof. Farhang Shadman, University of Arizona, Tucson
Risk is not necessarily from the nanoparticles themselves but what might be on them

a) Nano-particles in the gas phase
15 ppb VOC; 40 nm particles

- 10 ppb of Cu$^{++}$ in CMP wastewater results in $3 \times 10^6$ ppb of adsorbed copper on 90 nm CeO$_2$ nano-particles

b) Nano-particles in the wastewater

- 10 ppb of PFOS in wastewater results in $2.8 \times 10^4$ ppb of contaminated 10 nm carbon nano-particles
Types of Risk Enquiry

1. Risk from exposure to nanoparticles
   - impact on humans during manufacturing practices
   - impact on ecosystems during dispersion
   resulting from products in their life cycle in the environment

2. Risk from exposure to consumer products
   - direct exposure to humans
   - to ecosystems after disposal
Sustainability analysis of nanotech products is no different than that of any other product.
Sustainability issues associated with modern products and processes

We use:
- Bath: 50 gallons
- Shower: 25 gallons
- Dishwasher: 20 g/load
- Washing machine: 10 g/load

Industry uses:
- 2.2 lbs of beef: 11,624 g
- Dozen eggs: 1,219 g
- Hamburger & Fries: 2,087 g
- Paper ream: 99 g
- Microchip: 144 g
- Car manufacture: 99,065 g
**OUTLINE**

**Purpose:**
Incorporating Sustainability Considerations into Products/Processes

**Sustainability Analysis:**
- Engineering Definition
- Systems and LCA thinking
- Sustainability metrics, classification, selection for Processes
- Consolidation of metrics for easy decision making for sustainability
President’s Council for Sustainable Development

- Sustainable development is an evolving process that improves the **economy**, the **environment**, and **society** for the benefit of current and future generations.
WCED (Bruntlund) idea of sustainable development

Economic development (i.e. by technology application) with decreasing environmental impact and improving societal benefit

An Engineering Definition:

For a man-made system, sustainable development is continual improvement in one or more of the three domains of sustainability, i.e., economic, environmental, and societal without causing degradation in any one of them, either now or in the future, when compared, with quantifiable metrics, to a similar system it is intended to replace.

P.S. Even though continual improvement simultaneously in all domains provides a practical approach, this is still a high bar. In practice, an overall improvement is feasible.
System-Surrounding Paradigm

**System:** maximum space over which the process owner has control

**Sustainability Analysis** is essentially an accounting of what the system is doing to itself and to the surrounding in terms of environmental, societal, and economic impacts, and how these impacts can be minimized

**Corollary:** Maximization of benefits with cost minimization
Differences between Environmental Impact Assessment (EIA) and Sustainability

• Estimation of all applicable environmental impacts in quantitative terms

• Assessment is in absolute terms

• Can be done on an LCA basis

• Decision on cost-benefit term

• Estimation of all applicable environmental, economic, and societal impacts in comparison to a reference case

• No absolute in sustainability

• Should be done on an LCA basis

• Decision on overall quantitative desirability compared to the reference
Engineering Approaches to Sustainability

• Impact accounting: on a life cycle basis
• Analysis: comparative among processes, or over time
• Reference system: the one to supersede
• A single aggregate index composed of applicable metrics: to be used in the comparative study
Environmental, Economic, and Societal Impacts from a Life Cycle Basis

**Input**
- Energy
- Material
- Workforce

**Output**
- Product
- Emissions
- Discharge
- Waste

**Impact Category**
- Environmental Impacts
- Economic Benefits
- Social Impacts

**Production Process**
- Energy
- Material
- Workforce

**Use**
- Energy
- Material
- Workforce

**End of Life**
- Energy
- Material
- Workforce
1. Incremental improvement in the journey towards sustainable development:

