Life-Cycle Approaches for Assessing Green Chemistry Technologies

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To meet the goals of sustainability and to enable industrial ecology, green chemistry and engineering needs to be studied from a life-cycle perspective. When designed correctly, green chemistry and engineering can affect multiple stages of the life cycle of a product or process. Successful implementations of green chemistry and engineering research are improving the environmental impacts of chemical products and processes in every stage of the life cycle while also offering economic incentives. Analysis of new and existing green chemistry and engineering technologies with quantitative and qualitative metrics can identify and quantify these benefits. The examples presented illustrate the principles of life-cycle assessment as applied to green chemistry and engineering.

Introduction

Since the late 1970s, academic, governmental, and industrial communities worldwide have been discussing the meaning of "sustainability" and "sustainable development". Sustainability can have many interpretations, and it can be used to refer to economic, environmental, or social sustainability. This is an important point to note, because when many people hear the term sustainable, they think about environmental protection and preservation, but this is not always an accurate assumption. In 1987, the United Nations Bruntland Commission broadly defined sustainability as meeting the needs of the present without compromising the ability of future generations to meet their own needs.[1]

In the past decade, there have been numerous publications describing the principles of sustainability and characteristics of sustainable systems (see, for example, refs 2−6). However, there is no one definitive method for implementing and applying these ideas to current industrial and economic activities. A variety of qualitative or semiquantitative tools and concepts have become popularized, such as cleaner production, eco-efficiency, full-cost accounting, green chemistry and engineering (GC&E), industrial ecology, life-cycle assessment (LCA), the Natural Step, pollution prevention, triple bottom line, and others.

These concepts are interrelated and can be thought of in a hierarchical fashion, as illustrated in Figure 1. Consider the broad concept of sustainable development to be at the top of a pyramid. At the middle level are the concepts and ideas that try to define and discuss the achievement of environmental sustainability qualitatively. At the bottom of the pyramid are the most specific tools and concepts in this hierarchy; they are the more quantitative and tangible methods of analysis and implementation. Here, we discuss the opportunities and tangible benefits that green chemistry and engineering can provide to industrial ecology, using LCA as an analysis tool, as well as the use of quantitative metrics. These concepts are discussed further below.

Industrial Ecology

Industrial ecology takes a systematic approach to interactions between industry and the environment to evaluate and minimize impacts.[7] Industrial ecology includes the study of material and energy flows in industrial and consumer activities, the effects of these flows on the environment, and the influence of economic, political, regulatory, and social factors on the flow, use, and transformation of resources.[7] Industrial ecology is a collection of ideas and tools geared toward achieving sustainable development; it can be considered as a subset of sustainable development, because the goal of industrial ecology is to promote environmental sustainability while also maintaining or increasing economic viability.

Life-Cycle Assessment

Life-cycle assessment is one of the methods of analysis in the industrial ecology toolbox. The function of LCA is to evaluate environmental burdens of a product, process, or activity; quantify resource use and emissions; assess the environmental and human health impact; and evaluate and implement opportunities for improvements. An LCA has four primary components: (1) definition of the scope and boundaries of the assessment; (2) inventory analysis, where energy use and materials flows are quantified through the use of mass and energy balances; (3) impact analysis to determine the effects on the external environment and human health; and (4) improvement analysis, which can be implemented through methods such as green chemistry and "design for the environment", for example.

LCA is a flexible, interdisciplinary tool in that engineers, scientists, policy makers, and economists, plus members of other disciplines, can all contribute special expertise to an LCA study. Furthermore, the principles

