GREENSCOPE: A Tool for Chemical Process Sustainability Assessment and Design

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What is GREENSCOPE?

• Foundations
• Quantification of Sustainability for Chemical Processes
• Methodology
  – Taxonomy
  – Data Needs
• Application
• Tool
  – Excel®
  – Java
• Global Sustainability Assessment
• Conclusions
Motivation

The finite availability and accelerated depletion of ecological goods and services: The role of the chemical Industry

- Fundamental business sector for the global economy and society’s quality of life
- 5% of the U.S. nominal gross domestic product
- directly employs ≅ 800,000 people nationwide
- 11% of all U.S. patents /yr
- 96% of all final goods are directly influenced

- Exposure of workers to toxic and carcinogenic substances
- Water pollution, air emissions and solid waste
- Product use impacts: e.g., agrochemicals, fossil fuels
- Disposal impacts: e.g., flame retardant substances, paint pigments
- 6% of the total U.S. energy consumption
Sustainability for Chemical Processes

- Guidelines to achieve quality of life improvements
  - without affecting the availability of ecological goods & services
  - for new and existing manufacturing processes
- Address and assess environmental, social, and economic aspects that may be affected by industry
  - identify which system components are affected
  - localize process and product aspects which generate them
  - redesign relevant processes and products
  - demonstrate system improvements
- Minimize or eliminate the environmental impacts and maximizing the social/economic benefits
From qualitative to quantitative

- Improvements achieved in one area may simultaneously affect other areas negatively

- A more sustainable process is the result of an optimal tradeoff
Sustainable Process Design Procedure

- Support decision-makers to determine whether a process is becoming more or less sustainable
  - Are we doing relatively good / bad?
- What benchmarks to use?
- How close are we to achieving absolute targets?
Specific process changes to improve sustainability at early design stages will have greater potential influence on the sustainability of the process during operation.
Taxonomy of Chemical Process Indicators

• Triple dimensions of Sustainable Development
  – Environment, Society, Economy
  – Corporate level indicators
  – Assessment at corporate level

• Four areas of sustainable chemical processes
  – Environmental, Efficiency, Economics, Energy (4E’s)
  – Process design level
  – Taxonomy of chemical process indicators for use in process design
The GREENSCOPE Tool

• Clear, practical, and user-friendly approach
• Monitor and predict sustainability at any stage of process design
• Currently developed into a spreadsheet tool, capable of calculating 139+ different metrics
• User can choose which indicators / metrics to calculate
• User can redefine absolute limits to fit circumstances
• Identification and selection of two reference states for each sustainability indicator:
  – Best target: 100% of sustainability
  – Worst-case: 0% of sustainability

• Two scenarios for normalizing the indicators on a realistic measurement scale

• Dimensionless scale for evaluating a current process or tracking modifications/designs of a new (part of a) process

\[
\text{Percent Sustainability Score} = \frac{(\text{Actual-Worst})}{(\text{Best-Worst})} \times 100\%
\]
GREENSCOPE: Systematic Evaluation Procedure
• 66 indicators
• Specifications of process input material
• Health & Safety hazards: operating conditions and operation failures
• Impact of components utilized in the system and releases
• 100% sustainability, best target, is no releases of pollutants and no hazardous material use or generation
• 0% sustainability, worst cases, all inputs are classified as hazardous, and/or all generated waste for each potential EHS hazard is released out of the process
Environmental Indicators: Example

Safety hazard, fire explosion

\[ SH_{\text{fire/explosion}} = \frac{\text{Probable energy potential for reaction with } O_2}{\text{Mass of product}} \]

\[ SH_{\text{fire/explosion}} = \left( -\Delta H_{c,i} \times 10^{4 \times \text{IndVal}_i - 4} \right) m^*_i / m^*_\text{product} \]

If \( \Delta T\text{\_flash} \) is known

\[ \begin{align*}
\text{IndVal}_i &= -0.005 \Delta T\text{\_flash}_i + 1.0 & \text{if } 0 < \Delta T\text{\_flash} < 200 \\
1 & & \text{if } \Delta T\text{\_flash} \leq 0 \\
0 & & \text{if } \Delta T\text{\_flash} \geq 200
\end{align*} \]

