Sustainability Metrics: Life Cycle Assessment and Green Design in Polymers

MICHAELANGELO D. TABONE,[†,‡] JAMES J. CREGG,[†,§] ERIC J. BECKMAN,[†,∥] AND AMY E. LANDIS*[,†]

Mascaro Center for Sustainable Innovation, Department of Chemical Engineering, Department of Chemistry, Department of Civil and Environmental Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania 15261

Received May 13, 2010. Revised manuscript received August 27, 2010. Accepted September 2, 2010.

This study evaluates the efficacy of green design principles such as the "12 Principles of Green Chemistry," and the "12 Principles of Green Engineering" with respect to environmental impacts found using life cycle assessment (LCA) methodology. A case study of 12 polymers is presented, seven derived from petroleum, four derived from biological sources, and one derived from both. The environmental impacts of each polymer's production are assessed using LCA methodology standardized by the International Organization for Standardization (ISO). Each polymer is also assessed for its adherence to green design principles using metrics generated specifically for this paper. Metrics include atom economy, mass from renewable sources, biodegradability, percent recycled, distance of furthest feedstock, price, life cycle health hazards and life cycle energy use. A decision matrix is used to generate single value metrics for each polymer evaluating either adherence to green design principles or life-cycle environmental impacts. Results from this study show a qualified positive correlation between adherence to green design principles and a reduction of the environmental impacts of production. The qualification results from a disparity between biopolymers and petroleum polymers. While biopolymers rank highly in terms of green design, they exhibit relatively large environmental impacts from production. Biopolymers rank 1, 2, 3, and 4 based on green design metrics; however they rank in the middle of the LCA rankings. Polyolefins rank 1, 2, and 3 in the LCA rankings, whereas complex polymers, such as PET, PVC, and PC place at the bottom of both ranking systems.

Introduction

Sustainable, or green, products are increasing in popularity, as evidenced by the growth in green labeling initiatives, eco-marketing, and biobased materials. Unfortunately there is no universally recognized standard system for evaluating the sustainability of a product or process. Instead, sustainable design is guided by principles such as the "12 Principles of Green Chemistry," the "12 Additional Principles of Green Chemistry," and the "12 Principles of Green Engineering" (*1–3*), as well as by similar conceptions of sustainable design, such as "Cradle to Cradle," "Design for the Environment," "Industrial Ecology," and "Pollution Prevention" (*4–6*). These principles increased in status over the past two decades with the creation of the United States Environmental Protection Agency (EPA) "Green Chemistry Program" in 1993, the adoption of similar government programs in Italy and the United Kingdom, and the inaugural publication of the journal *Green Chemistry* by the Royal Society of Chemistry in 1999 (*7*). The application and efficacy of green chemistry and other green design principles are documented for many case studies, including biodegradable polymers, and the production of polymers from biomaterials (*1, 7–10*).

Life cycle assessment (LCA) is a tool that quantifies the environmental impacts resulting from the production, use, and disposal of a product or process. LCA has many benefits for making informed environmental decisions: (1) products are compared in defined environmental impact categories, which can be conceptualized by real environmental detriment, (2) unintended environmental trade-offs can be identified between impact categories and (3), a standardized methodology allows life cycle assessments from separate studies to be used to compare product choices (*11*). Previous publications have outlined the effect of green chemistry on various aspects of a product's life-cycle (*9*). Lankey et al. points out the benefit of using LCA within green chemistry to assess the trade-offs in switching between supply chemicals or processes (*10*). However, no published study quantitatively assesses the effect of adherence to green design principles on the life-cycle environmental impacts of similar products.

This study empirically compares adherence to green design principles in currently available plastics to the life-cycle environmental impacts of each plastic's production. Twelve polymers are assessed in this study. Seven polymers are generated from petroleum or other fossil fuel feedstocks: polyethylene terephthalate (PET), high and low density polyethylene (HDPE, LDPE), polypropylene (PP), polycarbonate (PC), polyvinyl chloride (PVC), and general purpose polystyrene (GPPS). Two biopolymers are assessed via different production processes: polylactic acid made via a general process (PLA-G) and a process reported by NatureWorks LLC (PLA-NW) as defined in the ecoinvent database, and polyhydroxyalkanoate was assessed separately as derived from corn grain (PHA-G) and from corn stover (PHA-S). Lastly, one hybrid bio/petroleum polymer is assessed, biopolyethylene terephthalate (B-PET) which is made from one fossil fuel feedstock and one biological feedstock.

