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Life Cycle Inventory Assessment as a Sustainable Chemistry and Engineering Education Tool

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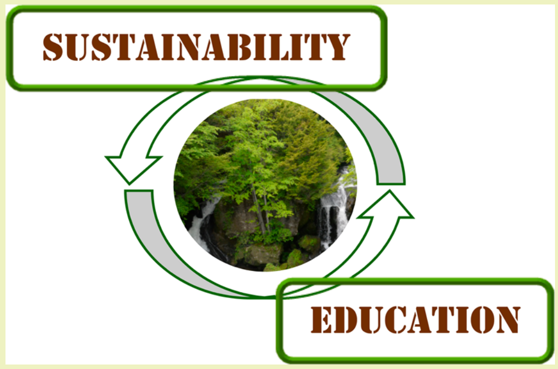
ABSTRACT: Chemists and chemical engineers are involved in and responsible for the life of a product from the discovery stage to manufacturing, market introduction, and end of life. They participate in and contribute to all segments of the supply chain, from cradle to grave. In the industrial sector, they work hand in hand with other professionals in engineering, business, intellectual property, and environmental safety and health. To better prepare students to understand industry-focused grand challenges and contribute to the long-term sustainability of the enterprise, we designed a course for advanced undergraduate and graduate students in the Schools of Chemistry & Biochemistry and Chemical & Biomolecular Engineering at the Georgia Institute of Technology. The pilot class of 26 students was introduced to chemical manufacturing, the eight sustainability grand challenges, intellectual property, regulatory and registration, and process hazard and safety. Invited speakers from industries such as Albemarle, BASF, Dow, ExxonMobil, GSK, Solvay, and PepsiCo presented their companies' approach to sustainability. Life cycle inventory (LCI) assessment of an existing product in the market was the main thrust of course, whereby student teams were charged to develop a virtual manufacturing process based on their review of patented literature. The groups completed nine LCI assessment projects, and by applying mass metrics and GC&E principles, they offered recommendations for rendering the processes more sustainable. This perspective presents the course objectives, approach, LCI methodology, results, conclusions, and lessons learned.



KEYWORDS: *Life cycle inventory, Life cycle assessment, Sustainability, Circular economy, Process and product design*

INTRODUCTION

"The public doesn't want to smell anything in their water," said Djanette Khiari, research manager at the Water Research Foundation as reported in the July 3, 2017, issue of Chemical and Engineering News.[1] Access to water, food, and energy are among the leading challenges facing global society today.[2,3] What better motivation for education and research and development in sustainable chemistry and chemical engineering than access to clean water! It has been predicted that we will need enough water, food, and energy to sustain a population as high as 9.8 billion by 2050 and 11.2 billion by the turn of century.[4] Key to meeting these challenges will be continued advances in chemistry, chemical engineering and materials science and engineering. Their products are ubiquitous in our daily lives—from pharmaceutical and biomedical technologies to electronics and communications to transportation and infrastructure. As discoveries continue to be made and technologies advance, how do we ensure the health and well-being of our planet for generations to come?

Increasingly, the grand challenges identified in the United Nations report[5] are driving new research initiatives. Reports such as that recently released from the 2016 NSF Workshop related to polymer science and engineering[6] discuss those challenges within the context of a somewhat more focused discipline. Note one of the grand challenges identified in that report: "Achieve accessible, scalable polymers that match or exceed the property matrix of existing materials, yet have a green life-cycle." The authors go further to point out the importance of life-cycle thinking.

The above report, along with many similar studies, comes a full decade after the National Research Council (NRC) of the National Academies released a report detailing eight grand challenges that must be addressed to secure a long-term sustainable future,[7] and the broad concept of sustainability has caught the attention of many leaders in the scientific, engineering, industrial, and regulatory communities. Education, or rather sustainability education which was called out as one of the eight grand challenges in the 2006 National Academies

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report, is of paramount importance to instilling "life-cycle thinking" into product and process design and development. Examples of how one might implement sustainability within science and engineering curricula are beginning to emerge. In 2009, Murphy et al. reported the results of their benchmarking studies on the incorporation of principles of green engineering into engineering curricula across the United States.[8] Allen and Shonnard provided a perspective on the knowledge base required for chemical engineering education.[9] They defined three major elements: framing the challenge, assessment and design, and systems perspectives. The major component of their "systems perspective" element is the use of life cycle assessment case studies. Allen et al., in 2016, provided an update on progress in incorporating green engineering content in chemical engineering curricula.[10] They concluded that incorporation of global perspectives, environmental literacy, and sustainability into the existing curricula will better prepare graduates for the challenges of future. Further, Yosie et al.,[11] suggested the following: "Engineering schools must include sustainability in curricula by adapting initiatives that are both internal and external to the university". They recommended lowering the barriers across disciplines and expanding participation by faculty and students in learning opportunities outside the classroom.

Recognizing the need for incorporating sustainability education into chemistry curricula, a visioning workshop was organized by the American Chemical Society Green Chemistry Institute (ACS GCI) in September 2015 to bring together key stakeholders to articulate a vision for a roadmap and identify the future state that will be achieved through that roadmap. The vision that emerged was the need for "Chemistry education that equips and inspires chemists to help solve the grand challenges of sustainability."[12] Discussions during the workshop focused on the current state of chemistry education and the steps needed to achieve the vision, at which point all chemistry will be green. As the ACS GCI Roadmap vision statement aptly pointed out, "the practice of chemistry should change from chemistry focused on academic and economic value with minimal regard for environmental, safety, or health impacts; to process and product design to minimize adverse environmental, health, and safety impacts while enhancing desired performance throughout the product life cycle."[12] The 2015 ACS GCI discussions laid the foundation for a draft set of green chemistry and engineering core competencies that embody the knowledge, skills, and abilities that a chemistry or chemical engineering graduate should possess. Graduates should be able to do the following:

- Design and/or select chemicals that improve product and sustainability (societal/human, environmental, and economic) performance from a life cycle perspective
- Design and/or select chemical processes that are highly efficient, that take advantage of alternative feedstocks, and that do so while generating the least amount of waste
- Understand how chemicals can be used/integrated into products to achieve the best benefit to customers while minimizing life cycle sustainability impacts
- Think about and make decisions taking into account life cycle thinking and systems analysis

A critical insight stemming from the workshop was that an overarching competency in sustainability requires systems thinking, which could serve as a key anchoring concept for chemistry education as our global society struggles to address the grand challenges of sustainability. The systems approach has been embraced by the chemical enterprise. The business needs of this enterprise, the major employer of chemistry and chemical engineering graduates, demand it. The business of chemistry continuously adjusts to evolving market needs, regulations, globalization, and supply chain demands. On the other hand, chemistry and chemical engineering curricula have remained largely unchanged over several decades. In the classroom, students rarely engage in multidisciplinary project teams, whereas in industrial settings, chemists and engineers routinely work together to develop new products and processes and bring those products to the market. In the U.S. alone, the business of chemistry was valued at about $800 billion in 2016, supported nearly 26% of the US GDP, provided 810,000 skilled good-paying American jobs, and invested $44 billion in R&D.[13] U.S. chemical sales are expected to exceed $1 trillion by 2020.[14] The global perspective is equally impressive. Europe is home to over 28,000 companies with a turnover of €520.2 billion, 1,155,000 direct employees, and R&D spending of €9.14 billion;[15,16] China's 2015 chemical sales were €1408.7 billion. The United Nations Environmental Program Global Chemicals Outlook Report[17] estimated that in developed countries the chemical industry output will be $3000 billion by 2020. For developing regions and countries with economies in transition, chemical output was estimated to grow to $3300 billion.

Clearly, the chemistry enterprise is global, with global supply chains and markets. Within that context, the enterprise must adjust to global regulations designed to improve the sustainability of products and processes. Perhaps the most stringent regulations are those of the EU, where the cost of compliance doubled during the 2004−2014 decade. The average cost of the EU regulations presented in Table 1 was estimated at €10 billion per year. The major contributors to those costs were industrial emissions (33%), chemicals (30%), and worker safety (24%). Regulatory compliance also impacted capital spending: as reported by Cefic, during 2005−2015, EU spending increased from €17.2 to 20.7 billion, while the U.S. and China saw increases from €9.8 to 32.5 billion and €14.4 to 95.6 billion, respectively.[15]

Table 1. Regulatory Legislation Introduced in the EU during the 2004−2014 Decade

Year	Legislation
2007	REACH (Registration, Evaluation, Authorization of Chemicals)
2008	CLP (Classification, Labeling, and Packaging)
2012	Seveso III (Health, Safety, and Environment)
2013	ETS Phase 3 (Emission Trading System)

To continue to grow and support our economy, the chemical enterprise needs an agile, flexible workforce that thinks "systems and sustainability". Quite simply, global regulations require businesses/industries to adopt practices that support a *circular economy*. In a 2016 briefing, the European Parliamentary Research Service discussed "opportunities and challenges" for moving toward just that, a circular economy.[18] One of the four identified challenges was the need for technical skills "which are currently not present in the workforce", namely, skills for scientists and engineers that would enable them to design products with circularity in mind. The briefing emphasized that the lack of such skills would be particularly problematic for scientists, mathematicians, and engineers.

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Thus, the roles and responsibilities of chemists, chemical engineers, and materials scientists and engineers should extend not only to the life of products in the market but, importantly, to the "end of life" and environmental fate of those products.

Leading chemical and pharmaceutical companies have established sustainability programs to assess their products and manufacturing processes. In some cases, they have developed their own special tools, while in others existing tools and databases have been used. Figure 1 presents an example of a toolbox developed by BASF, which consists of life cycle inventory (LCI) and life cycle assessment (LCA) for impact on the environment, total cost of ownership for cost from cradle to grave, eco-efficiency for impact on the environment and costs, and SEEBALANCE for impact on environment, costs, and society.[19,20] The social impact categories include employees, the international population, future generations, consumers, and local and national communities.[21]

Figure 1. Image depicting the elements of the sustainability toolbox developed by BASF (courtesy of BASF).

Borregaard, a Norwegian chemical company, also routinely conducts life cycle assessments. In 2008, they evaluated their products (cellulose, ethanol, lignin, and vanillin) for greenhouse gas emissions. Later, they performed a complete LCA on the same products. To establish the environmental profile of all their products from the Sarpsborg biorefinery plant, another LCA was carried out; Environmental Product Declarations (EPDs) were filed and are available on the Norwegian EPD Foundation Web site.[22−24]

Other companies, or company associations, have also developed toolboxes to assess the sustainability footprint of products and processes. Table 2 presents a handful of examples that have been reported recently.[25−30] All are used to assess the sustainability of product, process, and service ideas in the early stages of research and development. Notably, the GCI Pharmaceutical Roundtable believes that green chemistry and engineering are an imperative and is pursuing the implementation of green chemistry and engineering into all facets of drug production from discovery to development and manufacturing.[31]

Although some companies have developed their own methodologies, others have commissioned LCI assessments from consulting organizations. For instance, the Plastics Division of the American Chemistry Council (ACC) commissioned the life cycle assessment of nine plastic resins and four polyurethane precursors using manufacturing data provided by member and nonmember companies.[32] Also, PlasticsEurope, the European trade association of plastics manufacturers, provides access to eco-profiles of many chemicals on their Web site.[33]

Motivated by the recognized societal need for the design and development of sustainable chemical and materials technologies, coupled with the need for scientists and engineers to be educated in life cycle thinking, we developed an elective course entitled "Fundamentals & Challenges of a Sustainable Chemical Enterprise", which built on aspects introduced in a chemical engineering elective taught in Spring 2015 at the Chemical Engineering Department of Louisiana State University. Taught for the first time in Spring 2017, the Georgia Tech multidisciplinary team project-based course was aimed toward graduate and advanced undergraduate students in the Schools of Chemistry & Biochemistry and Chemical & Biomolecular Engineering at the Georgia Institute of Technology. The course and approach was the first of its kind at Georgia Tech; it is arguably the first course in North America to bring the chemistry and chemical engineering communities together with active participation from sustainability experts in the enterprise, where the whole chemical product value chain was represented. This perspective provides a view on the course objectives and outcomes and suggests next steps to accomplish more widespread sustainability curriculum design and implementation strategies.