Elseif \( R\text{\_code} \) is known

\[ \begin{align*}
\text{IndVal}_i &= 1 & \text{if } R\text{\_code} = 12, 15, 17, 18 \\
0.875 & & \text{if } R\text{\_code} = 11, 30 \\
0.75 & & \text{if } R\text{\_code} = 10 \\
0 & & \text{if } R\text{\_code} = \text{other}
\end{align*} \]

Elseif NFPA-f is known

\[ \begin{align*}
\text{IndVal}_i &= 1 & \text{if } \text{NFPA-flamm}=4 \\
0.833 & & \text{if } \text{NFPA-flamm}=3 \\
0.667 & & \text{if } \text{NFPA-flamm}=2 \\
0.5 & & \text{if } \text{NFPA-flamm}=1 \\
0 & & \text{if } \text{NFPA-flamm}=0
\end{align*} \]

Sustainability value

<table>
<thead>
<tr>
<th>Best, 100%</th>
<th>Worst, 0%</th>
</tr>
</thead>
<tbody>
<tr>
<td>All combustion enthalpy</td>
<td></td>
</tr>
<tr>
<td>0 kJ/kg of each process substance is released</td>
<td></td>
</tr>
</tbody>
</table>

\( \Delta H_c \): combustion enthalpy, kJ/kg

\( \Delta T\text{\_flash} \): temperature difference between the standard flash point and process temperature, \(^\circ\text{C}\)

\( R\text{\_code} \): Risk phrases of European community

NFPA-f: flammability hazard class according to the U.S. National Fire Protection Agency (NFPA)
Efficiency Indicators

• 26 indicators

• Amount of materials and inputs required to generate the desired product (reaction) or complete a specific process task (e.g., separation)

• Mass transfer operations have implicit influence in the amount of energy demand, equipment size, costs, raw materials, releases, etc.

• Efficiency indicators connect material input/output with the product or intermediate generated in the process or operating unit
Efficiency Indicators: Example

Actual atom economy

\[ AAE = AE \times \varepsilon \]

\[ AE_j = \frac{\left(\text{Molecular weight} \times \text{stoichiometric coefficient}\right)_{\text{product}} \times m^*_{\text{product}}}{\sum_{\text{reagents}} \left(\text{Molecular weight} \times \text{stoichiometric coefficient}\right)_{\text{reagent}}} \]

\[ \varepsilon = \frac{\text{Mass of product}}{\text{Theoretical mass of product}} \]

\[ AAE = \frac{\left(\beta \times \text{MW}\right)_{\text{product}} \times m^*_{\text{product}}}{\sum_{j=1}^{i} \left(\alpha \times \text{MW}\right)_{\text{reagent},j} \times \frac{m^*_{\text{limit. reagent}}}{\text{MW}_{\text{limit. reagent}}} \times \frac{\beta_{\text{product}}}{\alpha_{\text{limit. reagent}}} \times \text{MW}_{\text{product}}} \]

Value mass intensity

\[ MI_v = \frac{\text{Total mass input}}{\text{Sales revenue or value added}} \]

\[ MI_v = \frac{\sum_{j=1}^{i} m^*_{m,j}}{S_m} \]

\[ S_m = \sum_{i=1}^{i} m^*_{m,\text{product},i} \times C_{m,\text{product},i} \]

<table>
<thead>
<tr>
<th>Sustainability value</th>
<th>Best,</th>
<th>Worst,</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>100%</td>
<td>0%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sustainability value</th>
<th>Best,</th>
<th>Worst,</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>40</td>
</tr>
</tbody>
</table>

- \( m^\text{product}_{i} \): mass flow of product \( i \), kg/h
- \( m^\text{in}_{\text{limit. reagent},i} \): input mass flow rate of the limiting reagent, kg/h
- \( \text{MW}_{i} \): molecular weight of the component \( i \), kg/kmol
- \( \alpha_{i} \): stoichiometric coefficient of the reagent \( i \)
- \( \beta _{\text{product}} \): stoichiometric coefficient of the desired product
- \( m^\text{in}_{m,i} \): input mass flow rate of the limiting reagent, kg/h
- \( S_m \): total income from all sales in year \( m \), $/yr
- \( C_{m,i} \): cost of material \( i \) in year \( m \), $/kg
- \( m^*_{m,\text{product},i} \): annual mass flow of product \( i \) in year \( m \), kg/yr
Economic Indicators

• 33 indicators

• A sustainable economic outcome must be achieved for any new process technology or modification proposed for the commercial scale