Methods. Life cycle assessments were completed for each polymer using the ecoinvent v1.2 database, the EPA Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI 2 v.3.01) (*12*), and data from peer reviewed literature. Green Design Principles found in literature were reduced into quantifiable green design metrics. Each polymer's adherence to green design principles was assessed via these metrics. A decision matrix was used to normalize the results of both assessments and rank each polymer for preference in either assessment. Single-value metrics generated by the decision matrix were also used to compare the adherence to green design principles and the life-cycle environmental impacts in a two-dimensional chart.

Life Cycle Assessment. Life cycle assessments were completed in accordance with the ISO 14040−14043 series (*11*). The functional unit of comparison was one liter of polymer contained in pellets (prior to product molding). Previous material assessments compared impacts based on mass (*13–15*),

* Corresponding author phone (412) 624-3989; e-mail: ael30@pitt.edu.
[†] Mascaro Center for Sustainable Innovation.
[‡] Department of Chemical Engineering.
[§] Department of Chemistry.
[∥] Department of Civil and Environmental Engineering.

 © XXXX American Chemical Society

however varying physical properties for each plastic (e.g., density and modulus) cause vastly different masses to be required for the same plastic product, for example see Pietrini et al. 2007 (*16*). Volume was chosen as a functional unit for this study due to the approximately standard size of many plastic products (e.g., gift cards, bottles, and cups). The scope of each life cycle assessment was "cradle-to-gate," including only the impacts resulting from the production of each plastic and not the use or disposal. The use phase is excluded because each polymer can be used in multiple products that are consumed at different rates. The disposal phase is excluded because the environmental impacts of biopolymer disposal have yet to be studied and adequate data on the emissions and energy use of degradation are unavailable. A qualitative discussion on the effects of product disposal methods is included in the discussion.

Life cycle inventories in the ecoinvent v1.2 were used for all petroleum based polymers (PET, HDPE, LDPE, PP, PC, PVC, GPPS) and both polylactic acid scenarios (PLA-G and PLA-NW). The B-PET life-cycle inventory was completed specifically for this study, and is discussed in further detail in the following paragraph. No inventory was available for PHA; instead data from the impact assessment stage was obtained using a literature review of published life cycle assessments (*16–22*).

A life cycle inventory for B-PET was created for this study. The chemical composition of B-PET is identical to traditional PET and the production methods for both polymers are similar. In the B-PET production method, one monomer, ethylene glycol, is generated from sugar cane ethanol instead of natural gas. Ecoinvent inventory data on ethanol fuel and PET as well as literature sources were used to complete this inventory. Figure S.1 and Table S.1 in the Supporting Information (SI) display a full process schematic for production and data sources for the LCA. Additional detail describing the LCA is also found in the SI.

The life cycle impact assessment was completed using the Tool for the Reduction and Assessment of Chemical and environmental Impacts (TRACI) (*12*). Ten different impact categories were assessed: acidification, carcinogenic human health hazards, ecotoxicity, eutrophication, global warming potential, noncarcinogenic human health hazards, ozone depletion, respiratory effects, smog, and nonrenewable energy use (NREU).

No life cycle inventory data were available for PHA within the ecoinvent v1.2 database. Impact assessment data were obtained from previously published life cycle assessments, shown in the SI, Tables S.7 and Table S.8 (*16–22*). All studies contain assessments of NREU and greenhouse gas emissions; one study also includes eutrophication potential, smog formation, and acidification potential. To maintain complete assessments for use in the decision matrix, the average impact from the PLA scenarios is used as substitutes for PHA's impacts on human health, respiratory effects, ozone depletion, and ecotoxicity.

Green Design Metrics. Figure 1 summarizes previously published green design principles used in this study. Principles were reduced into "themes" which are quantitatively or qualitatively evaluated by metrics. Table 1 lists each theme, each associated metric, and specific principles associated with each theme/metric. The metrics from Table 1 were evaluated for each polymer in order to measure adherence to each design principles.