■ OBJECTIVES

The syllabus (Table 3) was designed with the aim of introducing students to the diverse and fascinating world of the chemical enterprise. Key objectives included the desire to expose students to the value chain—commodity products, pharmaceuticals, and consumer products—and for students to appreciate the crucial role and responsibilities chemists and engineers hold within the chemical enterprise. The aim was to provide them with the tools they will need to design and develop sustainable products and processes, while effectively addressing the grand challenges associated with sustainability. Within these contexts, the course offered students the opportunity to apply sustainable chemistry and engineering knowledge/learning to solve real world challenges through a multidisciplinary approach leading to innovative solutions and have the opportunity to interact with sustainability leaders in the chemical enterprise.

Table 2. Additional Examples of Sustainability Tools Developed in the Enterprise

Company	Toolbox	Sustainability dimensions	Ref
DowDuPont	DCSFT (Dow Chemical Sustainability Footprint Tool)	economic, social, resource use, water, greenhouse gas (GHG), Dow organization	25
	Dow Dimension Tool	resource quality, renewable-recycled raw materials, conversion efficiency, process safety, chemicals management, water, energy, GHG	
GlaxoSmithKline (GSK)	FLASC (Fast Life Cycle Assessment of Synthetic Chemistry)	synthesis route selection in early stages of pharmaceutical research; resource efficiency; materials environmental health and safety	26−28
GCI Pharmaceutical Roundtable	PMI/LCA (Process Mass Intensity/Life Cycle Assessment)	pharmaceutical industry mass-based green metric	29, 30

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Table 3. Syllabus for Course on "Fundamentals & Challenges of a Sustainable Chemical Enterprise"—Spring 2017

No. of sessions	Session Topic
1	History of chemical industry
2	Introduction to manufacturing: cradle-to-gate
2	Green Chemistry and Engineering
1	Role of chemists and engineers in industry
2	Material balance and green metrics
2	Life Cycle Inventory and Life Cycle Assessment
1	IP, patents, and patenting process
1	Toxicology basics
1	Energy intensity of chemical processes
1	Sustainability at BASF
1	Renewable feedstocks
1	Separation, sequestration, and utilization of CO_2
1	Class sustainability debate
1	Sustainability at ExxonMobil
1	Sustainability at Dow
1	Process safety and hazard analysis – Albemarle
1	Sustainability at Solvay
1	Sustainability at PepsiCo
1	Sustainability at GSK
1	Team poster presentations

To do so effectively, students were also introduced to the complexities of the global supply chain and its management; they became familiar with key elements of intellectual property and patent law, safety and health, regulatory requirements and product registration, and environmental challenges. Further, they learned the importance of effective communication to all stakeholders, namely, business leaders, shareholders, customers and, most critically, the communities in which they live and work.

From an educational perspective, most leading Chemical Engineering programs are accredited by ABET, the Accreditation Board for Engineering and Technology, where accreditation criteria include a requirement for documentation of key, desired student outcomes. As is evident from examination of Figure 2, the course objectives presented above map directly onto the desired outcomes.[34] From a chemistry perspective, the American Chemical Society[35] provides guidelines for undergraduate chemistry degrees; however they are more specifically focused on core chemistry course content.

■ APPROACH

The course began with a discussion of how the chemical industry evolved and the historical health and environmental events that led to the creation of regulatory agencies and laws, the birth of green chemistry and engineering concepts, and ultimately to sustainability and industry's grand challenges. To provide students with a better understanding of the chemical enterprise, leaders from several sectors of the industrial community were invited to visit and share their respective companies' sustainability programs. Companies such as BASF, Dow, ExxonMobil, Solvay, Albemarle, Pepsico, and GSK welcomed the opportunity. Included in the curriculum were topics such as green chemistry and engineering principles, toxicology, renewable feedstocks, LCA and LCI, energy intensity of chemical processes, renewable fuels, and CO_2 separation, sequestration,

