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Using GREENSCOPE for Sustainable Process Design: An Educational Opportunity

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Abstract

Increasing sustainability can be approached through the education of those who design, construct, and operate facilities. As chemical engineers learn elements of process systems engineering, they can be introduced to sustainability concepts. The EPA's GREENSCOPE methodology and tool, valuable in the evaluation and design of chemical processes, can be used to teach these concepts. This work describes example calculations of GREENSCOPE indicators for the oxidation of toluene and puts the indicators into context with best- and worst-case limits. The data available from the process is developed into understandable information which describes sustainability. Targets for more sustainable process designs are understood, and enhancements can be considered to improve designs, either for real-world processes or in an educational environment.

Keywords: chemical, process, sustainability, education, GREENSCOPE

1. Introduction and Background

While both private organizations and the public are asking for increased attention to sustainability (economic, environmental, and social aspects), the amount of information available on the topic continues to expand. People from many fields, for instance accountants and related business professionals, are also getting involved. The Sustainability Accounting Standards Board (SASB, 2013) looks for evidence of interest and financial impact in establishing the materiality of sustainability issues. Sustainable "materiality" can be defined as sustainability information which when omitted misleads investors about expectations of a company (IRI, 2012). These accounting impacts can be direct (e.g., scarcity of resources) or indirect, when consumer, NGO, or other groups could affect company performance (SASB, 2013). The Initiative for Responsible Investment (2012) points out that the Securities and Exchange Commission (SEC) has a number of social and environmental disclosure requirements which apply whether or not there is an immediate impact on financial results. This expansion beyond financial results is the focus of such groups as the Global Reporting Initiative (GRI, 2013), whose G4 Sustainability Reporting Guidelines help organizations measure performance, with the intent that sustainability performance disclosure leads to increasing sustainability.

Increasing sustainability can be approached by other means, including through the education of those who design, construct, and operate facilities. When the facilities of interest are manufacturing processes, then introducing sustainability into the engineering curricula helps satisfy the need. In addition, learning about sustainability simultaneously along with conventional process system engineering (PSE) knowledge will help students to incorporate sustainability with PSE at early education stages rather than just as an add-on during their professional careers. Sustainability in the engineering curricula has been the subject of recent interest (e.g., Hawkins et al., 2013), where objectives (i.e., desired results) are put forth as well as principles for achieving them (e.g., using systems thinking). When the function of a facility is the production of chemical products, the substantial need for sustainability education falls upon chemical engineers. As Allen and Shonnard (2012) state, there is a new need in chemical engineering to systematically address sustainability at multiple scales in a global setting with multiple objectives. They further suggest three elements are needed to educate chemical engineers: framing challenges to put sustainability into context, considering multiple system-level perspectives, and assessing and designing for sustainability.

The final element, assessing and designing for sustainability, demonstrates the need for tools and methodologies that are capable of providing an assessment and informing of design needs which consider and implement aspects of sustainability. In this work, an opportunity for addressing this needed element in chemical engineering education is suggested. This evaluation technique is based on the EPA's GREENSCOPE methodology and its tool application for designing more sustainable processes.

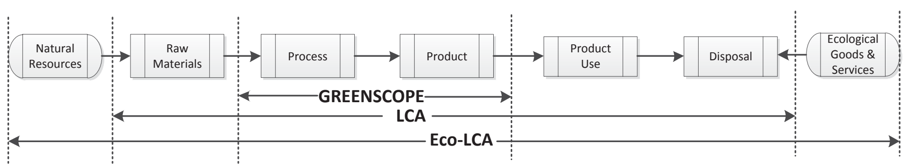

Figure 1. Framework for multiple-system level sustainability assessments based on characteristics of a chemical production facility and product.

Fig.(1) describes a framework for a methodology to connect a set of sustainability assessment approaches with different levels (multiple-system levels) and actions relative to the performance impact of product manufacturing. The GREENSCOPE portion represents a gate-to-gate sustainability evaluation and quantifies the contribution the facility provides to the next higher level of sustainability evaluation, a life cycle assessment (LCA) of the chemical product (and supply chain). Finally, the next higher level, Eco-LCA, encompasses sustainable system indicators which represent the interaction of the chemical facility and its inputs and outputs with the surrounding ecosystem. This approach demonstrates the domino effect alterations at the process level can have on the entire ecosystem, and by applying sustainability assessment and design tools significant improvements to the entire ecosystem can be realized.