Waste Prevention. Waste reduction is measured through atom economy, defined in eq 1 where M_{input} is the mass of chemicals input to all reactions and $M_{product}$ is the mass of the final chemical product. Atom economy is evaluated for the entire synthesis of each polymer using the method defined within Blowers et al. (*24*). The scope of each atom economy calculation begins with chemicals refined from petroleum or fructose in the case of plant sugars and ends with the final chemical structure of the polymer.

$$\text{atom economy} = \frac{M_{product}}{M_{input}} \quad (1)$$

Green Design Principles

12 Principles of Green Chemistry

GC 1. Prevention (Overall)
GC 2. Atom Economy
GC 3. Less Hazardous Chemical Synthesis
GC 4. Designing Safer Chemicals
GC 5. Safer Solvents and Auxiliaries
GC 6. Design for Energy Efficiency
GC 7. Use of Renewable Feedstocks
GC 8. Reduce Derivatives
GC 9. Catalysis
GC 10. Design for Degradation
GC 11. Real Time Analysis of Pollution Prevention
GC 12. Inherently Safer Chemistry for Accident Prevention

12 Additional Principles of Green Chemistry

A 1. Identify byproducts; quantify if possible
A 2. Report conversions, selectivities, and productivities
A 3. Establish a full mass balance for the process
A 4. Quantify catalyst and solvent losses
A 5. Investigate basic thermochemistry to identify
A 6. Anticipate other potential mass and energy transfer
A 7. Consult a chemical or process engineer
A 8. Consider the effect of the overall process on
A 9. Help develop and apply sustainable measures
A 10. Minimize use of utilities and other inputs
A 11. Identify safety and waste minimization are incompatible
A 12. Monitor, report and minimize wastes

12 Principles of Green Engineering

GE 1. Inherent rather than circumstantial
GE 2. Prevention instead of treatment
GE 3. Design for separation
GE 4. Maximize mass, energy, space, and time
GE 5. Output-pulled versus input-pushed
GE 6. Conserve complexity
GE 7. Durability rather than immortality
GE 8. Meet need, minimize excess
GE 9. Minimize material diversity
GE 10. Integrate local material and energy flows
GE 11. Design for commercial "afterlife"
GE 12. Renewable rather than depleting

FIGURE 1. Previously published green design principles.

TABLE 1. Metrics for Green Design Principles

theme	metric	principles referenced
avoid waste	atom economy	GC 2, A1, A3
material efficiency	density	GE 8, GE 4
avoid hazardous materials/pollution	TRACI health and ecotoxicity impacts	GC 3−5, 11; GE 2
maximize energy efficiency	Total Energy Demand	GC 6, A 10, GE 3, 4, 10
use of renewable sources	percent from renewable sources	GC 7, GE 12
use local sources	feedstock distance	GE 10
design products for recycle	percent recycled	GE 3, 6, 9, and 11
design to degrade	biodegradability	GC 10
cost efficiency	price	GE 9

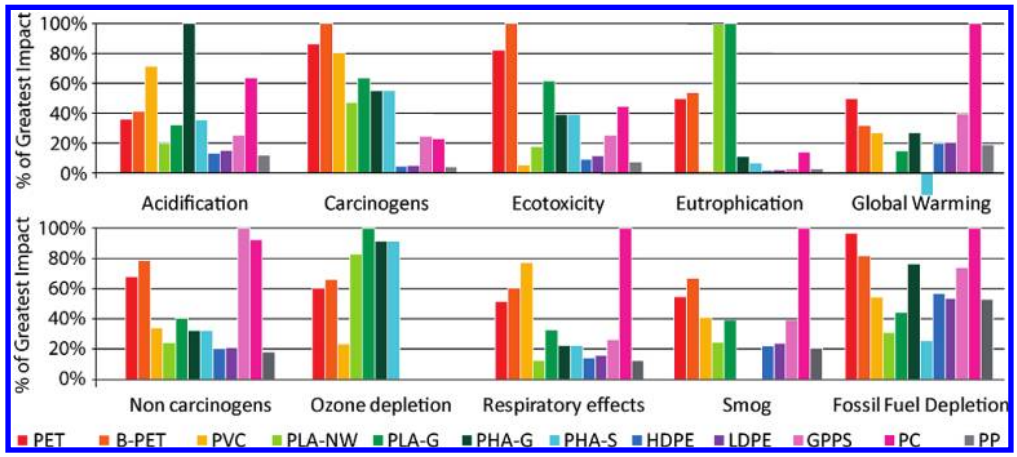

FIGURE 2. Life cycle assessment results for each of the polymers in TRACI impact categories. The top chart displays each polymer's relative impact in acidification, carcinogenic health hazards, exotoxicity, eutrophication, and global warming potential. The bottom chart displays each polymer's relative impact in the noncarcinogenic health hazards, ozone depletion, respiratory effects, photochemical smog, and fossil fuel depletion categories. All impacts are normalized from their original units to their relative impact as compared to the greatest impact exhibited in this study.

Material Efficiency. The ability of a material to promote efficient use is measured through its density, which is reflected in the volumetric functional unit used for all assessments. Less dense materials are able to serve many purposes with less mass, thus a lower density plastic is more preferable.