   *Think globally, Act locally*

2. Radical changes for attaining an envisioned outcome:

   *Think globally, Act globally*
Ecosystems Modeling
Credit Trading Design
Watershed Protection
Industrial Ecology
Impact Assessment
Risk Assessment
Risk Management
Benign by Design
Waste Minimization
Clean Energy
Renewable Sources
Electrochemistry
Solar, Wind, Biomass
Clean Products
Separation Chinoologies
Computer Modeling
Green Chemistry
Clean Catalysts
Life Cycle Assessment (LCA)
Systems Analysis
SLOW Roadwork Ahead
Scale and Nesting of Sustainable Systems

Five levels of scales for sustainable systems:

1. Global Scale (e.g. global CO2 budgeting)
2. National Scale (e.g. energy system, material flow)
3. Regional Scale (e.g. watersheds, Brownfields)
4. Business Systems (e.g. business networks, waste exchange networks)
5. Sustainable technologies (e.g. green materials, sustainable products)

System-Surrounding Paradigm

Sustainability analysis is essentially an accounting of what impacts (environmental, economic, and societal) the system is causing to itself and to the surrounding, and how these impacts can be minimized.
A SYSTEMS VIEW OF SUSTAINABILITY

Economy (economic capital)
- economic value is created for society
- some waste is recovered and recycled
- ecological goods and services are utilized in society

Environment (natural capital)
- waste and emissions may degrade the environment

Society (human capital)
- emissions may harm humans
- ecological goods and services are utilized in society

Courtesy of Joseph Fiksel, Ohio State University
Sustainability metrics (or indicators) need to be chosen for each problem system. Indicators can be grouped into three categories:

**Group I:** One dimensional: economic, ecological, societal

**Group II:** Two dimensional: socio-economic, eco-efficiency, and socio-ecological

**Group III:** Three dimensional: sustainability
Sustainability as the intersection of three domains

- Economic aspects
  - wastes
  - water use

- Socio-economic indicators
  - cost/benefit
  - employment
  - Disease

- Sociological aspects
  - energy intensity
  - material intensity
  - chemical risk
  - environmental risk

- Sustainability indicators
  - materials intensity
  - chemical risk
  - environmental risk
  - wastes
  - land use
  - GHG

- Environmental aspects
  - biodiversity

11/20/2012
The indicators

Interconnectivity of

Material intensity

Energy Intensity

Water Intensity

Environmental

Economic

Societal

emissions

Waste/emissions

discharges

health effects

value

value

value

costs

Economic

Societal

Interconnectivity of

The indicators
The system analysis must satisfy the following:

• Must be **comparative** to a reference system
• Must be based on **life cycle** of material, energy, and cost through the appropriate supply chain
• Must consider **quantitative measure** to represent environmental, economic, and societal domains
• Must identify the necessary and sufficient number of **critical metrics** that characterize the system
• Must lead to a **decision** of better or worse than the reference system, preferably with a single aggregate metric (or index)
Sustainability Analysis with Metrics

One way is to present sustainability results on a spider diagram for two states of a system or two similar systems.

But, for too many metrics and/or too many alternatives, visual comparison is impossible, and dealing with too many numbers is difficult.
Euclidean Distance:

\[ D_e = \sqrt{\sum_{i=1}^{n} c_i^2 (x_i - x_{i0})^2} \]

Where

- \( D_e (t, x_i) \) is relative sustainability of a candidate from a designated reference n Dimensional point.
- \( x_i \) is the value of metric i for candidate (process, product etc.)
- \( X_{i0} \) is the value of metric i for the reference point.
- \( c_i \) is the weighting factor for metric i.
- \( n \) is the number of metrics used.