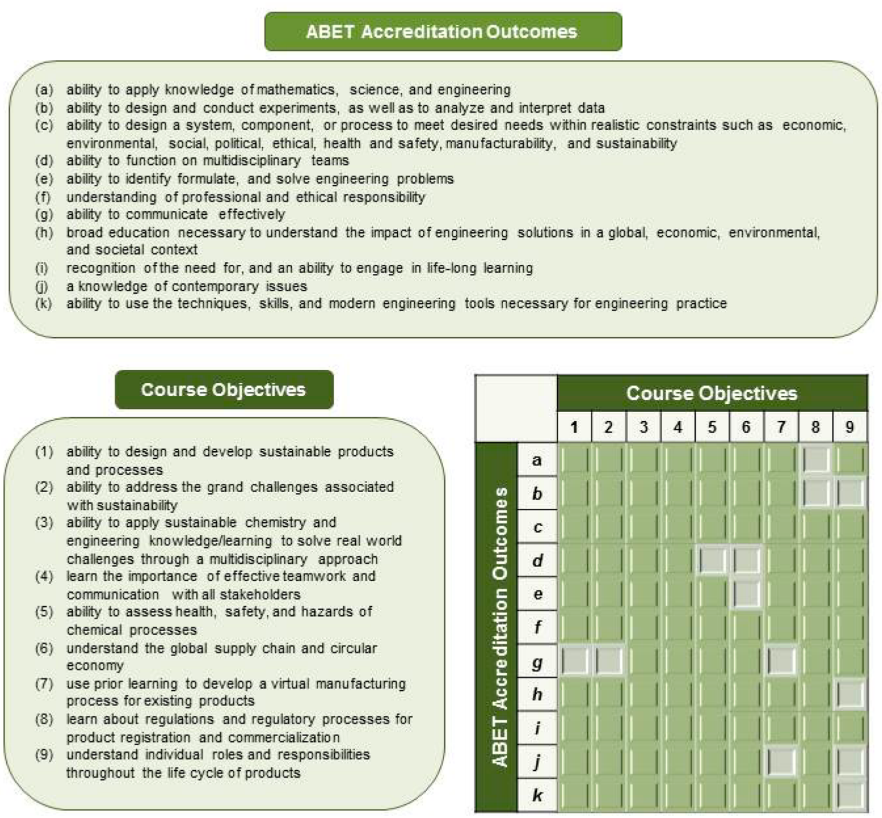

Figure 2. Presentation of desired ABET student outcomes, course objectives, and a map showing overlapping features between the objectives and outcomes.

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and utilization. Since students were required to complete an LCI project, they were also introduced to issues surrounding intellectual property, product registration and regulation, supply chains, new product/process development processes, and process safety and process/reaction hazard analysis.

Life cycle inventory is the foundation for assessing the sustainability of products and manufacturing processes. Companies in the enterprise either have developed their own proprietary tools such as SEEBALANCE, FLASC, and DCSFT which use proprietary manufacturing data or they provide manufacturing information under confidentiality to companies or organizations who carry out the study. Good examples of the latter are Borregaard and the Plastics Division of ACC. Thus, an LCI assessment of a selected group of existing products in the marketplace was chosen as the central element of the course. In the absence of real manufacturing data, and recognizing that patent applications are usually filed in the early stages of development and published after 18 months from filing date, we believe they provide the best source for manufacturing data regarding mass of components and process conditions. Cleary, this applies more to products and not as much to commodity raw materials which have been around for a long time.

The products interrogated by the project teams were vanillin, polyethylene terephthalate (PET), and polylactic acid (PLA). These particular products were chosen because they are (i) ubiquitous in our daily lives and have a wide range of applications, (ii) produced through multiple manufacturing routes by several vendors, and (iii) manufactured from petroleum as well as renewable resources. In addition, they provide an excellent opportunity for in-depth side-by-side sustainability analysis and, importantly, *systems thinking*. The approach to learning about the grand sustainability challenges relied heavily on the design of a virtual manufacturing process for products in the market that everyone could relate to easily. Through this action-based team-oriented exercise, students were inspired to apply the knowledge and skills acquired in this course and throughout their education to identify and address the grand sustainability challenges. The course objectives were achieved through a series of steps highlighted in the following:

- Establish communication and dialogue between chemists and engineers by creating three-membered teams that functioned throughout the semester
- Develop a virtual manufacturing process with a complete mass balance from a published experimental procedure from the *Journal of Organic Chemistry*
- Apply green chemistry and engineering principles to this virtual manufacturing process to identify challenges and opportunities for rendering the process more sustainable
- Compare existing commercial manufacturing processes from industrial literature with the virtual manufacturing process using green chemistry and engineering principles and mass metrics
- Assign an existing commercial product to each team for LCI and sustainability analysis
- Conduct a class debate on the sustainability and regulatory challenges associated with bisphenol A
- Have each team select a sustainability subject and prepare a short video to be evaluated by their peers in the class
- Require a final detailed LCI written report and presentation of results in a poster session to be evaluated by industry judges

The LCI Teams and their assigned projects are presented in Table 4.

Table 4. Life Cycle Inventory Project Teams

Team	Project
1	Polylactic acid (PLA) from corn
2	Polylactic acid (PLA) from oil
3	PET Production − PlantBottle from Coca Cola
4	PET production from oil through oxidation of *p*-xylene and ethylene glycol
5	PEF (polyethylene furanoate)
6	Vanillin from oil through guaiacol
7	Vanillin from rice bran−ferulic acid (Rhovanil)
8	Vanillin from sulfite black liquor
9	Novolac production

Determination of an accurate mass balance for all chemical reactions and ultimately for the manufacturing processes and mass closures for each step of the process were essential. Also, labeling of each stream as raw material, product, coproduct, auxiliary, catalyst, solvent, waste, emission, etc. was required, as was the identification of the recyclable streams. Developing an accurate mass balance (accounting for every gram of material input) for each step of the manufacturing processes posed a challenge at the beginning of the course, especially for chemistry students who were introduced to the concept for the first time. Through several assignments, students were shown how to develop mass balance spreadsheets for each step of a manufacturing process with the specific purpose of determining and accounting for mass input, output, and waste and recycle streams.

Believing that mass metrics are the foundation for sustainability assessment of manufacturing processes, our top priority was sustainability assessment by applying mass metrics. Energy and carbon footprint analyses were optional. Additionally, while a spreadsheet for a "back of the envelope" process economic evaluation was developed for student teams to carry out a process economic evaluation to complement their projects, this aspect was eliminated from the requirements in this first course iteration because of the heavy course load of many of the students and the project timeline.