Avoid Hazardous Materials and Pollution. The avoidance of hazardous materials and pollution is measured via an average of the normalized life-cycle impacts in TRACI categories of respiratory effects, human health cancer, human health noncancer, and ecotoxicity (*12*).

Maximize Energy Efficiency. Overall energy efficiency was measured by the cumulative life-cycle energy use found by the cumulative energy demand life cycle impact assessment (LCIA) method. This energy demand includes all energy use in the production of the product, as well as any embedded energy in input materials such as oil, natural gas, or biomass, calculated using the higher heating value (HHV) as explained by Huijbregts et al. (*25*).

Use of Renewable Sources. The use of renewable sources is measured by the percent of material from biological sources in the final product, by mass.

Design Products for Recycle. Adherence to these principles is measured through the percent recovery of a material in the U.S. municipal recycle stream (*26*).

Design Biodegradable Products. The biodegradability of a product is measured through categorical classifications: nonbiodegradable, biodegradable in an industrial facility, or biodegradable in typical backyard conditions. For quantitative purposes, these categories are assigned values of 1, 2, and 3, respectively.

Use Local Sources. The categorical distance of the furthest feedstock location is assessed as a metric. Petroleum sources are categorized as international, often traveling to the U.S. through Canada or from the Middle East. Renewable sources may be local or not. Bioethylene for use in B-PET is only produced in India, and is assumed to be an international source for the U.S. PLA and PHA are often produced from regional corn crops. For quantitative purposes, categorical distances of international, national, and regional (roughly 600 mile radius) are assigned values of 1, 2, and 3, respectively.

Cost Efficiency. Sustainable products that are competitively priced will more effectively integrate into markets. The cost effectiveness of each polymer was measured via a median price per liter of the polymer, as reported by ICIS (*27*).

Decision Matrix. A decision matrix was used to create two single-value-metrics for each polymer, one evaluating each polymer for life-cycle environmental impacts and the other evaluating each polymer for adherence to green design principles. Results from both assessments were normalized to the average across all polymers, shown in eq 2, where N_{ij} is the normalized value for polymer i in metric/impact j, V_{ij} is the value for polymer i in metric/impact j, n is the total number of polymers studied, and Ψ_j is a multiplication factor which is 1 for metrics/impacts in which higher values are more preferable and −1 for metrics/impacts in which lower values are more preferable. The resulting normalized values in each category all average to either 1 or −1 depending on the value of Ψ_j. An alternate normalization method employs the maximum value in place of the average value and was also completed for comparison.

$$N_{ij} = \frac{V_{ij}{}^{*n}}{\sum_i (V_{ij})} * \Psi_j \qquad (2)$$

Single-value metrics were created in order to rank polymers with respect to adherence to green design principles or life-cycle environmental impacts. The single value metrics are the sum of the normalized impacts for each polymer in either the life cycle assessment or the green design assessment. Each impact category or green design metric is equally weighted in the single value metric system. While equal weighting is arguably nonideal, it reduces bias toward specific metrics and maintains clear transparency.

Life Cycle Assessment Results. The cradle-to-gate environmental impacts resulting from the production of each packaging polymer are shown in Figure 2. The resulting life cycle impacts are normalized to the largest impact found in this study. Figure 2 shows biopolymer production resulting in the highest impact in 5 of the 10 categories: ozone depletion, acidification, eutrophication, carcinogens, and ecotoxicity. PLA-G results in the greatest eutrophication potential, most likely as a result of fertilizer use (*28*). B-PET results in the greatest impact in ecotoxicity and human health cancer categories, this impact is largely attributed to sugar cane farming and ethanol production which accounts for anywhere from 13 to 21% of impacts in each category (see SI Figure S.2). It should be noted that the high eutrophication impact of B-PET is not solely attributable to agriculture/ethanol production; traditional PET production produces the second highest impact in this category. PHA-G results in the greatest acidification impact.