P.S. If necessary, \( x_i - x_{i0} \) can be normalized to render them dimensionless.
Consolidation of Metrics

For metrics $m_1, m_2, \ldots$, applied to a base case $X$ and a new case $Y$, we introduce the composite measure $D$ as

$$D = \left( \prod_{i=1}^{n} \left[ c_i \left( \frac{y_i}{x_i} \right) \right] \right)^{1/n}$$

Where $c_i$ is the weighting factor ($0 < c_i$) for metric $i$
$y_i$ is the value of metric $i$ for $Y$
$x_i$ is the value of metric $i$ for $X$ ($x_i$ or $y_i \neq 0$ or $\infty$)

and $n$ is the number of metrics used.

• Idea based on geometric mean of the ratios (dimensionless) of the values of the metrics between the two states being representative of the difference between the two states $X$ and $Y$. The geometric can be looked upon as the statistical distance between the two states.
Shifting the reference point to
(1) Place all data in the positive side for calculating $D_e$
(2) To avoid zero and infinity in calculating $D$

\[
D_e = \sqrt{\sum_{i}^{n} \left[ c_i \frac{(y_i - x_{i0})}{(y_i - x_{i0})_{\text{max}}} \right]^2}
\]

\[
D = \left( \prod_{i}^{n} \left[ c_i \left( \frac{y_i'}{x_i'} \right) \right] \right)^{1/n}
\]

\[
y_i' = y_i - \left( x_{i0} - C_{\text{offset}} \right)
\]

\[
x_i' = x_i - \left( x_{i0} - C_{\text{offset}} \right)
\]
Finding the minimum number of indicators for sustainability analysis

• The Principle of Parsimonious Parameterization: necessary and sufficient number of indicators for sustainability analysis

• Use of Principal Component Analysis on the indicator data space constructing an Eigenvalue Problem:
  \[ A \mathbf{x} = \lambda \mathbf{x} \]
  where \( A \) is the \( n \times n \) indicator correlation matrix, \( \mathbf{x} \) is an \( n \) dimensional eigenvector (called principal component) corresponding to eigenvalue \( \lambda \)

• Use of Partial Least Squares (PLS) and Variable importance in Projection (VIP) method to determine the least number of indicators that will provide reliable \( D_e \) or \( D \) data for comparing relative sustainability of options
Hierarchical Analysis

- **Step 1:** Select the metrics to be used
Hierarchical Analysis

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- Step 2: Classify them in 3D, 2D, and 1D metrics
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- “Strong Sustainability”: Examine for sustainability improvement against the definition that when at least one metric improves, the other metrics do not decline (Pareto optimality)
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• **Step 5:** “**Weak Sustainability**” (Real World): Compute Aggregate Index (D or D_e) for alternatives for relative sustainability decisions.
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- **Step 6:** Prioritize metrics using Principal Component Analysis-Identification Protocol (PCA-VIP) to arrive at the number of necessary and sufficient metrics.
Hierarchical Analysis

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- **Step 7:** Redo the D (or D_e) analyses using metrics of step 6
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**Potential outcome:** The analysis will help in finding conditions that improve Aggregate Index to targeted values (process development)
BASF: five coating formulation

Environmental Fingerprints of alternate Curing Processes
Shonnard, Kirchner, and Saling, ES&T: 2003, 37, 5340-5348

• **Processes:**
  • Aqueous Coating
  • 2C-PU Coating
  • AC-Coating
  • NC-Coating
  • UV-Coating

• **Metric Used**
  • Energy consumption
  • Raw material consumption
  • Risk potential
  • Toxicity potential
  • Emissions into media
  • Land area
Sustainability of Engineered Processes

Mapping the BASF Metrics

- Socio-economic
- Economic
- Eco-efficiency
- Land area
- Energy
- Toxicity potential
- Raw materials
- Process risk
- Waste/emissions
- Societal
- Socio-ecological
- Ecological

Economic
Societal
Socio-ecological
Socio-ecological
Eco-efficiency

Mapping the BASF Metrics
Environmental Fingerprints of alternate Curing Processes
Shonnard, Kirchner, and Saling, ES&T: 2003, 37, 5340-5348