• Based in profitability criteria for projects (process, operating unit), may or may not account for the time value of money

• Indicators supported in cost criteria:
  – Processing costs: capital cost, manufacturing cost
  – Process input costs: raw material cost, utility costs
  – Process output costs: waste treatment costs
Economic Indicators: Example

Net present value

\[
NPV = \text{The total of the present value of all cash flows minus the present value of all capital investments}
\]

\[
NPV = \sum_{m=1}^{n} \text{PWF}_{cf,m} \left[ (S_m - \text{COM}_m - d_m)(1 - \Phi) + \text{rec}_m + d_m \right] - \sum_{m=-b}^{n} \text{PWF}_{v,m} \text{TCI}_m
\]

\[
S_m = \sum_{i=1}^{j} m^*_i \times C_{m,\text{product } i}
\]

\[
\text{COM}_m = 0.280 \text{FCI}_{L,m} + 2.73 C_{OL,m} + 1.23 \left( C_{WT,m} + C_{WT,m} + C_{BM,m} \right)
\]

\[
d_m = 0.1 \text{FCI}_L
\]

\[
\text{rec}_m = \begin{cases} 
C_{\text{Land}} + WC + \text{FCI}_L - \sum_{m=1}^{n} d_m & \text{if } m = n \\
0 & \text{if } m \neq n
\end{cases}
\]

\[
\text{TCI}_m = C_{\text{Land},m} + \text{FCI}_{L,m} + WC_m
\]

\[
\text{FCI}_L = C_{TM} = 1.18 \sum_{i=1}^{n} C_{BM,i}
\]

\[
C_{BM,i} = C_{p,i} F_{BM,i}
\]

\[
C_{OL} = 4.5 N_{OL} \times (\text{annual salary})
\]

\[
N_{OL} = \left( 6.29 + 31.7 P^2 + 0.23 N_{np} \right)^{0.5}
\]

\[
N_{np} = \sum \text{Equipment}
\]

Sustainability value

<table>
<thead>
<tr>
<th>Best, 100%</th>
<th>Worst, 0%</th>
</tr>
</thead>
<tbody>
<tr>
<td>NPV @ ( r_d = ) minimum</td>
<td></td>
</tr>
<tr>
<td>NPV @ discount rate ( (r_d) = 0% ) (MARR) = 40% for very high risk projects</td>
<td></td>
</tr>
</tbody>
</table>

\( n \): life of the plant or equipment, yr

\( \text{PWF}_{cf,m} \): the selected present worth factor

\( S_m \): total income from all sales in year \( m \), $

\( \text{COM}_m \): cost of manufacture without depreciation, $

\( \text{FCI}_L \): Fixed capital investment without including the land value

\( d_m \): depreciation charge. Here, it is assumed as 10% of the \( \text{FCI}_L \) evaluated in year \( m \), however it can be estimated by different methods

\( \Phi \): fixed income tax rate given by the IRS

\( \text{rec}_m \): salvage-value recovered from the working capital, land value, and the sale of physical assets evaluated at the end of the plant life. Often this salvage value is neglected,
Energy Indicators

- 14 indicators
- Different thermodynamic assessments for obtaining an energetic sustainability score
  - Energy (caloric); exergy (available); emergy (embodied)
- Zero energy consumption per unit of product is the best target (more products per unit of consumed energy)
- Most of the worst cases do not have a predefined value
  - They depend on the particular process or process equipment
  - The designer has to choose which value is unacceptable
  - Some worst cases can be assigned by taking the lowest scores found through comparing several sustainability corporate reports
Energy Indicators: Example

Exergy intensity

\[ R_{Ex} = \frac{\text{Net exergy used}}{\text{Mass of product}} \]

\[ R_{Ex} = \frac{\text{Ex}^{*\text{in}} - \text{Ex}^{*\text{lost}}}{m_{\text{product}}} \]

\[ \text{Ex}^{*\text{in}} = [\text{Ex}^{*}\text{ (physical)} + \text{Ex}^{*}\text{ (chemical)}]\text{input flows} + \text{Ex}^{*}\text{ (work)} + \text{Ex}^{*}\text{ (heat)} \]

\[ \text{Ex}^{*\text{in}} = \sum_{j=1}^{n} m_j^{*\text{in}} (\Delta H - T_0 \Delta S)_j + \sum_{j=1}^{n} \sum_{i=1}^{e} (x_i \text{Ex}_{ij}^{\text{ch}} + RT_0 x_i \text{ln}(x_i)) \]