LCI METHODOLOGY

Personal experience with LCI assessment of two commercial flame retardant manufacturing processes[36] demonstrated the immense value of the methodology to better understand the associated environmental and economic challenges and identify the significant contributors to those challenges, and the "hotspots" associated with the manufacturing processes. Addressing those challenges can bring economic and health and environmental rewards. For the pilot course, we adapted the methodology developed by Overcash and Jimenez-Gonzalez[37,38] which uses a modular data-based approach that extends throughout the supply chain.[39−41] Our primary focus was on designing a virtual manufacturing process based on patent literature, developing the cradle-to-gate (CtG) mass balance for production of 1000 kg of target product, and identifying all streams as either product, coproduct, recycle, waste, or emissions. This was followed by the application of green chemistry and engineering metrics and health

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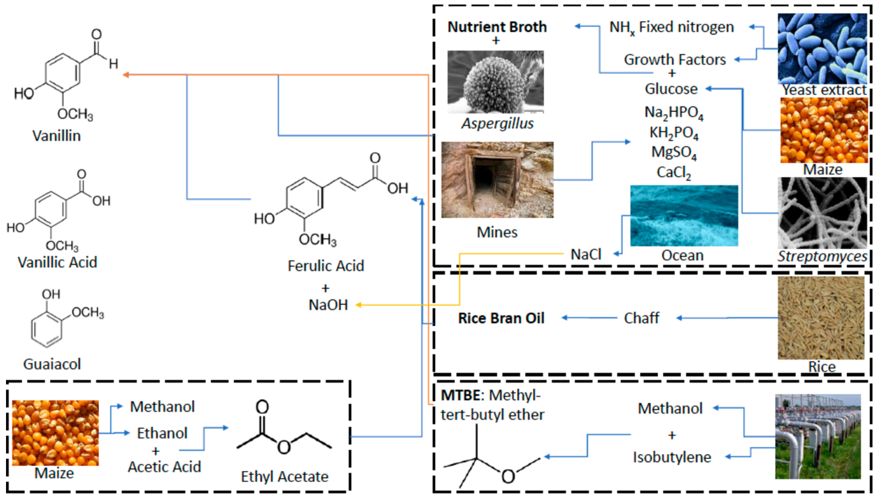

Figure 3. Representative block flow diagram for production of vanillin from rice bran.

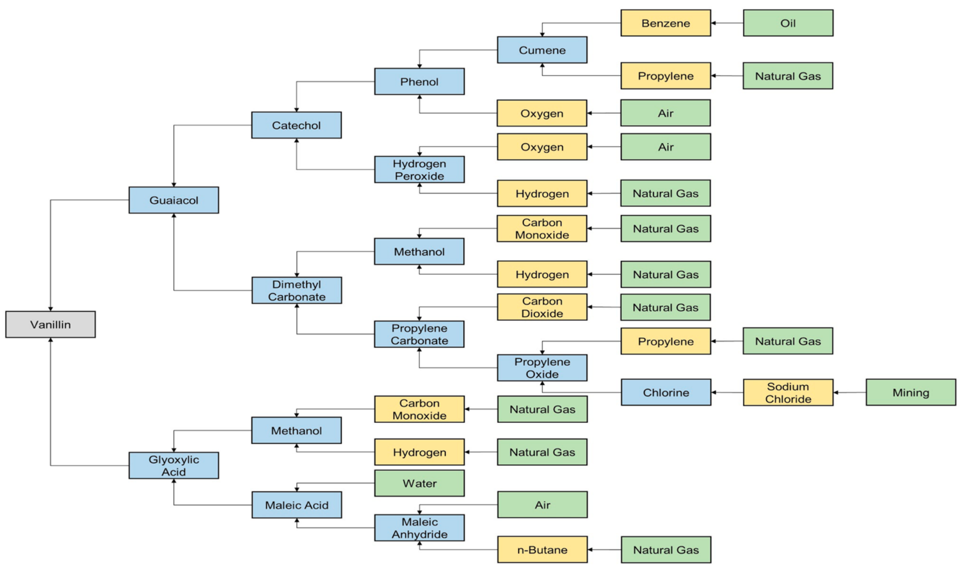

Figure 4. Representative block flow diagram for production of vanillin from crude oil.

and environmental impact assessments of materials involved in the process. Determination of the energy balance and carbon footprint of the manufacturing process was optional.

The first step in the development of a transparent LCI assessment of a product was to define the cradle-to-gate (CtG) synthesis/manufacturing route and to select a reliable and representative manufacturing process from literature sources, whereby patents were the preferred source of such information. Through this exercise, students learned to search the patent literature and to identify the best available manufacturing information that they believed came closest to actual manufacturing practices. Occasionally, patented information needed to be complemented with more recent published literature. The *Kirk-Othmer Encyclopedia of Chemical Technologies*[42] and *Ullmann's Encyclopedia of Industrial Chemistry*[43] were suggested as excellent resources for manufacturing routes of raw materials.

The second step required development of a block flow diagram (BFD) for manufacturing the target product from the pertinent natural resource (cradle) to the final product (gate). This CtG diagram includes _all_ raw materials, auxiliaries, solvents, and catalysts used in the production process. Two examples of block flow diagrams for production of vanillin from rice bran and crude oil are shown in Figures 3 and 4. The design of the BFDs provides a solid base for the development of associated process flow diagrams (PFD), mass balances, and ultimately the manufacturing process for each production module.

The third step involved development of an accurate mass balance for each module of the BFD with the objective of producing 1000 kg of the target product. This is the most important part of an LCI assessment and was the most challenging step in the project. The students were required to account for each gram of materials input and identify the output as valuable products, byproducts, recycle streams, wastes, or emissions. This third step was most revealing, especially for chemistry students who are trained to assess efficiencies of chemical reactions only by yield, disregarding solvents, water, coproducts, wastes, and emissions. With the information gathered in the first three steps, the teams had all the necessary data to design a process flow diagram (PFD) for the CtG virtual manufacturing process.

At this stage, the information needed to assess the sustainability of the overall manufacturing process from both qualitative

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and quantitative perspectives was available. By applying green chemistry and engineering principles and metrics to each block of the manufacturing process, students could identify "hotspots" associated with each GtG block and the overall (CtG) manufacturing process and pinpoint opportunities for rendering those processes more sustainable. Calculation of mass, waste, solvent and water intensities, emissions, and recycle streams identified the most significant components that affect the sustainability of an overall manufacturing process. At the same time, by assessing the health and safety hazards of raw materials, process conditions, and products of each manufacturing block, students learned to reconcile mass metrics with safety and health challenges. At this point, students also had all the necessary data to assess energy intensity, carbon footprint, and process economics.