<table>
<thead>
<tr>
<th>Process</th>
<th>Aggregated metric, D</th>
<th>Metrics used:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aqueous coating:</td>
<td>1.0</td>
<td>energy consumption, raw</td>
</tr>
<tr>
<td>2 C-PU Coating</td>
<td>0.987</td>
<td>matl consumption, risk</td>
</tr>
<tr>
<td>AC-Coating</td>
<td>0.868</td>
<td>potential, toxicity potential</td>
</tr>
<tr>
<td>NC-Coating</td>
<td>1.034</td>
<td>emissions into media, land</td>
</tr>
<tr>
<td>UV-Coating</td>
<td>0.196</td>
<td>area</td>
</tr>
</tbody>
</table>

![Graph showing environmental fingerprints](chart.png)
### Fender Case Study

- **Impact Assessment results - total**

<table>
<thead>
<tr>
<th></th>
<th>AI</th>
<th>St</th>
<th>PC/PBT</th>
<th>PP/EPDM</th>
<th>PPO/PA</th>
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<tbody>
<tr>
<td>energy</td>
<td>1290</td>
<td>1120</td>
<td>1060</td>
<td>810</td>
<td>1080</td>
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<tr>
<td>resources</td>
<td>15</td>
<td>25</td>
<td>18</td>
<td>14</td>
<td>21</td>
</tr>
<tr>
<td>water</td>
<td>36</td>
<td>27</td>
<td>22</td>
<td>17</td>
<td>25</td>
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<tr>
<td>GWP</td>
<td>104</td>
<td>105</td>
<td>83</td>
<td>62</td>
<td>115</td>
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<tr>
<td>ODP</td>
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<td>0.1</td>
<td>0.4</td>
<td>0.2</td>
<td>1.2</td>
</tr>
<tr>
<td>AP</td>
<td>28</td>
<td>19</td>
<td>20</td>
<td>16</td>
<td>20</td>
</tr>
<tr>
<td>EP</td>
<td>4.4</td>
<td>4.2</td>
<td>3.9</td>
<td>3.5</td>
<td>7.2</td>
</tr>
<tr>
<td>POCP</td>
<td>6.7</td>
<td>9.2</td>
<td>8.7</td>
<td>8</td>
<td>9.1</td>
</tr>
<tr>
<td>Htox air</td>
<td>3.8</td>
<td>3.7</td>
<td>2.5</td>
<td>1.9</td>
<td>2.5</td>
</tr>
<tr>
<td>Htox water</td>
<td>0.66</td>
<td>0.92</td>
<td>0.99</td>
<td>0.62</td>
<td>0.74</td>
</tr>
<tr>
<td>Eco tox</td>
<td>2.9</td>
<td>3.4</td>
<td>2.7</td>
<td>1.9</td>
<td>2.4</td>
</tr>
<tr>
<td>waste</td>
<td>3.7</td>
<td>1.2</td>
<td>1</td>
<td>0.25</td>
<td>0.25</td>
</tr>
</tbody>
</table>
Sustainability of Engineered Processes

Societal

Socio-economic

Economic

Eco-efficiency

Energy resources

Water
SWP
ODP
AP, EP, POCP, waste

Ecotox
Htox air
Htox water

Mapping the fender Metrics
Fender Case Study: comparison of the alternatives

![Spider diagram comparing various environmental impacts of different materials.]

- Materials compared: Al, St, PC/PBT, PP/EPDM, PPO/PA
- Metrics: GWP, ODP, EP, POCP, Htox (air, water), Eco tox, energy, resources, waste, water

Legend:
- Al
- St
- PC/PBT
- PP/EPDM
- PPO/PA
Automobile Fender Study D Results

Comparison with steel

<table>
<thead>
<tr>
<th>Material</th>
<th>Aggregate Metric, D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel</td>
<td>1</td>
</tr>
<tr>
<td>Al</td>
<td>1.2</td>
</tr>
<tr>
<td>PC/PBT</td>
<td>1.4</td>
</tr>
<tr>
<td>PP/EPDM</td>
<td>1.0</td>
</tr>
<tr>
<td>PPO/PA</td>
<td>1.2</td>
</tr>
</tbody>
</table>