2. GREENSCOPE

GREENSCOPE (Gauging Reaction Effectiveness for the ENvironmental Sustainability of Chemistries with a multi-Objective Process Evaluator) presents a methodology and tool for evaluating and designing more sustainable processes (Gonzalez and Smith, 2003). Other tools one could consider include ENVOPexpert (Halim and Srinivasan, 2002), which provides an expert system for identifying the root causes of waste flows and changing them; and SustainPro from Gani and co-workers (Carvalho et al, 2013), which has indicator analysis, evaluation, and generation of alternatives in addition to various connections to other tools. The Waste Reduction (WAR) Algorithm (U.S. EPA, 2013) is a tool openly available for use to evaluate chemical processes in eight environmental impact categories. Use of the WAR Algorithm by academics has been widespread, with over 270 citations and 1800 downloads of the software (Martin, 2013).

A benefit of GREENSCOPE is the intent to become a relatively simple and widely used tool for the evaluation and design of chemical processes which are more sustainable; thus, it offers an opportunity for direct integration and impact in process design classes. Additional features include the ability to apply GREENSCOPE at any point from conceptual design to pilot-scale to full-plant scale and on partial or complete processes. Recent advances of the method and tool started with a taxonomy of indicators representing the sustainability of a chemical process (Ruiz-Mercado et al, 2012a). This resulted in nearly 140 indicators which are defined in four basis areas (the four *Es*): environment, economics, efficiency, and energy. In particular, the strength of the method was demonstrated through the definition of best-target and worst-case limits for each of the indicators. These limits create a dimensionless scale for each indicator,

$$\text{Percent Score} = \frac{(\text{Actual-Worst})}{(\text{Best-Worst})} \times 100\% \tag{1}$$

so that actual processes are within the best- and worst-case limits, which define 100% and 0% sustainability, respectively. One of the powerful aspects of this methodology is the ability to compare disparate processes on the same scales, by using the same limits. Of course, users are able to select indicators of interest or use the complete set.

An analysis with these indicators may require significant amounts of data. Thus, a description of data requirements and data-source alternatives was developed (Ruiz-Mercado et al, 2012b). Diagrams were also developed to allow one to visualize the relationships between process data, external data inputs, and the corresponding indicator(s). The most recent contribution (Ruiz-Mercado et al, 2013), demonstrates the successful implementation and use of the GREENSCOPE process evaluation and design tool. The tool is operational within Microsoft Excel®, and the authors are working to develop a standalone software version. In this mentioned contribution, the manufacture of biodiesel is undertaken as a case study to demonstrate and describe this achievement. All of the proposed indicators were calculated and presented graphically. The case study identifies positive aspects and opportunities for improvement in the process.

3. Using GREENSCOPE for Education

Abundant methods for accomplishing chemical process design are described in the literature. For example, Allen and Shonnard (2002) describe methods for evaluating and improving the environmental performance of processes. There are many instances when GREENSCOPE could be used advantageously. Examples include, an individual performing laboratory experiments could use GREENSCOPE to quickly evaluate alternative synthesis routes, a conceptual designer could generate basic process-oriented results, someone doing front end loading could add more safety and relative detail, or a detailed designer could analyze a final design. In addition, retrofit analyses can be done with GREENSCOPE, using appropriate sets of the available indicators. Finally, GREENSCOPE offers an opportunity to educate engineers and scientists on the potential results of their choices. In recognizing the effects on sustainability, it is also important to realize that the process sustainability evaluation areas (the four *Es*) are related to each other through implicit relationships. Improvements achieved in one area (e.g., energy) simultaneously could affect other area(s) negatively (e.g., economics). Therefore, decision making in process design could result in a tradeoff to achieve a net overall improvement in process sustainability.

Educational opportunities using GREENSCOPE are plentiful, from laboratory work to chemical process designs. Here, the focus will be on a process design, using toluene oxidation as an example. The process considered follows the work of Smith and Gonzalez (2004), where a number of what-if calculations were performed to evaluate sustainability indicators for possible process modifications. An emphasis placed here is on determining the best- and worst-case limits for the indicators, allowing various process alternatives to be compared on the same basis. The expectation is that showing the ease of determining the limits and indicator calculations will provide stimulation for educational use, as well as the ability to quantify sustainability on the process level.

3.1 Toluene Oxidation Process

The toluene oxidation process, pictured in Fig.(2), is designed to produce 6.8×10^5 kg of benzaldehyde per year. Benzoic acid is also made as a valuable co-product.