RESULTS AND DISCUSSION

Creation of an action-based, collaborative environment for assessing the LCI of a product ubiquitous in everyday life was an effective strategy to encourage "systems thinking" and educate chemistry and chemical engineering students about the grand challenges of sustainability. The complementary knowledge and skills of engineers and chemists facilitated identification of those sustainability challenges leading to recommendations for appropriate solutions. By bringing speakers from a diverse group of companies that covered the whole supply chain from petroleum products (ExxonMobil) to chemicals (BASF, DowDuPont, Solvay) to pharmaceuticals (GSK) and finally consumer products (PepsiCo), students were introduced to a diverse set of sustainability programs. These lectures were extremely popular with students, and the interactions with speakers during and after class were insightful. The speakers were impressed with the level of interest and depth of students' understanding of sustainability and challenges thereof.

The concepts of team work and collaboration were fostered from the beginning of the semester; students were encouraged to form teams and work on assignments together with major emphasis placed on report quality. They independently formed functional teams that worked together throughout the semester. Through this exercise, students learned how to manage their project by breaking it down into specific tasks and assigning responsibilities and timelines. They were cognizant and respectful of each other's course/research schedules/deadlines.

For the in-depth life cycle inventory of each product, students had to dig deep into a type of literature that they were not accustomed to. We recommended the *Kirk-Othmer Encyclopedia of Chemical Technology*[42] and *Ullmans Encyclopedia of Chemical Technology*[43] as the best starting points, followed by the SciFinder and Reaxys databases. These proved to be a challenge especially for undergraduate students. Patent searches *via* the World Intellectual Property Organization (WIPO), the United Stated Patent and Trademark Office (USPTO), and Google Patents helped students identify the best available information related to manufacturing of the desired products and raw materials. To assist students in extracting appropriate information from patent literature, the topic was covered in two class sessions, and students were provided additional assistance in how to study patents in order to extract the best manufacturing information. In some cases, students needed to complement patent information with more recent reports from the scientific literature.

Construction of manufacturing modules and the block flow diagram from cradle (nature) to the final manufactured product (gate) helped students to identify all the necessary raw materials including solvents, auxiliaries, catalysts, water, and nitrogen for production of the final product—a practice that is not customary for chemists used to developing synthetic pathways. The inclusion of processes such as mining, farming, harvesting, etc. were not required. The block flow diagram for production of PET from oil is presented in Figure 5; BFDs for

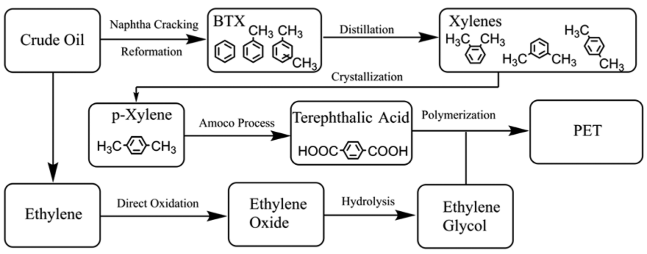

Figure 5. Representative block flow diagram for the production of polyethylene terephthalate (PET) from crude oil.

production of vanillin from rice bran and oil (Figures 3 and 4, respectively) were presented above.

The most challenging and tedious steps were construction of the mass balance tables for the GtG inventory of each raw material and CtG inventory of the final product; and identification of each component of the outputs of each GtG block as *product, coproduct, recycle,* or *waste.* By doing so, students were able to keep track of all materials throughout the CtG manufacturing process. Table 5 presents an example GtG mass balance for production of vanillin from guaiacol and glyoxylic acid. Next, students built process flow diagrams (PFD) for each manufacturing block using their process design knowledge, and finalized their CtG manufacturing process. Chemical process optimization programs such as AspenPlus were used to further refine the manufacturing processes, however using such programs for polymer manufacturing processes proved difficult.

With the final virtual manufacturing process in hand, teams performed qualitative and quantitative sustainability assessments of each module and the final CtG process. Application of mass metrics to each GtG block and the CtG production process identified process "hotspots" facilitating recommendations on how to make those processes environmentally "friendlier". By using the principles of green chemistry and engineering, students identified challenges and opportunities for rendering the process more sustainable.

Effective communication of their findings through a poster presentation and a final comprehensive written report was the last stop for their journey. Judges from industry complemented our judging of the posters: prizes were awarded for the top two posters. Interactions with industry speakers and judges were lively and their insights and feedback offered students a glimpse into real world challenges and opportunities.

The LCI project report for the production of PLA from corn provides a good example for our methodology and the students' approach in identifying so-called "hotspots" and the application of sustainability principles. In the absence of an integrated patented manufacturing process, the team used three different publications that reported the hydrolysis of maize starch to glucose,[44] production of crude calcium lactate from glucose,[45] and production of polymer grade lactic acid *via* methyl lactate.[46] For the polymerization of biolactic acid to PLA through ring opening polymerization, they used well-known

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Table 5. Material Balance for Production of Vanillin from Guaiacol and Glyoxylic Acid

