2006-279: GREEN ENGINEERING DESIGN THROUGH PROJECT-BASED INDUSTRIAL PARTNERSHIPS

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Green Engineering Design through Project-based Industrial Partnerships

Abstract

Student projects have examined the impact of green engineering on both R&D and manufacturing in several chemical industries. This has been accomplished through industry-university partnerships with pharmaceutical and petrochemical companies. Several grants from the US Environmental Protection Agency have supported initiatives in green chemistry, engineering and design. These projects have the broader goal of supporting sustainability in the chemical industry.

Introduction

Too often the teaching of a technical subject like green engineering is limited to an individual class experience or one dimensional laboratory or design experience. The teaching of green engineering in the curriculum is greatly enhanced by active participation of students throughout the curriculum and in real-world projects. Green engineering is a multidisciplinary topic that if practiced to the fullest would greatly impact how industry operates and provide a sustainable future. Rowan University is incorporating green engineering into its curricula in various course and our latest efforts (as described in this paper) are to actively involve industry in green engineering projects through our engineering clinic program.

The EPA originally defined green engineering as the design, commercialization and use of processes and products that are feasible and economical while minimizing the generation of pollution at the source and also minimizing risk to human health and the environment [1]. The definition of green engineering was more broadly defined in a recent conference (Sandestin, Florida, 2003) to transforming existing engineering disciplines and practices to those that lead to sustainability. Green engineering incorporates development and implementation of products, processes, and systems that meet technical and cost objectives while protecting human health and welfare and elevating the protection of the biosphere as a criterion in engineering solutions [2]. Nine green engineering principles were developed as a result of this conference. Engineers should follow these principles to fully implement green engineering solutions:

1. Engineer processes and products holistically, use systems analysis, and integrate environmental impact assessment tools.
2. Conserve and improve natural ecosystems while protecting human health and well-being.
3. Use life cycle thinking in all engineering activities.
4. Ensure that all material and energy inputs and outputs are as inherently safe and benign as possible.
5. Minimize depletion of natural resources.
6. Strive to prevent waste.
7. Develop and apply engineering solutions, while being cognizant of local geography, aspirations and cultures.

8. Create engineering solutions beyond current or dominant technologies; improve, innovate and invent (technologies) to achieve sustainability.
9. Actively engage communities and stakeholders in development of engineering solutions.

Educational Approach

The traditional and probably most common method of introducing aspects of green engineering has been through a senior and graduate level elective course on environmental engineering, with an emphasis on process treatment. Courses were developed that focus on methods to minimize or prevent waste streams from existing chemical plants in the 1990's. The educational progression mirrors the progression in industry. In industry initial efforts were applied to waste treatment whereas current efforts are aimed at reducing the total volume of effluent treated as well as the nature of the chemicals treated. Currently, many of the environmental and pollution prevention courses have been replaced by courses in green engineering, environmentally conscious chemical process engineering, and engineering for sustainable development and a discussion of some of these efforts has been previously presented [3]. These courses are typically offered during the senior year and are optional engineering courses. These stand-alone courses are excellent in providing detailed coverage of the subject and are needed in the engineering curriculum. Students may get the impression that green engineering is either optional or something done at the end of the design process, since this course is usually both optional and at the end of their undergraduate education.

A better method is to introduce these concepts throughout the curriculum [4] which helps to emphasize that engineers should be using green engineering and sustainability throughout the design process. Implementing this integrated approach, in which students see green engineering throughout their 4 years of engineering shows the importance of this subject to the students and reinforces the need to employ this subject in industry. Both of these methods of education should be encouraged and further development is needed.

In 1998 a program was initiated with support from the EPA to develop a text book on green engineering, "Green Engineering: Environmentally Conscious Design of Chemical Processes" [5] by Allen and Shonnard; disseminate these materials and assist university faculty in using these materials through national and regional workshops coordinated with the American Society for Engineering Education (ASEE), Chemical Engineering Division [6]. Rowan University took the lead in developing curriculum modules that can be used to easily integrate green engineering concepts throughout the curriculum. These efforts include the development of instructor guides, case studies, homework problems and in-class examples. These efforts originally piloted at Rowan were expanded involving faculty from across the country in module development and implementation. These green engineering course modules can be found on the green engineering web site (www.rowan.edu/greenengineering) [7], [8] and are described in several papers [9], [10], 11.