3.2 Efficiency Indicators for Toluene Oxidation

One can calculate a couple of efficiency indicators to understand how mass is being used by the process. In the case of toluene oxidation to benzaldehyde, the reaction is:

$$C_6H_6\text{-}CH_3 + O_2 \rightarrow C_6H_6\text{-}CHO + H_2O \tag{2}$$

An efficiency indicator for this reaction is atom economy (Ruiz-Mercado et al, 2012a, indicator Eff-2), which is calculated as the mass of product (benzaldehyde) divided by the mass of reactants. A perfect value (100% sustainability) would use all reactants in the product, and the atom economy would be one. If no product were formed the atom economy would be zero (worst-case scenario, 0% sustainability). The actual value observed here is 85.49% (reported in Table 1). If one discounts oxygen as being free from air, then only a single oxygen atom is counted, and atom economy is 98.14%.

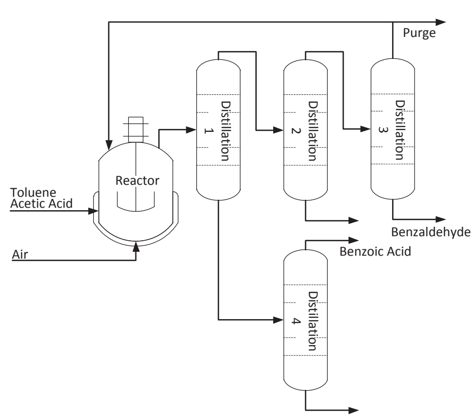

Figure 2. A conceptual design for the oxidation of toluene in acetic acid solvent, with a train of distillation columns used for separations.

Table 1. GREENSCOPE indicators, percent scores, and best- and worst-case limits.

Indicator Name	Indicator Value	Units	GREENSCOPE Percent Score	Best Case	Worst Case
Atom Economy	0.8549	kg/kg	85.49%	1	0
Reaction Yield	0.8042	kg/kg	80.42%	1	0
Net Present Value	0.48×10^6	$	49.48%	2.67×10^6	-1.66×10^6
Payback Period	5.24	y	57.60%	1	11
Specific Energy Intensity	0.04×10^6	kJ/kg	97.73%	0	1.95×10^6
Specific Toxic Release	0.1391	kg/kg	43.14%	0	0.2446
Ecotoxicity to Aquatic Life Potential	5.48×10^6	CTU/ CTU	79.03%	0	26.13×10^6
Photochemical Oxidation Potential	0.6477	kgO_3eq/ kg	48.21%	0	1.2507

Another efficiency indicator is reaction yield (ibid., Eff-1), defined as the mass of product divided by the theoretical mass of product. Again, the best- and worst-case limits are easy to calculate, with a distribution of benzaldehyde and benzoic acid products as 0.9822kg per kg fed for the best-case, and thus the ratio limits are one and zero for the best- and worst-case limits (shown in Table 1). An actual value for the process is 0.7899kg/kg, which gives a GREENSCOPE score of 80.42%.

3.3 Economic Indicators for Toluene Oxidation

The net present value and payback period were calculated with a spreadsheet following the chemical facility project table listed in Peters and Timmerhaus (1980). Net present value limits were determined as defined by Ruiz-Mercado et al., 2012a, Econ-1. The payback period limits were set as the first and last year of production.

3.4 Energy Indicators for Toluene Oxidation

An energy indicator and its limits have been calculated as shown in Table 1 for specific energy intensity. The limits were taken directly from ibid., Energy-2, and the indicator value was calculated using the Excel® GREENSCOPE tool.

3.5 Environmental Indicators for Toluene Oxidation

Three environmental indicators were calculated as shown in Table 1. The specific toxic release indicator (ibid., Env-14) ratios the TRI-listed waste per year over the mass of products per year. The worst-case limit was calculated by assuming that all waste is TRI-listed. Similar calculations were done for ecotoxicity and smog formation (ibid., Env-39 and Env-27), using the Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI) available from the U.S. EPA (Bare, 2013). While the method in TRACI for Env-39 differs from Ruiz-Mercado et al. (2012a), this example shows the flexibility of the GREENSCOPE methodology, which can be used even when specific aspects are changed to fit the desires and available data of users.

4. Discussion and Conclusions

The above indicator calculations provide a wealth of information developed from process data. The key advantage of the indicators is the ability to see information in context, represented by the indicator limits. Knowing the basis of the best- and worst-case limit calculations, the percent GREENSCOPE scores show how close or far a process is from desired targets. The engineer can then propose process changes to improve a process towards such targets and see tradeoffs when they occur.

Chemical engineering education provides knowledge on process aspects such as mass and energy use, economics, and where possible, the environment. The sustainability evaluation and design tool GREENSCOPE ties directly to these education elements. Thus, the commonly taught concepts can be further elucidated by using the GREENSCOPE methodology and/or tool.

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