The production of polyolefin polymers, (HDPE, LDPE, and PP) does not result in the maximum impact in any category. This result is likely due to the limited chemical

TABLE 2. Evaluation of Polymers Using Green Design Metrics. Darker Green Cells Symbolize More Preferable Values

Material	Overall Atom Economy (%)	Carcinogens (kg benz. eq /L)	Non-Carcinogens (kg tolu. eq/ L)	Respiratory Effects (kg PM2.5 eq/ L)	Ecotoxicity (kg benz. eq/ L)	Cumulative Energy Demand (MJ eq/ L)	% Renewable Material	Distance of Feedstocks	% Recovery	Biodegradeable	Price (USD/ L)
PET	80%	$1.1x10^{-2}$	62.9	$4.9x10^{-3}$	5.72	123.8	0%	Intern.	18%	N/A	4.13
B-PET	62%	$1.3x10^{-2}$	72.7	$5.7x10^{-3}$	6.98	146.2	15%	Intern.	18%	N/A	4.13
PVC	55%	$1.1x10^{-2}$	31.7	$7.3x10^{-3}$	0.40	82.9	0%	Intern.	0%	N/A	4.02
PLA-NW	80%	$6.1x10^{-2}$	22.5	$1.2x10^{-3}$	1.21	79.4	100%	Region.	0%	Indus.	4.66
PLA-G	80%	$8.4x10^{-3}$	37.5	$3.1x10^{-3}$	4.31	98.3	100%	Region.	0%	Indus.	4.66
PHA-G	48%	$7.2x10^{-3}$	30.0	$3.1x10^{-3}$	2.76	91.5	100%	Region.	0%	Backyard	6.20
PHA-S	48%	$1.1x10^{-2}$	30.0	$2.1x10^{-3}$	2.76	91.5	100%	Region.	0%	Backyard	6.20
HDPE	100%	$6.5x10^{-4}$	18.7	$1.3x10^{-3}$	0.65	73.4	0%	Intern.	10%	N/A	1.52
LDPE	100%	$6.9x10^{-4}$	19.6	$1.5x10^{-3}$	0.82	72.3	0%	Intern.	5%	N/A	1.58
GPPS	98%	$3.2x10^{-3}$	92.7	$2.5x10^{-3}$	1.79	92.2	0%	Intern.	1%	N/A	2.35
PC	59%	$3.0x10^{-3}$	85.6	$9.5x10^{-3}$	3.13	128.9	0%	Intern.	0%	N/A	5.25
PP	100%	$5.8x10^{-4}$	16.8	$1.2x10^{-3}$	0.54	67.6	0%	Intern.	0%	N/A	1.78

processing required for polyolefin polymers. Monomers for polyolefin polymers are the direct products of oil refining. The more complex petro-polymers (PET, PC, and PS) require additional synthetic steps between the oil refinery and polymerization. Additional processing requires additional transportation and chemical process emissions, thus increasing the likelihood of emissions and environmental impact.

Green Principles Assessment Results. Table 2 shows the results of the green principles assessment for each of the 12 polymers studied. The biopolymers adhere well to several green design principles: the use of renewable and regional resources, low emissions of carcinogens, and low emissions of particulates. Polyolefin polymers exhibit the highest atom economy, the lowest price, and low pollutant emissions.

Comparison. Rankings generated by the decision matrices are shown in Table 3. The two ranking systems represent design choices based on either the green design principles or the life cycle assessment results. Biodegradable polymers sit on top of the green design rankings, owing mostly to their low energy demand, use of renewable materials, and biodegradability.

Comparing the green design rankings to the life cycle assessment rankings, the biopolymers, which ranked 1, 2, 3, and 4, in the green design system, are 6, 4, 8, and 9 respectively in the LCA rankings (as shown in Table 3). Polyolefins (PP, LDPE, HDPE) rank 1, 2, and 3 in the LCA rankings. Complex polymers, such as PET, PVC, and PC place at the bottom of both ranking systems. Specifically, B-PET ranked eighth in the green design ranking and last in the LCA ranking. The production of B-PET requires agriculture, fermentation, and multiple chemical processing steps, resulting in a low atom economy and a large potential for emissions and environmental impact.

To further study the relationship between green design metrics and environmental impacts, the single-value metrics used to rank each polymer are presented in Figure 3, where the *x*-axis represents adherence to green design principles and the *y*-axis represents life-cycle environmental impacts. The close relationship between many of the polymers in the green design principles dimension shows the relatively small differentiation between rankings 1−5, as well as rankings 6−8. In contrast, single-values in the life-cycle environmental impacts dimension are relatively continuous, exhibiting tight differentiation only between the polyolefin polymers, ranking 1−3.