Green Engineering Project-based Learning

We have sought to improve on our concept of green engineering education integration in a way that not only enhances student learning, but improves the environment. This is through real-world projects in our engineering clinic sequence [9]. The green engineering projects use a vertically integrated student team of junior, senior and masters level engineering students who work with the industrial partner on approaches to pollution prevention. These projects provide an illustration of how companies can take advantage of universities in their region to assist in sustainable development and manufacturing. Students are able to learn about green engineering design and apply their knowledge directly to a real industrial case. The industries involved partner by providing support in terms of senior staff, scientific/engineering process data, access to plant facilities, and take initiatives recommended forward to process improvements on the plant scale. The industries examined represent two distinct industrial sectors, thus providing student teams with unique challenges in designing for the environment. We expect these projects to yield the following green engineering outcomes which will be described in further detail in the paper.

Pharmaceutical industry : Bristol-Myers Squibb Co

- solvent reduction (in both quantities and toxicity)
- green engineering approach in initial phases of drug development to
  - increase efficiency in use of raw materials and energy
  - reduction in pollutant liquid waste
- energy conservation/recovery through life cycle assessment of processes

Petrochemical industry: Valero Energy Corp (Paulsboro, NJ)

- energy and water reduction/optimization
- increase efficiency in use of raw materials and energy
- emissions reduction/wastewater minimization

The role of academia in industrial projects in the green engineering area is vital to infuse fresh ideas into operations. The students and industrial personnel gain through training in the project briefings and plant visits where an exchange of ideas is encouraged. Each project starts with seminars by each party on their particular area of expertise thus fulfilling a goal of outreach. Students are encouraged to step back and look at the big picture and provide some points of view that draw upon both principles learned in prior courses or concepts learned in another clinic project. The clinic team will also develop a green engineering heuristic that will be applicable to other companies, thus expanding the outcomes of the projects.

Rowan University has experience in industrially-oriented projects through its Engineering Clinic program that partners academic experts with industry to solve real-world problems. Through the projects described in this paper we are extending our already successful program to pollution prevention and green manufacturing. Our record of success with industrial partners with clinic projects at Rowan has resulted in significant outcomes. [12, 13, 14, 15, 16, 17, 18, 19, 20, 21]

These projects are funded by grants from the U.S. Environmental Protection Agency, Region 2, through Pollution Prevention Grants Program and the Conservation Challenge Grants Program. Both of these competitive funding sources are administered by each region of the country. Matching and/or in-kind support is required for the pollution prevention grant program. Region 2, where Rowan University is located is comprised of New Jersey, New York, Puerto Rico, the U.S. Virgin Islands and the Tribal Nations.

Pharmaceutical Industry Initiatives

The pharmaceutical industry is a prominent commercial sector in EPA Region 2. The majority of the leading pharmaceutical companies have headquarters, research & development centers and manufacturing facilities in New Jersey, New York and/or Puerto Rico. This industry is vital to the regional economy as well as to national security and the standard of living, health, and welfare of the public at large. For the United States pharmaceutical industry to grow and develop in a sustainable way (while at the same time meeting current and future EPA regulations), adoption of green engineering principles is necessary from R&D through manufacturing. Through this project, a student-faculty team is working with Bristol-Myers Squibb scientists and engineers to develop green engineering protocols that can be adopted by the pharmaceutical industry.

The majority of drug products made through organic synthesis routes require many sequential reaction steps, large quantities of organic solvents (with varying degrees of toxicity), and are made in batch processes. All of the above are not optimal from a green engineering manufacturing standpoint. A significant impact on the use of solvents, in terms of quantities and toxicity, can be made if investigations into the early stages (Phase I or II) of drug development are performed. It is important to work with drugs in Phase I or II of development, since these changes can be incorporated into the final manufacturing steps that are approved by the FDA. By Phase III, “synthesis lock” and “process lock” prevent innovations from being easily implemented. The team is working on developing a heuristic that pharmaceutical companies can follow in the development of new drugs.