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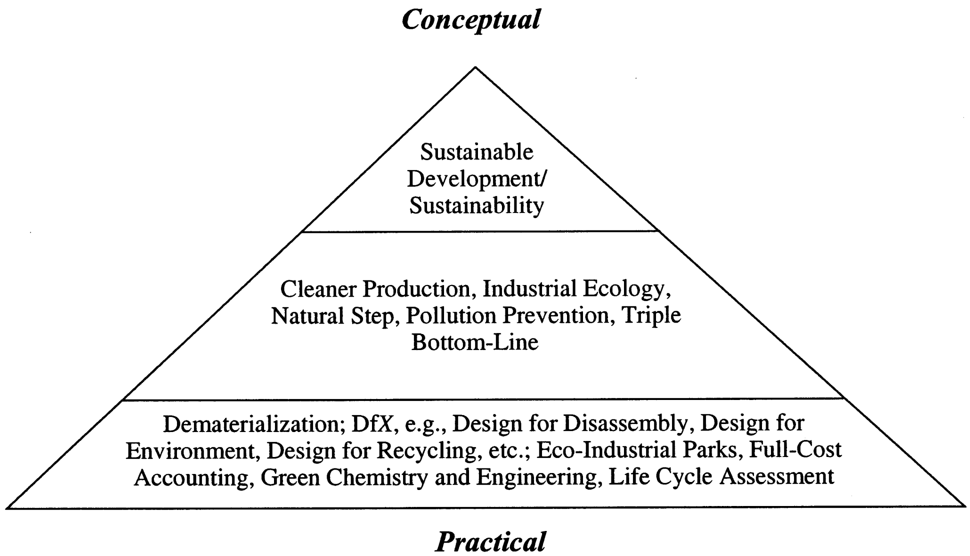

Figure 1. Hierarchy of concepts relating to sustainability.

of LCA can be applied to products and processes in any type of industry or sector.

Green Chemistry

Green chemistry began as a concept at the U.S. Environmental Protection Agency (EPA), developed into an EPA program, and has evolved into a worldwide community. As a concept, green chemistry is one of a set of tools that can be used to implement the ideas embodied in industrial ecology. The concepts of green chemistry are based on a set of twelve principles, given in Table 1, whose goal is to prevent pollution and, like industrial ecology, to help achieve more sustainable activities.

Green chemistry involves the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances. Although the concept name specifies chemistry, interdisciplinary collaboration is an important aspect of green chemistry, and GC&E is relevant to many of the scientific and engineering disciplines. Green chemistry and engineering technologies offer pollution prevention approaches toward environmentally sustainable manufacturing, an important strategy for protecting human health and the environment.[9]

Green chemistry and engineering effects changes in the hazard of a product at the most fundamental level, the molecular level. The types of hazards that are of concern for their impact on human health and the environment can be viewed simply as physical or chemical properties of the substances being used. Simply put, the molecular structure of a chemical substance is a determining factor in its properties, such as potential health hazards. Practitioners of GC&E focus on modifying these intrinsic properties to reduce or eliminate the hazardous nature of these substances. In the same way that the mechanical properties of a substance can be designed, it is possible to design substances such that they do not exhibit certain toxic or hazardous properties. It is for this reason that green chemistry and engineering is capable of accomplishing its goals throughout the life cycle of a product or process; inherent properties do not change merely by moving through the various life-cycle stages. Life-cycle innovation, therefore, is recognizing that, by designing the fundamental properties of the substances used in particular stages of the life cycle, GC&E has the power to impact the entire life cycle of a product or process.[10]

Table 1. The Twelve Principles of Green Chemistry[a]

1. Waste prevention is preferable to waste treatment or clean up after it has been formed.
2. Wherever practical, synthetic methodologies should be designed to use or generate substances that exhibit little or no toxicity to human health and the environment.
3. Synthetic methodologies should be designed to maximize the incorporation of all materials used in the process into the final product.
4. A raw material or feedstock should be renewable, rather than depleting, wherever technically and economically practical.
5. Selective catalytic reagents are superior to stoichiometric reagents, all other factors being equal.
6. Unnecessary derivatives (e.g., blocking groups, protecting groups, temporary modification of physical/chemical properties, etc.) should be avoided where possible.
7. The use of auxiliary substances (e.g., solvents, separation agents, etc.) should be eliminated wherever possible, and in cases where they are necessary, they should be innocuous.
8. Energy requirements should be recognized for their environmental and economic impacts and correspondingly minimized.
9. Chemical products should be designed to achieve efficacy of function while reducing toxicity.
10. Chemical products should be designed so that, at the end of their functional life, they do not persist in the environment and break down into innocuous degradation products.
11. Substances used in a chemical process, and the specific form of those substances, should minimize the potential for chemical accidents resulting from releases, explosions, and fires, for example.
12. Analytical methodologies should be developed and used to allow for real-time, in-process monitoring and control to reduce or eliminate the formation of hazardous or unwanted substances.