TABLE 3. Rankings for Each of the Polymers Based the Normalized Green Design Assessment Results and the Normalized Life Cycle Assessment Results

Material	Green Design Rank	LCA Rank
PLA (NatureWorks)	1	6
PHA (Utilizing Stover)	2	4
PHA (General)	2	8
PLA (General)	4	9
High Density Polyethylene	5	2
Polyethylene Terephthalate	6	10
Low Density Polyethylene	7	3
Bio-polyethylene Terephthalate	8	12
Polypropylene	9	1
General Purpose Polystyrene	10	5
Polyvinyl chloride	11	7
Polycarbonate	12	11

The relationship between green design principles and life-cycle environmental impacts shows a distinct difference between biopolymers and petroleum polymers. With the exception of PET, petroleum polymers exhibit lower life-cycle environmental impacts when they adhere more strictly to green design principles. Biopolymers exhibit a range of life-cycle environmental impacts, however their rank based on green design principles does not vary widely, with the exception of B-PET. Adhering to green design principles reduces environmental impact in either the petroleum or biological polymer categories. Switching from petroleum feedstocks to biofeedstocks does not necessarily reduce environmental impacts.

The use of maximum values instead of average values for normalization does not alter the LCA rankings; however this

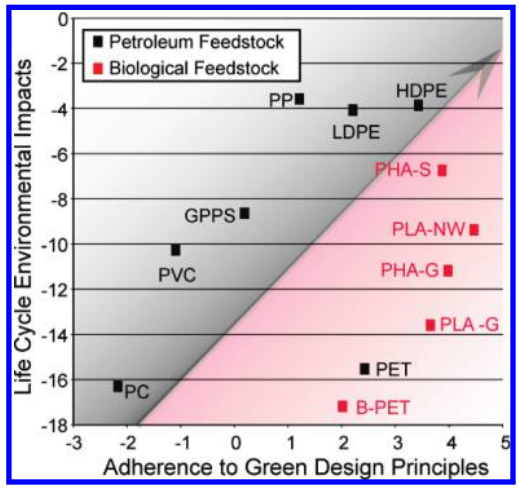

FIGURE 3. Polymer assessments displayed in two dimensions, with "adherence to green design principles" on the *x*-axis and "life-cycle environmental impacts" in the *y*-axis. In this system, greater values are more preferable, meaning greater adherence to principles, or lower normalized environmental impacts.

does alter the green design rankings. Regardless of normalization, the overall disparity between biological and petroleum polymers remains. Results for the maximum normalization method are shown in SI Figure S.3.

Discussion

Results from this study show a qualified positive correlation between adherence to green design principles and a reduction of the environmental impacts of production. The qualification results from the difference between biopolymers and petroleum polymers. While biopolymers uniformly rank highly in terms of green design, they exhibit relatively high environmental impacts from production. As shown through the LCA results, biopolymers represent decreases in fossil fuel use and global warming potential and increases in other impact categories such as eutrophication, human health impacts, and eco-toxicity. These impacts result both from fertilizer use, pesticide use, and land use change required for agriculture production as well as from the fermentation and other chemical processing steps (*28*).

Atom economy is shown to be an indicative predictor of low life-cycle environmental impacts. Polyolefin polymers exhibit 100% atom economy and result in the lowest environmental impacts. However, low atom economy does not necessarily represent poor environmental performance. The impacts of different synthetic stages in chemical plants vary widely; for example the production of ethylene glycol from ethylene oxide results in a relatively large eutrophication impact, and the production of chlorine gas from salt requires significantly high energy use.

Principles regarding the use of renewable resources should be redefined to prevent trade-offs related to the use of harmful chemicals on crops and the energy/emissions in the production and use of fertilizers and pesticides. For example the use of renewable sources could be limited to those that require below-average pesticide and fertilizer use. Principles should be further qualified to address the trade-offs involved in chemical processing from bio feedstock or chemicals. This study's example, B-PET, first required the conversion of sugar starch into ethanol, a process already under scrutiny for its environmental benefit (*29*). Following this conversion, B-PET must go through the same production process as traditional PET, thus resulting in greater environmental impacts in all impact categories with the exception of nonrenewable energy use and greenhouse gas emissions.

The LCAs in this study have a limited scope; to be comprehensive, the use and end of life should be included in future studies. The exclusion of disposal scenarios affects conclusions regarding biodegradable polymers and commonly recycled plastics. In 2007, recycling facilities in the U.S. processed 18% of total PET production, 10% of all HDPE production, and 5% of all LDPE production (*26*). Recycling rates can be increased through many factors including the improvement of collection processes and the design of high value, recyclable materials. Had the effect of recycled plastics on the reduction of virgin plastic production been included in the life cycle assessment, impacts resulting from each of these plastics would be reduced. However, the environmental impacts of the recycling process would also have to be included, most likely resulting additional impacts depending on the specific process. The environmental impacts of other waste scenarios such as incineration and land filling are also excluded. The proliferation of waste incinerators with energy recovery may provide benefit by reducing landfill waste and producing energy, however they may also produce environmental detriment by emitting additional pollutants to air and water. Finally, the environmental and human health impact of chemical byproducts of PLA or PHA biodegradation have yet to be studied. The biodegradation of these polymers inherently produce the greenhouse gases carbon dioxide and methane. Future work in environmental assessments of plastic products should include the creation of life cycle inventories for disposal scenarios of plastic products.