\[ + \sum_{k=1}^{b} W_k^{*} + \sum_{k=1}^{b} Q_k^{*} (1 - T_0 / T_{s,k}) \]

\[ \text{Ex}^{*\text{lost}} = T_0 S^{*}\text{generated} \]

\[ S_{\text{generated}} = \sum_{j=1}^{r} m_j^{*\text{in}} \Delta S_j - \sum_{j=1}^{r} m_j^{*\text{out}} \Delta S_j - \sum_{k=1}^{b} Q_k^{*} \]

\[ \Delta S_{i,j} = \sum_{i=1}^{c} \Delta S_{i,j} + \Delta S_{i,j}^{\text{mix}} \quad \Delta S_{j,i} = \sum_{i=1}^{c} y_{i,j} \Delta S_{j,i} + \Delta S_{j,i}^{\text{mix}} \]

Sustainability value

Best, 100%  Worst, 0%

0 Max Ex\text{total}/kg product
Indicators and Data Needs

• To generate a sustainability assessment a model must have available data
• Data is not the final goal, but it is mandatory to get there
• $M \& E$ flows, operating conditions and equipment specifications; substance properties: physicochemical, thermodynamic, and toxicity; manufacturing and capital costs
• Data-source alternatives can be used to fulfill potential data gaps
  – Simulators
  – Physiochemical
  – Toxicological
  – QSAR models
  – Databases
  – Classification lists
Indicators and Data Needs: Efficiency
Indicators and Data Needs: Economic
## Data Sources

<table>
<thead>
<tr>
<th>Data source</th>
<th>Property or type of provided data</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT, TOXNET, ACToR</td>
<td>Hazardous material list</td>
</tr>
<tr>
<td>TRI program TOXNET/HSDB</td>
<td>TRI PBT chemical list</td>
</tr>
<tr>
<td></td>
<td>ERPG-2, ERPG-3, MW, ΔH_c, ρ, pH, K_{OW}, P_v, T_{flash}, NFPA-r, NFPA-f, IDLH, EC_{50}, LC_{50}, LD_{50}, TWA</td>
</tr>
<tr>
<td>NIST Chemistry WebBook</td>
<td>MW, ΔH_r, C_p(T), ΔH_f, ΔH_c, ΔH_v, T_{flash}, P_v(T), U, ΔG_r,</td>
</tr>
<tr>
<td>AIHA</td>
<td>ERPG-2, ERPG-3</td>
</tr>
<tr>
<td>ACToR</td>
<td>MW, IDLH, LC_{50}, LD_{50}, ρ, K_{OW}, P_v, MAK-CH, TWA, hazard, acute toxicity, chronic toxicity, carcinogenicity, reproductive toxicity, neurotoxicity, immunotoxicity, dermal toxicity, respiratory toxicity, nephrotoxicity, endocrine effects, ecotoxicity</td>
</tr>
<tr>
<td>ACToR/ICSC</td>
<td>MW, EU_{class}, R_{code}, NFPA, MAK-CH, T_{flash}, μ, EC_{class}, TWA</td>
</tr>
<tr>
<td>IRIS</td>
<td>MW, P_v, K_{OW}, RfD, toxicity kinetics, pharmacokinetic modeling, hazard identification, mode-of-action and dose-response, cancer factors, and cancer descriptors</td>
</tr>
</tbody>
</table>
Sustainability Assessment: Biodiesel Case Study

- External data: ERPG, IDLH, $T_b$, $T_m$, $LC_{50}$, etc.
- Process data: $m_{\text{in}}$, $m_{\text{out}}$, $C_{\text{RM}}$, $C_{\text{UT}}$, $C_{\text{equipment}}$, etc.
- Definition of best & worst case scenarios
Biodiesel: Process Description

- Soybean oil
- 95% Oil conversion
- 1 Ton FAME/h
- 99.60% Purity
- 0.1 Ton Glycerol/h
- Utilities: steam, electricity, cooling water
- Solid, liquid, & air releases
Environmental Indicator Results