[a] Source: Anastas and Warner.[8]

Assessing the Impacts of Green Chemistry and Engineering Technologies

The primary question regarding GC&E technologies is how we can best qualitatively and quantitatively assess the design parameters for green chemistry as listed above and assess the environmental and economic impacts of green chemistry and engineering technologies. To be useful, metrics should help to complete the inventory analysis stage of LCA. Metrics need to be specific and detailed enough to provide useful information about the chemical product or process, but they also must be simple enough to address the environmental issues within a useful time frame. Some desired metrics for LCA include (1) amounts of inputs, e.g., materials, water, electricity; (2) emissions to air, water, and land; (3) relative toxicities of materials; (4) process or product costs; (5) use of recycled material (e.g., waste or byproduct used as an input); and percentage of waste produced where

$$\% \text{ waste} = (\text{mass of waste})/(\text{mass of product} + \text{mass of byproduct} + \text{mass of waste})$$

A primary difficulty in assessing green chemistry technologies is gathering the data desired for LCA. Often, laboratory researchers might not realize what data would be of interest to a practitioner of LCA, and so, such data might not be noted or reported. With research in industry, a concern often arises about confidentiality and protection of trade secrets. However, much of the data of interest are not so specific as to be of corporate concern. Alternatively, company-specific data could be aggregated by researchers so that the data for individual companies are not publicly identified. The Green Chemistry Institute (a not-for-profit organization under the auspices of the American Chemical Society) is currently collaborating with academic researchers at the University of Scranton, and industry to design a quantitative survey to elicit data on products and processes in such a way that the data would be of use in LCA but also would not raise concerns of corporate confidentiality.

Assessing Green Chemistry and Engineering Technologies Using LCA

An essential aspect of green chemistry and engineering is that it can facilitate environmental improvements at every stage of the life cycle, which typically includes the stages of materials extraction and acquisition; materials transformation, processing, and manufacturing; packaging, transportation, and distribution; consumer use; and end-of-life management. A second essential aspect is that effective implementation of a green chemistry technology can offer environmental benefits that propagate throughout the life cycle. Specific examples illustrating these two aspects have been described elsewhere.[10]

Within the LCA framework, the first step in assessing technologies is to define the boundaries of the study. A useful concept is to choose the boundaries to be within your sphere of influence. This is so that, once the study is completed, the changes indicated by the LCA study can be made.

As discussed above, several types of quantitative data throughout the life cycle of a product or process are desirable to form an inventory analysis. Metrics can be tailored to a particular study to compare the environmental impacts of a process or product. For example, we might want to know the electricity use required by a traditional chemical process as compared to a process designed following the principles of green chemistry.

The impact analysis portion of an LCA is often the most difficult and controversial, because of the complicated nature of chemical fate and transport studies and of risk assessment for human health and the environment. For example, in a life-cycle study of a paper-bleaching process using chlorine, an impact analysis might assess the potential risks to the ecological environment and human health in the associated geographic regions. However, such analyses can often be disputed by the affected parties. At the most basic level, appropriate metrics will allow us to extrapolate logically that certain impacts must be lessened, if not to what extent. In the case of the bleaching process, appropriate metrics can allow us to determine that the dissemination of organochlorines has decreased. This can be viewed as an improvement, even if it is not possible to quantify the exact benefits to the environment or human health.

Finally, studying the life-cycle impacts of a product or process and assigning metrics for the comparison of two options allow us to pinpoint where the most significant environmental stressors occur over the life cycle, and the findings can also help to determine where the most effective changes (regarding both environmental impact and cost) can be made.

Life-cycle studies can be performed within a range of complexities, cost, detail, time, and even methods, depending on the resources available to the researcher. A most important factor in any LCA study, however, is that the method be transparent, so that the analysis is understood and so that future work can build upon the study. Here, we do not attempt to address a life-cycle question in its entirety. Rather, we present two brief examples of the life-cycle issues associated with two green chemistry and engineering technologies so that the reader will have a flavor of the goals and benefits of life-cycle assessment.

Example: Life Cycle of Metals

A major benefit of using LCA to assess green chemistry and engineering technologies is that such an analysis can uncover environmental impacts that might not have previously been considered and can highlight the most pressing environmental issues. Consider as an example PPG Industries Inc.'s project to replace lead in their automobile primer with yttrium, a project for which PPG was recognized with the 2001 Presidential Green Chemistry Challenge Award in Designing Safer Chemicals.[11] Be sure to note, however, that similar life-cycle questions can be asked about any GC&E project.