The specific objectives of this project are to identify reductions in the use of hazardous chemicals in a drug synthesis. The Rowan team first met with the Bristol-Myers Squibb staff and discussed several possible drugs at various stages of development that we could examine. A confidentiality agreement was signed which limits the amount of information we can reveal about the drug and the manufacturing process. A cancer drug in the early stages of development was selected. The team then met to set and review project goals/objectives.

The initial part of the project involved a review of process development documentation and a pilot plant visit to understand equipment issues. The basic data on raw materials, products, byproducts of the process were analyzed. Green engineering metrics for lab-scale (discovery), intermediate and pilot-scale processes were compared. Life cycle assessment was made using overall material and energy balances along with environmental performance tools. Tier 1 tools such as economic criteria, environmental criteria, exposure limits, toxicity weighting in analyzing various drug production pathways.

Since organic solvents typically account for 80% of all chemicals in a pharmaceutical process, a significant part of the work focuses on process modifications to reduce solvents used. Several process opportunities for greener processes were explored. A life cycle assessment is conducted to compare these alternatives and show broader impacts on the ecosystem (greenhouse gas production, etc). These alternative production routes include new solvents and processing methods. Throughout this process, we are in constant contact with Bristol-Myers Squibb R&D

staff and get feedback for continuous improvement of our approach. The analyses of these alternative approaches are presented to the company in bimonthly progress meetings. One of the techniques develop that can gauge the “greenness” of these process improvements is a solvent selection table. This technique that the student team developed is described in the following section.

Green Engineering Example – Solvent Selection Guide

One of the particular issues that the team investigated was the solvents used in processing. By applying green engineering to the process development of a pharmaceutical, this will lead to protocols on how quantities of solvents can be reduced and also present a technique for systemic solvent examination that can be translated throughout the industry. An expected result would be to replace a traditional process in which 5 to 10 steps use 20 solvents with a new process that reduces both the number of solvents and the amount of solvent used.

A computer-based solvent selection guide was developed that compares the “greenness” of solvents used in various process steps. Methods to determine the most efficient solvent for a specific process take into consideration various factors. These considerations include basic engineering, economics, chemistry principles, and safety concerns, which are typically the primary concerns for solvent selection. This table provides guidance for selected solvents from an environmental perspective. The environmental categories are typically secondary consideration for solvent usage in the pharmaceutical industry. There are a large number of databases and information available for the various environmental criteria, but most of this information is not readily available for comparison. The user has to search for the data and re-enter the data into a spreadsheet if a comparison of two solvents is desired. This data is available from MSDS sheets, the EPISUITE software package, SOLV-DB website along with the metrics developed by IChemE [22], [23], [24] [25].

An Excel spreadsheet was developed which includes inhalation toxicity, ingestion toxicity, aquatic toxicity, ozone depletion, smog formation, global warming potential, carcinogenicity and acidification for typical solvents used in the pharmaceutical industry. The environmental metrics used for this solvent selection guide take into account safety and liability. This solvent selection guide is different from previous solvent selection guide because it takes into account parameters, which were not previously considered in other solvents selection tables. This table also provides the user with raw data, so a direct comparison can be made very quickly to determine if any process improvements were made in the environmental categories. Another advantage to this solvent selection guide is that the data can be expanded to include solvents which are proprietary.

The spreadsheet calculates greenness and workers’ safety in terms of a weighted scale, otherwise know as a pharmaceutical index. This index would allow quick and easy comparison between different process routes to determine which process is inherently greener. The program can also determine multiple green process solutions for the same process by factoring in different weighted scales defined by the user. The Excel program can be customized for the twelve metrics mentioned above. The total weighted index is the sum of each metric. Weighted values were calculated by multiplying a given parameter by the mass of that solvent used in the process.