<table>
<thead>
<tr>
<th>Indicator</th>
<th>Description</th>
<th>Sust. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. $N_{\text{haz. mat.}}$</td>
<td>Number of hazardous materials input</td>
<td>40.00</td>
</tr>
<tr>
<td>6. $H_H_{\text{irritation}}$</td>
<td>Health hazard, irritation factor</td>
<td>99.31</td>
</tr>
<tr>
<td>10. $SH_{\text{react/dec I}}$</td>
<td>Safety hazard, reaction / decomposition I</td>
<td>97.00</td>
</tr>
<tr>
<td>22. $EH_{\text{bioacc.}}$</td>
<td>Environmental hazard, bioaccumulation (the food chain or in soil)</td>
<td>98.34</td>
</tr>
<tr>
<td>27. $PCOP$</td>
<td>Photochemical oxidation (smog) potential</td>
<td>99.83</td>
</tr>
<tr>
<td>32. $WPI_{\text{acid. water}}$</td>
<td>Aquatic acidification intensity</td>
<td>99.88</td>
</tr>
<tr>
<td>38. $WPI_{O2 \text{dem.}}$</td>
<td>Aquatic oxygen demand intensity</td>
<td>0.60</td>
</tr>
<tr>
<td>43. $EP$</td>
<td>Eutrophication potential</td>
<td>98.89</td>
</tr>
</tbody>
</table>
## Efficiency Indicator Results

<table>
<thead>
<tr>
<th>Indicator</th>
<th>Description</th>
<th>Sust. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2. $\text{AE}_i$</td>
<td>Atom economy</td>
<td>90.60</td>
</tr>
<tr>
<td>7. $\text{MI}_v$</td>
<td>Value mass intensity</td>
<td>99.46</td>
</tr>
<tr>
<td>17. $\text{pROI}_M$</td>
<td>Physical return on investment</td>
<td>99.76</td>
</tr>
<tr>
<td>21. $w_{\text{recycl. prod.}}$</td>
<td>Mass fraction of product from recyclable materials</td>
<td>4.50</td>
</tr>
<tr>
<td>25. WI</td>
<td>Water intensity</td>
<td>100</td>
</tr>
</tbody>
</table>
Energy Indicator Results

<table>
<thead>
<tr>
<th>Indicator</th>
<th>Description</th>
<th>Sust. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2. $R_{SEI}$</td>
<td>Specific energy intensity</td>
<td>99.49</td>
</tr>
<tr>
<td>6. $\eta_E$</td>
<td>Resource-energy efficiency</td>
<td>63.26</td>
</tr>
<tr>
<td>8. $BF_E$</td>
<td>Breeding-energy factor</td>
<td>53.38</td>
</tr>
<tr>
<td>10. $Ex_{total}$</td>
<td>Exergy consumption</td>
<td>92.59</td>
</tr>
<tr>
<td>14. $BF_{Ex}$</td>
<td>Breeding-exergy factor</td>
<td>100.00</td>
</tr>
</tbody>
</table>
Economic Indicator Results

<table>
<thead>
<tr>
<th>Indicator</th>
<th>Description</th>
<th>Sust. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. NPV</td>
<td>Net present value</td>
<td>44.52</td>
</tr>
<tr>
<td>8. PBP</td>
<td>Payback Period</td>
<td>81.10</td>
</tr>
<tr>
<td>19. COM</td>
<td>Manufacturing cost</td>
<td>68.70</td>
</tr>
<tr>
<td>23. $C_E$, spec.</td>
<td>Specific energy costs</td>
<td>88.07</td>
</tr>
<tr>
<td>33. $C_{pur. air fract.}$</td>
<td>Fractional costs of purifying air</td>
<td>85.26</td>
</tr>
<tr>
<td>Indicator</td>
<td>Symbol</td>
<td>Equations</td>
</tr>
<tr>
<td>---------</td>
<td>--------</td>
<td>-----------</td>
</tr>
<tr>
<td>1. Total energy consumption</td>
<td>T</td>
<td>$E_{total} = E_1 + E_2 + \ldots + E_n$</td>
</tr>
<tr>
<td>2. Specific energy intensity</td>
<td>S</td>
<td>$E_{intensity} = \frac{E_{total}}{Q}$</td>
</tr>
<tr>
<td>3. Energy intensity</td>
<td>E</td>
<td>$E = \frac{E_{total}}{Q}$</td>
</tr>
<tr>
<td>4. Waste energy intensity</td>
<td>W</td>
<td>$W = \frac{E_{waste}}{Q}$</td>
</tr>
<tr>
<td>5. Solvent recyclying rate</td>
<td>R</td>
<td>$R = \frac{E_{recycled}}{E_{total}}$</td>
</tr>
<tr>
<td>6. Process energy efficiency</td>
<td>P</td>
<td>$P = \frac{E_{process}}{Q}$</td>
</tr>
<tr>
<td>7. Fixed energy intensity</td>
<td>F</td>
<td>$F = \frac{E_{fixed}}{Q}$</td>
</tr>
<tr>
<td>8. End-use energy factor</td>
<td>U</td>
<td>$U = \frac{E_{use}}{Q}$</td>
</tr>
<tr>
<td>9. Energy for recycling</td>
<td>R</td>
<td>$R = \frac{E_{recycled}}{Q}$</td>
</tr>
<tr>
<td>10. Energy consumption</td>
<td>C</td>
<td>$C = \frac{E_{consumption}}{Q}$</td>
</tr>
</tbody>
</table>

