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Integrating Simple Environmental Impact-Based Metrics into the Undergraduate Curriculum

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ABSTRACT: The most important learning objective in green chemistry education is the ability to identify the synthesis, process, or chemical that is least environmentally harmful. Existing metrics fall short for different reasons. Mass-based metrics fail to assess environmental harm, while life cycle assessment (LCA) is much too complex to insert into the existing curriculum without displacing a significant amount of content. However, individual environmental impact-based metrics derived from LCA can be easily incorporated into the curriculum with very little instruction time and no significant displacement of content. For first year or introductory chemistry, we show how typical first-year calculation questions can be expanded to allow students to use an impact-based metric to identify the least harmful of the presented options. For upper-year courses, we propose an activity that scaffolds the LCA process of compiling data, calculating individual impact-based metrics, combining metrics, and using context to make a decision. This activity was implemented using a problem-based learning model to support multivariate reasoning through peer discussions.

KEYWORDS: *first-year undergraduate/general, second-year undergraduate, upper-division undergraduate, curriculum, green chemistry*

■ INTRODUCTION

In 2020, Students Organizing for Sustainability International conducted a global survey into student experiences and perceptions of sustainability in postsecondary education.[1] From their results, 92% of respondents agreed that "sustainable development is something which all universities and colleges should actively incorporate and promote," and 85% agreed that "sustainable development is something I would like to learn more about." However, only 26% of respondents reported in-depth coverage of sustainable development in their courses, and 40% reported low or no coverage altogether. In postsecondary chemistry education, this leaves the next generation of chemists and chemical engineers unequipped to reshape chemistry practices in response to the climate crisis.

This issue is being addressed by promoting and integrating the principles of green chemistry into the curriculum. The ACS Green Chemistry Institute's Road Map envisions "Chemistry education that equips and inspires chemists to solve the grand challenges of sustainability."[2] While there has been progress globally,[3] there is still a need to grow the green chemistry education curriculum.[4] Efforts to teach green chemistry have taken different approaches, such as emphasizing simple mass-based metrics that consider the amount of waste generated (e.g., atom economy)[5] or reducing hazards and minimizing exposure in teaching laboratories. Another approach is to focus on molecular design principles, such as the molecular basis of toxicity[6] or sustainability.[7]

The ability to identify the least harmful of the available options is the most important learning objective in green chemistry education. This skill gives chemistry students a better understanding of the environmental impacts of their choices.[3,5] Yet green chemistry content, especially related to process metrics (e.g., yield, hazard, waste) is often viewed by educators as advanced or additional to the core chemistry curriculum.[8,9] Despite agreeing that environmental hazards, reaction efficiency, and impacts of chemicals are important topics, most educators feel they cannot include green chemistry without displacing other important course content.[2] This reveals some chemistry educators' perspective that the green chemistry content is incompatible with their course material.[9] Many also feel that they do not have the background or resources, including textbooks,[10] to add this content into their courses.[2,8]

Green chemistry is meant to be a responsible way of conducting science, rather than its own discipline.[11] The key to advancing green chemistry education is not to displace other

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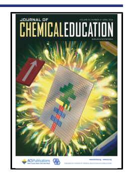

necessary content but to integrate green chemistry into this content and make chemistry inherently green.[3] But what do terms like "green" really mean?

Measures of "Green"

There is no "green" chemical or process; this term describes how environmentally friendly one thing is compared to another.[12] It is a relative indication of environmental impact. As such, one synthetic route might be greener than another, but none are inherently green. In the 1990s, various mass-based metrics were introduced to measure the "greenness" of a chemical process by the amount of waste produced, such as atom economy, E factor, and process mass intensity (PMI).[13] While a step in the right direction, these mass-based metrics are unclear indications of greenness. For example, the E factor, published by R.A. Sheldon in 1992, measures kilograms of waste per kilogram of product.[14] Using this metric, one can quickly determine E factors for several similar chemical processes and compare the values to deduce which process yields the least waste. The ease and speed with which mass-based metrics such as E and PMI can be calculated has value in settings where workload must be minimized, such as in a large company trying to reduce the harm of thousands of chemical processes. However, it is not always the case that the process yielding the least mass of waste is the greenest. Some waste is more harmful than others, but these metrics fail to consider the impact of the waste produced. Also, many aspects of environmental harm are not associated with waste, such as resource depletion, water consumption, and energy consumption. Thus, mass-based metrics are poor indicators of which process is the greenest[11] and inadequate for the task of teaching that most important learning objective.