Material input	Mass, kg	Material output	Mass, kg	Comment	Waste/recycle
		Condensation			
Guaiacol	1484	Guaiacol	413	To next step	
Glyoxylic acid monohydrate	876	Glyoxylic acid monohydrate	0	All consumed	
Water	495	Water	958	To next step	
Fe(acac)$_3$	106	Fe(acac)$_3$	106	To next step	
		4-Hydroxy-3-methoxymandelic acid	1401	To next step	
		2-Hydroxy-3-methoxymandelic acid	104	To next step	
		2-Hydroxy-3-methoxy-1,5-dimandelic acid	261	To next step	
Total	3252		3242		
		Organic extraction			
Guaiacol	413	Guaiacol	0		
Water	958	Water	958	Aqueous phase	
Fe(acac)$_3$	106	Fe(acac)$_3$	106	Aqueous phase	
4-Hydroxy-3-methoxymandelic acid	1401	4-Hydroxy-3-methoxymandelic acid	1401	Aqueous phase	
2-Hydroxy-3-methoxymandelic acid	104	2-Hydroxy-3-methoxymandelic acid	104	Aqueous phase	
2-Hydroxy-3-methoxy-1,5-dimandelic acid	261	2-Hydroxy-3-methoxy-1,5-dimandelic acid	261	Aqueous phase	
Toluene	958	Toluene + guaiacol	1371	Organic phase	Recycle
Total	4199		4199		
		Oxidation/Decarboxylation			
Water	958	Water	1131	Next step	
Fe(acac)$_3$	106	Fe(acac)$_3$	106	Next step	
4-Hydroxy-3-methoxymandelic acid	1401	4-Hydroxy-3-methoxymandelic acid	0	Converted to vanillin	
2-Hydroxy-3-methoxymandelic acid	104	2-Hydroxy-3-methoxymandelic acid	0	Converted to vanillin isomer	
2-Hydroxy-3-methoxy-1,5-dimandelic acid	261	2-Hydroxy-3-methoxy-1,5-dimandelic acid	0	Converted to 5-formyl vanillin	
Ammonium vanadate	21	Ammonium vanadate	21	Next step	
Air and nitrogen		Vanillin	1000	Next step	
		2-Hydroxy-3-methoxybenzaldehyde	80	Next step	
		5-Formylvanillin	173	Next step	
		Vanillylmandelic acid oxidation products	75	Next step	
		Carbon dioxide	419	Released	Waste
Total	2851		3005		
		Organic extraction			
Water	1131	Water	1258	Aqueous phase	Waste Treatment facility
Fe(acac)$_3$	106	Fe(acac)$_3$	1258	Aqueous phase	Waste Treatment facility
Ammonium vanadate	21	Ammonium vanadate	1258	Aqueous phase	Waste Treatment facility
Vanillin	1000	Vanillin	2448	Organic phase − To stripping and drying step	
2-Hydroxy-3-methoxybenzaldehyde	80	2-Hydroxy-3-methoxybenzaldehyde	2448	Organic phase − To stripping and drying step	
5-Formylvanillin	173	5-Formylvanillin	2448	Organic phase − To stripping and drying step	
Vanillylmandelic acid oxidation products	75	Vanillylmandelic acid oxidation products	2448	Organic phase − To stripping and drying step	
Toluene	1120	Toluene	2448	Organic phase − To stripping and drying step	
Total	3706		3706		
		Drying and stripping toluene			
Organic phase	2448	Toluene	1120	Recovered	Recycle
Organic phase	2448	Vanillin	1000	To crystallization step	
Organic phase	2448	2-Hydroxy-3-methoxybenzaldehyde	80	To crystallization step	
Organic phase	2448	5-Formylvanillin	173	To crystallization step	
Organic phase	2448	Vanillylmandelic acid oxidation products	75	To crystallization step	
Total	2448		2448		
		Crystallization and isolation			
Vanillin	1000	Vanillin	1000	Isolated product	
2-Hydroxy-3-methoxybenzaldehyde	80	2-Hydroxy-3-methoxybenzaldehyde	80	Valuable products − to be isolated	
5-Formylvanillin	173	5-Formylvanillin	173	Valuable products − to be isolated	
Vanillylmandelic acid oxidation products	75	Vanillylmandelic acid oxidation products	75	Valuable products − to be isolated	
Water	1000	Water and methanol mother liquor	2000	Methanol recovery	Waste water to treatment facility
Methanol	1000	Water and methanol mother liquor	2000	Methanol recovery	Waste water to treatment facility

information in the literature. With the virtual manufacturing process in hand, they developed the mass balance for producing 1000 kg of PLA and calculated mass and energy metrics in order to identify hotspots and to assess the sustainability of

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each individual step and the overall CtG manufacturing process. Mass, water, and solvent intensities, plus environmental impact and reaction mass efficiency, were the key mass metrics used by the team. Acidification of dilute aqueous calcium lactate solution and subsequent isolation of crude lactic acid created large quantities of aqueous effluent and calcium sulfate as coproduct, both of which contributed to the large water intensity and environmental impact. The team concluded that for every 10% drop in water consumption, water intensity would decrease by a factor of about 3.5. Purification of crude lactic acid, production of lactide, and its conversion to PLA required three reactors, large quantities of methanol, and multiple separation columns. These contributed to the high mass and energy intensity and large environmental impact of the production process and led to increased fixed and variable expenses. Sensitivity studies showed that by recycling 90% of the solvent, the environmental impact of the process would drop from 40 to 5! While polymerization of lactic acid is a highly exothermic process, the isolation and purification of PLA are energy intensive operations. Modeling work by the team indicated that by heat integration between the column and the reactor, they would be able to reduce the energy intensity of that step by 53%.