The type, location, and extraction method of fossil fuel feedstocks affect the emissions profiles for petroleum based products. For example, the extraction of crude oil from Canadian oil sands results in more than 5 times the global warming potential of crude oil produced in Iraq or Saudi Arabia (*31*). The ecoinvent v1.2 database assumes a European average for emissions resulting from the extraction, processing, and transportation of crude oil and natural gas; a majority of which is assumed to originate in the Middle East or Russia. Life cycle impacts will likely increase if assumptions are changed to reflect oil and gas use in the United States; or if assumptions include increased production from alternative fossil fuel sources such as oil sands or shale gas.

Future work in the field of sustainable design metrics should include the discussion of available data during the design phase of chemical products. In this study, life cycle assessment results are used to measure adherence to principles governing the use and design of safe chemicals. Of course, life cycle assessment results (particularly for the end of life) are not available before the production of a product, much less so during the design of a chemical synthesis. In future quantitative assessments of green design methods, data such as the toxicity of reactants and the heat of reaction can be used to measure adherence principles such as reduce energy use and avoid hazardous chemicals. Future work can also address the development of functional life cycle assessment design tools. Such tools can be designed to apply existing life cycle assessment data to nascent chemical design; they can increase the awareness of green chemists and aid the development of more environmentally beneficial chemical products.

Acknowledgments

We thank the National Science Foundation who provided funding for this research through a Research Experiences for Undergraduates Grant, EEC Award No. 0647397. We also thank the Mascaro Center for Sustainable Innovation for their

valuable undergraduate program and Dr. John Brigham and Dr. Melissa Bilec at the University of Pittsburgh for their support.

Supporting Information Available

A process outline and inventory information for the life cycle assessment of biopolyethylene terephthalate, results for the B-PET LCA, data used from the literature review on PHA production, and results from the maximum normalization method. This material is available free of charge via the Internet at http://pubs.acs.org.