Let us briefly consider the life-cycle environmental impacts of replacing the lead used with yttrium (Y), a rare earth metal. Most people are aware of the health hazards of lead, and finding a substitute material is certainly desirable and noteworthy. The environmental benefits presented publicly focused primarily on the human health impacts of lead use. However, the environmental impacts of yttrium use must also be considered. A review of the life-cycle impacts would bring to mind additional questions, such as (1) What is the source of yttrium, and what are the environmental impacts of mining it? (2) What will the increase in the use of yttrium be with this new technology? (3) What are the impacts of a dissipative use of yttrium, as with paint?

A few minutes of research will show that China is the main source of yttrium, with 92% of mining production. Thus, China will likely bear the brunt of the environmental burden of increased mining and processing

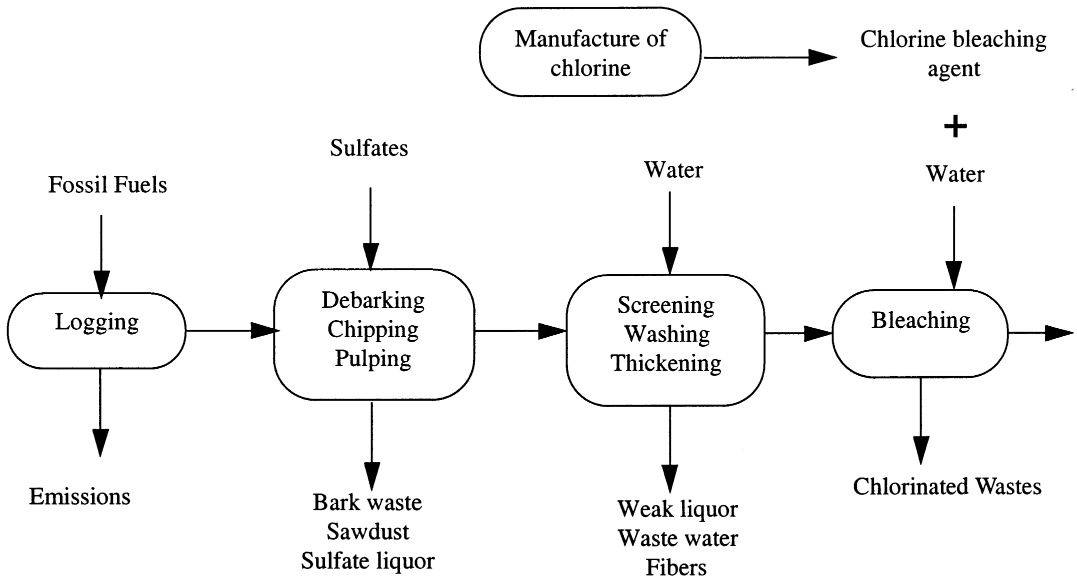

Figure 2. Flow diagram for the manufacture of bleached pulp. Modified from Ciambrone, D. F. *Environmental Life Cycle Analysis*; Lewis Publishers: Boca Raton, FL, 1997.

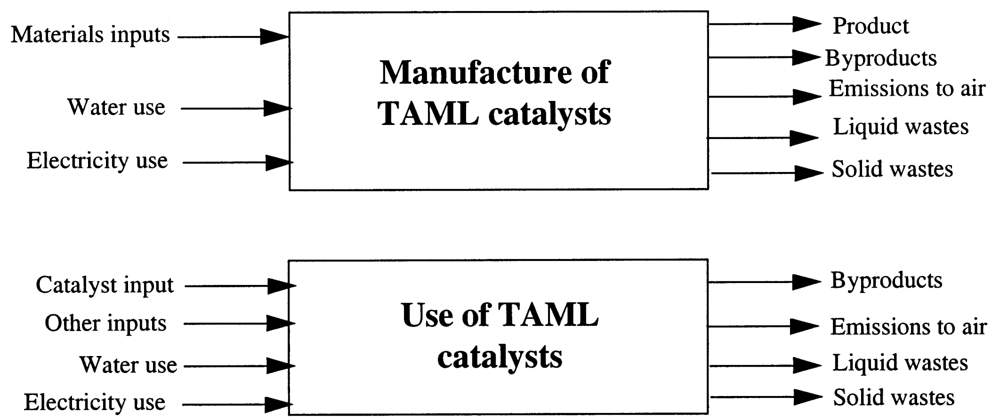

Figure 3. Diagram of inputs and outputs to be assessed in the manufacture and use of TCF bleaching catalysts.