The team also discussed safety issues associated with the manufacturing processes. They addressed flammability and health hazards of methanol and concentrated sulfuric acid and the need for proper use of personal protective equipment. They recommended process development and optimization efforts for development of a mass- and energy-integrated process that would lead to lower mass, water, and solvent intensity and reduced environmental impact. Citing a recent patent application, they recommended exploring the possibility of direct conversion of lactic acid to PLA using an organic acid catalyst.[47]

Process and personal safety, health, and environment (SHE) were also important components of the course. Recall that the course began with a historical perspective, which included a review of past major safety and environmental disasters that led to the creation of regulatory agencies such as the U.S. EPA and the U.S. Chemical Safety Board (CSB). In another lecture, two Georgia Tech safety officers discussed chemical and biological laboratory safety; toxins, toxicity, dose response, and exposure and risk assessment were also included. They also discussed and compared basic risk assessment processes in academia vs industry. Speakers from industry reiterated the significance of personal and process safety, and a few of them began their lecture with a safety "tailgate", a popular practice in industry. It was important to hear an industrial perspective on scale up of chemical reactions and reactive hazard evaluation processes. One speaker discussed an explosion that had occurred at their manufacturing facility that led to significant property damage and personnel injury and provided an analysis of the root cause of the incident. Students learned about the danger of "runaway" reactions which could lead to an explosion, a fireball, toxic release, or vapor cloud explosion. The need for a "reactive hazard screening program" before scale up of a chemical process was emphasized, and a number of "desktop screening methods" were recommended, including the following:

- Review the process and identify all chemical mixtures
- Review molecular structures and identify reactive and hazardous *functional groups*
- Consult Bretherick's Handbook and review literature[48]
- Identify incompatible mixtures *via* NOAA (National Oceanic and Atmospheric Administration) Chemical Reactivity Worksheet[49]
- Utilize CHETAH (ASTM Computer Program for Chemical Thermodynamic and Energy Release Evaluation) program to identify potential explosion hazards[50]
- Consult Material Safety Data Sheet (MSDS)

Using a Semenov Diagram, aspects such as the stable operating point (SOP), self accelerating decomposition temperature (SADT), temperature of no return (TNR), and unstable operating point were discussed. Students were reminded that often secondary reactions in a process are ignored, but they could lead to decomposition at elevated temperatures. It was noted that a wide range of calorimetric methods from small scale to larger scale are available and should be used to further assess the safety of any process before commercialization.

LESSONS LEARNED

Feedback from the class was sought and welcomed (Table 6). It was emphasized that student input is highly valued and needed for improving the course and creating added benefit. The best aspects of the course were the concept, content, learning from and interacting with industry experts, applied principles of sustainability by industry, and metrics and analytics. The interdisciplinary nature of the course was also appreciated as it demonstrated the benefits of teamwork across the aisle. Our unorthodox approach to teaching the class, high workload and expectations, and the scope of the LCI projects elicited some complaints. The workload proved especially high for the senior undergraduate engineering students who carried a heavy load, which included the required core chemical engineering process design course. Also, literature searching beyond Google and Wikipedia took undergraduate students out of their comfort zone. In general, finding the most recent manufacturing processes for commodity products from the patent literature was difficult. As a result, students were not able to find the best and

Table 6. Summary of Student Feedback

Course best aspects	Course improvement comments
Message and focus of the course: Sustainability of industry	Decrease time spent; this is an elective course
Learning sustainability metrics and analytics	Extremely high workload! Reduce LCI project scope
Great topic and concepts	More in-class preparation for LCI projects
Open discussion vibe of the class	High expectations from professors
Provided great insight into sustainability practices	Course has the potential to be very interesting and insightful
Best course I ever took	Dr. Sabahi wanted this course to be our everything!
Learning about applied principles of sustainability from industry	Promote the course at chemistry department
Excellent content and thoughtful arrangement of seminars	Learning about more individual learning opportunities would have added to the class
Thank you for the informative and beneficial course	I hope this course will become a core course down the road

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Table 7. Summary of Student Evaluations

Category	ChBE 4803	ChBE 8803	CHEM 8833
How prepared were you to take this course	4	3.8	4.5
Amount learned	4.1	4.8	4.5
Assignments facilitated learning	3.3	4.8	4.5
Assignments measured knowledge	4	4.8	4
Course effectiveness	3.5	4	4.5

most recent technologies for production of some key raw materials such as glyoxylic acid, and they relied on processes that may not be practiced. In most cases, the feedback from industrial judges during the poster presentations provided students with a better view of current industrial manufacturing practices. Also, energy intensity calculations and carbon footprint measurements demanded more time, and as a result, these were made optional. Some of the teams were able to make a rough estimate of the energy requirements for their products.

Students were also asked to evaluate the course on a scale from 1 to 5, and the results are summarized in Table 7. The highest ratings were given by the graduate students, while senior engineering students were most critical. The differences between the scores were striking. For instance, the category labeled "assignments facilitated learning" received the lowest score from seniors but highest from graduate engineering and chemistry students. This may reflect the workload and time pressure felt by seniors. Conceivably, graduate students are better prepared for a less-structured, project-oriented class that requires independent thinking, planning, and research.

The feedback from our volunteer industry speakers and judges was overwhelmingly positive. All expressed interest in continuing their participation in the future and offered recommendations to further improve the syllabus. They emphasized that sustainability education provides a definite advantage to graduates who are seeking employment in the industrial sector.

PATH FORWARD

Building on the extraordinary work done by our student teams and in collaboration with some of the course participants, publications detailing what we learned about vanillin production (three routes) and PET and its PlantBottle and PEF replacements are planned. The syllabus will be modified to better prepare students for their LCI projects, and an additional debate will be introduced to the schedule to encourage critical thinking. To build on the multidisciplinary nature of the course, participation by students in other engineering disciplines such as materials science and engineering and mechanical engineering will be encouraged. The scope of industries speaking on their sustainability programs will also be expanded. For instance, the biorefining industry is playing a much larger role as a supplier of raw materials and products.

The interest and enthusiasm of our students to learn and understand the challenges associated with sustainability and how they affect the future of humanity from the perspectives of economics, health and the environment, and society has encouraged us to strive to improve the course content. Students expressed interest in understanding the social impact of industry and of the broader concept of social justice issues both locally and internationally, which requires explicitly adding the subject to the syllabus. By expanding the interdisciplinary nature of the course and through improving the syllabus, we will be well positioned to prepare a generation of scientists and engineers who will be well equipped to address global sustainability challenges.

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Notes

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