The chart compares the aggregate metric, D, of different materials against steel. Aluminum (Al) has the highest value, followed by PC/PBT, PP/EPDM, and PPO/PA, with Steel having the lowest value.
Case: Automotive Shredder Residue Treatment (Catholique U, Leuven)  
(where improvement is described as negative)

<table>
<thead>
<tr>
<th>Treatment strategy</th>
<th>EI</th>
<th>MI</th>
<th>WC</th>
<th>LU</th>
<th>GW</th>
<th>HT</th>
<th>TC</th>
</tr>
</thead>
<tbody>
<tr>
<td>y</td>
<td>1.8</td>
<td>3.6</td>
<td>1.7</td>
<td>8.7</td>
<td>637</td>
<td>3844</td>
<td>472</td>
</tr>
<tr>
<td>Landfill</td>
<td>-13.1</td>
<td>-408</td>
<td>-4.3</td>
<td>-3.6</td>
<td>-641</td>
<td>1614</td>
<td>-675</td>
</tr>
<tr>
<td>Recycle+Landfill</td>
<td>-24.6</td>
<td>-48.2</td>
<td>-5.2</td>
<td>-11.5</td>
<td>841</td>
<td>841</td>
<td>12</td>
</tr>
<tr>
<td>Energy recovery</td>
<td>-26</td>
<td>-438</td>
<td>-7.8</td>
<td>-14.6</td>
<td>-325</td>
<td>-325</td>
<td>-812</td>
</tr>
<tr>
<td>recycle+Energy Recovery</td>
<td>-26</td>
<td>-438</td>
<td>-7.8</td>
<td>-14.6</td>
<td>-325</td>
<td>-325</td>
<td>-812</td>
</tr>
</tbody>
</table>

| Minimum            | -26    | -438   | -7.8   | -14.6  | -641   | -325   | -812   | -3000  | 106    |

| y'                 |        |        |        |        |        |        |        |        |
| Landfill-Minimum   | 27.8   | 441.6  | 9.5    | 23.3   | 1278   | 4169   | 1284   | 3533   | 0      |
| Recycle+Landfill-Minimum | 12.9   | 30     | 3.5    | 11     | 0      | 1939   | 137    | 383    | 55     |
| Energy recovery-Minimum | 1.4    | 389.8  | 2.6    | 3.1    | 1482   | 1166   | 824    | 2617   | 27     |
| recycle+Energy Recovery-Minimum | 0      | 0      | 0      | 0      | 316    | 0      | 0      | 0      | 71     |

| Maximum            | 27.8   | 441.6  | 9.5    | 23.3   | 1482   | 4169   | 1284   | 3533   | 71     |

| Normalized         |        |        |        |        |        |        |        |        |
| Landfill           | 1      | 1      | 1      | 1      | 0.86235| 1      | 1      | 1      | 0      | 2.78   |
| Recycle+Landfill   | 0.464029| 0.067935| 0.36842| 0.472103| 0      | 0.4651 | 0.1067 | 0.108406| 0.774648| 1.19   |
| Energy recovery    | 0.05036| 0.882699| 0.27368| 0.133047| 1      | 0.279683| 0.64174| 0.74073| 0.380282| 1.75   |
| recycle+Energy Recovery | 0      | 0      | 0      | 0      | 0.21323| 0      | 0      | 0      | 1      | 1.02   |

Best-->Worst D,B,C,A
Relative Sustainability of the Automotive Shredder Residue options
The PLS-VIP score shows that TC has the maximum contribution to overall sustainability. TC, HTST, HTLT, WC and MI are the important variables in that order for their contribution to overall sustainability. All variables have VIP scores more than 0.8.
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