activity to satisfy an increase in U.S. demand for yttrium. To recover yttrium, Y-containing metals are extracted as salts from ores using sulfuric acid (H_2SO_4), hydrochloric acid (HCl), and sodium hydroxide (NaOH). The U.S. estimated consumption of yttrium for 2000 is only 400 t of yttrium oxide (Y_2O_3), essentially all of which is imported. Yttrium metal is also quite expensive, costing about \$80−100/kg.[12] Although finding a substitute for lead is important, it is also important to acknowledge that the use of yttrium will incur environmental impacts and to recognize that trade-offs are being made.

Of course, this is not to say that the substitution of yttrium for lead should not be made. Incremental improvements are an essential aspect of GC&E. Small changes can often result in significant environmental benefits, and incremental changes are often easier and less expensive to implement than sweeping changes. The important point of using LCA in this way is to recognize and understand the tradeoffs that can be made when processes or materials are altered and to consider in advance the new environmental issues that might arise. Ideally, an LCA would describe the tradeoffs being made and would quantitatively show that the benefits of the process change outweigh any new environmental issues that arise and also that these potential new issues can be addressed satisfactorily.

Example: Alternatives to Chlorine Bleaching in the Pulp and Paper Industry

The widespread generation and dissipation of organochlorines is a recognized hazard to the health of people and wildlife.[13] Chlorine bleaching has been used widely in the pulp and paper industry; Figure 2 shows a flow diagram for the manufacture of bleached pulp. Much research is being done to find safer alternatives, and one alternative is using elemental-chlorine-free (ECF) technologies. Even more environmentally friendly is the replacement of chlorine-based bleaching with totally chlorine-free (TCF) methods (see, for example, refs 14−19).

One example of TCF methods is the use of the so-called TAML (a trademark owned by Carnegie Mellon University) catalysts as alternative reagents for paper bleaching.[14−16] To assess this green chemistry technology, we would like to be able to compare the resource use and environmental impacts of the manufacture of alternative whitening agents in the pulp and paper industry to those of traditional chlorine or ECF methods. Ideally, we would be able to collect and assess quantitative data on the processes, as illustrated in Figure 3.

Applications and Benefits of LCA

This type of methodology can be applied to the assessment of all types of advances in green chemistry, green engineering, and other disciplines. The boundaries of the study and level of detail can be tailored toward an assessment of the desired metrics. A life-cycle study of GC&E technologies can potentially save time and money by helping to identifying important issues, but LCA can also help to determine the full credit due to these technologies for their environmental and economic benefits.

This is especially important for an emerging and interdisciplinary area of research such as green chemistry. Often, reports on green chemistry and engineering technologies will focus on the immediate successes of the product or process developed. This is important, but for long-term investment and support for these technologies, it is necessary to understand the full life-cycle impacts. Collaborative and interdisciplinary research activities are an essential aspect of being able to study the life cycle of products and processes effectively and efficiently. Being able to demonstrate the life-cycle environmental and economic benefits of green chemistry and engineering technologies quantitatively will encourage government officials, industrial management, and academic researchers to invest the time, effort, and capital needed into further research and development and into the implementation of these and similar environmentally friendly technologies.

Summary

Green chemistry and engineering research offers a wide variety of demonstrable achievements and future potential for improving process and product environmental impacts, both at a particular life-cycle stage and also up- and downstream of a process improvement. Advances in green chemistry and engineering are essential to providing the specific innovations at all stages of a product or process life cycle by which we can implement the goals of industrial ecology while also maintaining a sustainable economy. Developing quantitative metrics and assessing GC&E technologies with these metrics and with life-cycle assessment are important steps toward demonstrating the full range of benefits of these technologies. Having both researchers and those who support or manage research understand the basic concepts and benefits of life-cycle assessment will help to bridge the gaps between broad goals and models, basic and applied research, and successful implementation of environmentally friendly and economically sustainable technologies.

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