Note: The equations and values are hypothetical and for demonstration purposes only.
Stand Alone GREENSCOPE Software

- Currently in development
- Dr. Rajib Mukherjee (ORISE Post-Doc)
- JAVA Language
- Based on the Excel® version
- User can define
  - level of interaction
  - which indicators to calculate
  - best and worst case scenarios
### Efficiency Information

<table>
<thead>
<tr>
<th>Compound ID</th>
<th>Compound Name</th>
<th>Product</th>
<th>Hazardous</th>
<th>Renewable</th>
<th>Recyclable</th>
<th># of C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>FAME</td>
<td>Y</td>
<td>N</td>
<td>Y</td>
<td>N</td>
<td>19</td>
</tr>
<tr>
<td>2</td>
<td>Glycerol</td>
<td>Y</td>
<td>N</td>
<td>Y</td>
<td>N</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>Methanol</td>
<td>N</td>
<td>Y</td>
<td>Y</td>
<td>N</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>Phosphoric acid</td>
<td>N</td>
<td>Y</td>
<td>N</td>
<td>Y</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>Trisodium Phos</td>
<td>Y</td>
<td>N</td>
<td>N</td>
<td>N</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>OIL</td>
<td>N</td>
<td>N</td>
<td>Y</td>
<td>Y</td>
<td>57</td>
</tr>
<tr>
<td>7</td>
<td>Water</td>
<td>N</td>
<td>N</td>
<td>N</td>
<td>N</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>Sodium Hydrox</td>
<td>N</td>
<td>Y</td>
<td>N</td>
<td>Y</td>
<td>0</td>
</tr>
</tbody>
</table>
Calculate efficiency indicators, choose from the list:

1. Reaction Yield
2. Atom Economy
3. Actual Atom Economy
4. Stoichiometric Factor
5. Reaction Mass Efficiency
6. Total material consumption
7. Mass Intensity
8. Value mass intensity
9. Mass Productivity
10. Environmental Factor
11. Mass Loss Index
12. Environmental Factor based on molecular weight
13. Effective Mass Yield
14. Carbon Efficiency
15. Material Recovery Parameter
16. Solvent and Catalyst Environmental Impact Parameter
17. Physical Return on Investment
18. Renewability-Material Index
20. Recycled material fraction
21. Mass fraction of products from recyclable materials
22. Mass fraction of products designed for disassembly, reuse or recycling
23. Total water consumption
24. Fractional water consumption
25. Water intensity
26. Volume fraction of water type

Select All
Global Sustainability Assessment

- Impact assessment beyond the process to decide which design alternative is more sustainable based on the life-cycle considerations
- Identifying stages contributing greater than any other stage to the global life-cycle impact within the product life cycle
Global Sustainability Assessment

A complete quantification of sustainability performance requires an extensive evaluation of the entire system beyond the manufacturing facility.
Conclusions

• Performance indicators for designing sustainable chemical processes at any level:
  – Provides direction to the designer (0% and 100% sustainability)
  – Modifying existing processes as well as implementing new chemistries
  – Approximates manufacturing scale sustainability from a bench or pilot scale

• With GREENSCOPE, the results of sustainable chemical practices are quantified:
  – Modifications in the type and magnitude of goods and services
  – Preventing and minimizing all types of releases
  – Manufacturing the desired product without negatively affecting the economic profitability

• GREENSCOPE can be used as a reliable and robust tool for the development of chemical processes
Disclaimer

The views expressed in this presentation are those of the author and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

References

Thanks!

Questions?