A weighted index was established to measure which solvent would be more applicable for a particular process. Each metric was scaled and summed to generate an overall index dependent upon amount of solvent used in the process. To accomplish this, each parameter was normalized from 0-1 so that the lower numbers reflect greener material for a given category. These values were then summed by a weighting factor to stress the category of greatest concern. To accomplish this, each category (i.e. Ingestion toxicity, biodegradation, aquatic toxicity, etc.) was initially weighed on a log scale with a log base equivalent to the maximum value of that particular parameter. These values were then scaled in a linearly fashion utilizing the following formulas:

$$1 - \frac{\log_b x - \log_b x_{\min}}{\log_b x_{\max} - \log_b x_{\min}} \tag{1a}$$

$$\frac{\log_b x - \log_b x_{\min}}{\log_b x_{\max} - \log_b x_{\min}} \tag{1b}$$

where $\log_b x$ is the log base value of specified solvent
$\log_b x_{MIN}$ is the minimum log base value of solvent for known parameter
$\log_b x_{MAX}$ is the maximum log base value of solvent for known parameter
b represents highest value witnessed in known parameter
x represents value of specified solvent

For example, given values from Table 1 and Equation 1a,

Table 1 Max/Min Values of Ingestion Toxicity in which Solvent is Scaled upon based on all 64 Solvents in Database

	$X_{Acetonitrile}$ (PPM)	**Xmin (PPM)**	**Xmax (PPM)**	**log min**	**log max**
Ingestion toxicity (rat mg/kg)	3800	24	25000	0.3	1

*Xmax and Xmin values are obtained from Solvent Selection Table. These are the highest and lowest values of the specified parameter (in this case, ingestion toxicity) witnessed within the database. Similarly, logmin and logmax are are the highest and lowest values of the log scale specified parameter witnessed within the database.

Ingestion toxicity for acetonitrile can be scaled as follows

$$\text{Ingestion Toxicity}_{\text{Acetonitrile}} = 1 - \frac{\log_{25000} 3800 - \log_{25000} 24}{\log_{25000} 25000 - \log_{25000} 24} = 0.27$$

Both equations 1a and 1b enable our scales to invert between 0-1 and 1-0. High values in specified parameters that signified relative greenness would employ Equation 1a to generate low weighted scales. Equation 1b is used to generate low weighted scales if the parameters have low values signifying relative greenness. This issue becomes extremely important when summing parameters into an overall weighted index factor where those that are judged greener are lower than those deemed toxic. Table 3 below depicts how each factor was scaled in terms of greenness due to relatively high/low parameter values.

Table 2: Greeness with Respect to Relative Values Set in Specified Metric Parameters

	HIGH VALUES	LOW VALUES
Threshold Limit Value	Greener	
Ingestion	Greener	
Biodegradation	Greener	
Aquatic Toxicity	Greener	
Carcinogenicity		Greener
Half Life		Greener
Ozone Depletion		Greener
Global Warming Potential		Greener
Smog Formation		Greener
Acidification		Greener
Soil Adsorption		Greener
Bio Concentration Factor		Greener

According to this table, TLV, ingestion, biodegradation and aquatic toxicity are scaled using Equation 1a. The remaining parameters were scaled using Equation 2a. The overall weighted indexed was then tabulated as a summation of these parameters with several factors weighted more so than others. For our specific case working with pharmaceuticals, workers' safety was of primary concern when establishing a weighted index. Therefore, threshold limit values, ingestion toxicity, and carcinogenicity were weighed more heavily than others in establishing a pharmaceutical greenness index. The tabulation determined using the following equation:

$$\begin{aligned}\text{Pharmaceutical Index} &= 2*(\text{TLV} + \text{Ingestion} + \text{Carcinogenicity}) + \\ &\text{Biodegradation} + \text{Aquatic Toxicity} + \text{Half-Life} + \text{Ozone Depletion} + \text{GWP} \\ &+ \text{Smog Formation} + \text{Acidification} + \text{Soil Adsorption} + \text{BCF}\end{aligned} \qquad (2)$$

Since low values for the parameters signify greenness, intuitively low values for pharmaceutical index indicate relative greenness. The index is used as a guide to quantitatively assess the greenness between two or more solvents or processes. An overall pharmaceutical index calculation for acetonitrile would be