Literature Cited

(1) Anastas, P.; Warner, J., *Green Chemistry: Theory and Practice*; Oxford University Press:USA: 2000.
(2) Anastas, P. T.; Zimmerman, J. B. Design through the 12 principles of green engineering. *Environ. Sci. Technol.* **2003**, *37* (5), 94A–101A.
(3) Gonzalez, M. A.; Smith, R. L. A methodology to evaluate process sustainability. *Environ. Prog.* **2003**, *22* (4), 269–276.
(4) McDonough, W.; Braungart, M., *Cradle to Cradle: Remaking the Way We Make Things*; North Point Press: New York, 2002.
(5) Graedel, T.; Allenby, B., *Design for Environment*; Prentice Hall: Englewood Cliffs, NJ, 1996.
(6) Graedel, T.; Allenby, B., *Industrial Ecology*; Prentice Hall: Englewood Cliffs, NJ, 1995.
(7) Anastas, P. T.; Kirchhoff, M. M. Origins, current status, and future challenges of green chemistry. *Acc. Chem. Res.* **2002**, *35* (9), 686–694.
(8) Lankey, R.; Anastas, P., *Advancing Sustainability Through Green Chemistry and Engineering*; American Chemical Society: Washington, DC, 2002.
(9) Anastas, P.; Lankey, R. Life cycle assessment and green chemistry: The yin and yang of industrial ecology. *Green Chem.* **2000**, *2* (6), 289–295.
(10) Lankey, R. L.; Anastas, P. T. Life-cycle approaches for assessing green chemistry technologies. *Ind. Eng. Chem. Res.* **2002**, *41* (18), 4498–4502.
(11) Guinée, J. Handbook on life cycle assessment operational guide to the ISO standards. *Int. J. Life Cycle Assess.* **2002**, *7* (5), 311–313.
(12) Bare, J.; Norris, G.; Pennington, D.; McKone, T. The tool for the reduction and assessment of chemical and other environmental impacts. *J. Ind. Ecol.* **2002**, *6* (3−4), 49–78.
(13) Erwin, T. H.; Vink, K. R. R.; Glassner, David A.; Springs, Bob; O'Connor, Ryan P.; Kolstad, Jeff; Gruber, Patrick, R. The sustainability of NatureWorks™ polylactide polymers and Ingeo™ polylactide fibers: An update of the future. *Macromol. Biosci.* **2004**, *4* (6), 551–564.
(14) Vink, E.; Rabago, K.; Glassner, D.; Gruber, P. Applications of life cycle assessment to NatureWorks™ polylactide (PLA) production. *Polym. Degrad. Stab.* **2003**, *80* (3), 403–419.
(15) Shen, L.; Patel, M. Life cycle assessment of polysaccharide materials: A review. *J. Polym. Environ.* **2008**, *16* (2), 154–167.
(16) Pietrini, M.; Roes, L.; Patel, M.; Chiellini, E. Comparative life cycle studies on poly (3-hydroxybutyrate)-based composites as potential replacement for conventional petrochemical plastics. *Biomacromolecules* **2007**, *8* (7), 2210–2218.
(17) Heyde, M. Ecological considerations on the use and production of biosynthetic and synthetic biodegradable polymers. *Polym. Degrad. Stab.* **1998**, *59* (1−3), 3–6.
(18) Kim, S.; Dale, B. Life cycle assessment study of biopolymers (polyhydroxyalkanoates) derived from no-tilled corn. *Int. J. Life Cycle Assess.* **2005**, *10* (3), 200–209.
(19) Kim, S.; Dale, B. Energy and greenhouse gas profiles of polyhydroxybutyrates derived from corn grain: A life cycle perspective. *Environ. Sci. Technol.* **2008**, *42* (20), 7690–7695.
(20) Yu, J.; Chen, L. The greenhouse gas emissions and fossil energy requirement of bioplastics from cradle to gate of a biomass refinery. *Environ. Sci. Technol.* **2008**, *42* (18), 6961–6966.
(21) Akiyama, M.; Tsuge, T.; Doi, Y. Environmental life cycle comparison of polyhydroxyalkanoates produced from renewable carbon resources by bacterial fermentation. *Polym. Degrad. Stab.* **2003**, *80* (1), 183–194.
(22) Kurdikar, D.; Fournet, L.; Slater, S.; Paster, M.; Gruys, K.; Gerngross, T.; Coulon, R. Greenhouse gas profile of a plastic material derived from a genetically modified plant. *J. Ind. Ecol.* **2000**, *4* (3), 107–122.
(23) India Glycols Limited. http://www.indiaglycols.com/ (accessed June 8, 2009).
(24) Blowers, P.; Zhao, H.; Case, P.; Swan, J., Atom economy, expanding boundaries to incorporate upstream reactions. In *Proceedings of the 2004 AIChE Annual Meeting*; Austin, TX., November 7−12, 2004.
(25) Huijbregts, M. A. J.; Rombouts, L. J. A.; Hellweg, S.; Frischknecht, R.; Hendriks, A. J.; van de Meent, D.; Ragas, A. M. J.; Reijnders, L.; Struijs, J. Is Cumulative fossil energy demand a useful indicator for the environmental performance of products? *Environ. Sci. Technol.* **2005**, *40* (3), 641–648.
(26) Municipal Solid Waste in the United States; U.S. Environmental Protection Agency: Washington, DC, 2008.
(27) ICIS, "Indicative Chemical Prices." http://www.icis.com/StaticPages/A-E.htm (accessed January 14, 2010).
(28) Landis, A.; Miller, S.; Theis, T. Life cycle of the corn-soybean agroecosystem for biobased production. *Environ. Sci. Technol.* **2007**, *41* (4), 1457–1464.
(29) Searchinger, T.; Heimlich, R.; Houghton, R.; Dong, F.; Elobeid, A.; Fabiosa, J.; Tokgoz, S.; Hayes, D.; Yu, T. Use of US croplands for biofuels increases greenhouse gases through emissions from land-use change. *Science* **2008**, *319* (5867), 1238.
(30) Varisli, D.; Dogu, T.; Dogu, G. Ethylene and diethyl-ether production by dehydration reaction of ethanol over different heteropolyacid catalysts. *Chem. Eng. Sci.* **2007**, *62* (18−20), 5349–5352.
(31) *Development of Baseline Data and Analysis of Life Cycle Greenhouse Gas Emissions of Petroleum-Based Fuels*, DOE/NETL-2009/1346; United States Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2008; http://www.netl.doe.gov/energy-analyses/pubs/NETL%20LCA%20Petroleum-based%20Fuels%20Nov%202008.pdf.

ES101640N