Table 3: Scaled Values (0-1) of each metric derived for Acetonitrile

Acetonitrile	
TLV (ppm)	0.45
Ingestion (rat mg/kg)	0.27
Carcinogenicity (unitless)	0
Biodegradation (log Biodegradation)	0.27
Aquatic Toxicity (mg/L)	0.3
Half-Life (12 hr days)	0.73
Ozone Depletion (unitless)	0
GWP (unitless)	0.33

Smog Formation (unitless)	0.2
Acidification (unitless)	0
Soil Adsorption (log Koc)	0.72
Bio Concentration Factor (log BCF)	0.27

Overall Index Scale of Acetonitrile is derived in equation 2.

$$OIS_{Acetonitrile} = 2\times(0.45+.27+0)+0.27+0.3+0.73+0+0.33+0.2+0+0.72+0.27 = 4.3$$

Similar calculations can be performed for other solvents used in the process. These are then combined into an overall greenness score using the mass of the solvents used in the manufacturing operation. Thereby a comparison of the relative greenness of the processes can be made.

Petroleum Refining Industry Initiative

Some of the largest and most visible manufacturing plants in EPA Region 2 are the petroleum refineries that are situated near the major transportation arteries in New Jersey. They are excellent candidates for applying green engineering methods because of their size, quantities of material processed and emissions issues. Since no new refineries have been built in the United States in over 25 years, the industry needs to take existing older facilities and upgrade and optimize them to allow operations to be conducted in an economic and environmental way. This upgrade is necessary since refining operations are vital to national security and energy policy.

The U.S. petroleum refining industry has come under considerable strain because of several important factors and changes in the industry. Over the years, there has been an increased domestic demand for petroleum products and a decrease in U.S. production; however, there has been no new capacity added. This lack of infrastructure growth has caused a tremendous strain on the industry in meeting existing demand, and the U.S. has had to increase the amounts of imports to meet these needs.

A number of Federal regulations such as the Clean Air Act and the Clean Water Act along with stringent state regulations have also caused the industry to incur high costs for environmental compliance. These costs are accrued because refineries must produce reformulated, cleaner-burning gasoline, which require companies to replace or modify existing equipment with devices for controlling emissions. These costs of compliance are having an effect on refineries trying to expand and to keep pace with the country's increasing demand.

Through this project we are assisting industry in innovative and cost-effective pollution prevention strategies and improve their methods through on-site training and implementation. The initial exploratory phase of the project involves a series of brainstorming sessions with engineers from various refinery operations to look at challenges and opportunities in pollution prevention and green engineering.

A team of Rowan faculty and students is currently working side-by-side with Valero staff investigating various aspects of pollution prevention strategies. Some of the areas that we anticipate being involved in are wastewater minimization through water reuse and recycle and energy optimization though heat integration and heat exchanger network retrofitting [12], [13], [14], [15], [16]. Complete details will be presented in the conference. The overall energy optimization is a multi-step process that involves

- Simulation of existing units:
- Flowsheet simplication
- Determination of the basic energy savings horizons
- Synthesis of the horizon networks
- Retrofit network
- Test the feasibility of the new retrofit network
- Cost Analysis

The overall water use optimization will also be conducted using a methodology developed by Savelski [21]. In this case, the proposed procedure identifies the minimum water usage (target) of a given set of water-using/water-disposing processes (desalters, hydrodesulphurization processes, distillation, etc), and then determines a network of interconnections of water streams among the processes so that the overall fresh water consumption is minimized while the processes receive water of adequate quality. As with the energy optimization method, the water-use minimization involves several steps,

- Fresh Water Targeting
- Network Construction
- Alternative Networks

Summary

Two EPA-sponsored projects in pollution prevention have been started that focus on solving real-world industrial problems. These projects tackle pollution prevention issues of two distinctly different industry with similar goals of water, energy, and pollution reduction through green chemistry and engineering strategies. The students involved in these projects will be analyzing process operations and examining methods to quantify material and energy usage and proposing approaches for green engineering design.

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