Compared to mass-based metrics, life cycle assessment (LCA) is a better way of determining the relative "greenness" of two or more chemicals or processes because the method considers the harm of chemicals, not just their mass, and includes resource depletion and water and energy consumption.[14] To measure the harm of chemicals, LCA uses impact-based metrics that can illustrate a comprehensive picture of the chemical or process' effect on the environment.[15] Examples of impact-based metrics include global warming, smog formation, ozone depletion, human toxicity, eco-toxicity, acidification, and eutrophication.[13] These metrics describe the chemical's potential for environmental harm compared to a reference compound (e.g., the global warming potential of methane is 28, while carbon dioxide, the reference compound for this metric, is 1).[16] The environmental impact of the release of a specified amount of a chemical is governed by eq 1,

$$I = P \times m_{\text{emitted}} \quad (1)$$

in which I represents the impact index, P is the impact potential for a substance, and m is the mass of a substance emitted to the environment, including as fugitive emissions or as waste. P is the ratio of the harm caused by the emission of 1 kg of the substance to the harm caused by 1 kg of the reference substance (CO_2 for global warming, phosphate anion for eutrophication, etc.). Thus, the global warming potential (P_{GW}) for methane is 28 kg CO_2 equivalents per kg of methane (or 28 g CO_2 eq per g of methane), although potentials are often shown as being unitless for simplicity. To determine the total impact index for a reaction, one must sum the indices of all substances at any stage of the process.

The downside of LCA is that it is time-consuming and complex. It requires hours of searching for methodological details and impact potentials published in different industry tables and technical resources. LCA is also challenging to teach and learn, since it requires setting system boundaries[13,17] and multivariate decision-making[18] through combining several different impact-based metrics to where, in the end, the choice for which option is "greenest" still depends on the context. As a result, mass-based metrics are usually taught instead despite being much less effective indicators of greenness.

This Work

This article presents approaches to integrating green chemistry into the introductory and upper postsecondary chemistry curriculum using environmental impact-based metrics. First, we outline ways to teach simple impact-based metrics in general chemistry courses and provide a detailed resource for educators interested in using this approach. Second, we present an upper-year activity that scaffolds the life cycle assessment (LCA) process. This article provides a detailed description of the activity, results from its implementation, and teacher reflections.

■ GENERAL CHEMISTRY: INTRODUCING IMPACT-BASED METRICS

The time-consuming and difficult aspects of doing an LCA are associated with the early steps, such as scope determination and building an inventory of all input and output chemicals at each stage in the life cycle, and the late steps of making a decision from all the available information. Fortunately, the math involved in assessing the harm from each chemical, as represented by eq 1, is simple. The concept of impact and impact metrics can be easily incorporated into common first-year undergraduate chemistry problems which involve calculating mass, pressure, or equivalents (to name only some examples). The framing of the question becomes "which does less harm?", and mass values derived from the problem are simply multiplied by given potentials to determine the answer. This approach contextualizes the skills a modern chemist needs to make decisions,[19] empowering students to judge better which of two or more chemicals is the least harmful to the environment. The concept of choosing the least harmful option is therefore conveyed primarily through practice questions and requires only enough classroom time to teach eq 1.

Examples of Impact-Based Questions for General Chemistry

The questions herein aim to seamlessly integrate green chemistry into the curriculum without displacing other important content. They accomplish this by adding a green decision, using impact-based metrics, to the type of practice questions typically found in a first or second-year chemistry course, such as the ideal gas law or mole calculations. The standard calculation exercise is retained, but the student subsequently must perform basic impact calculations and then choose the greener of two or more alternatives. Box 1 provides an example question appropriate for early first-year undergraduates or high school.

Box 2 provides an example question for first-year undergraduate discussion of ideal gases. (For more examples, see the educator resource in the Supporting Information). This will help students begin considering different substances or processes based on their environmental impacts and then

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Box 1. Mole calculations sample problem

Question: Garbage decomposing in landfills releases methane gas, which is often "flared" (burned) rather than being vented into the atmosphere. Calculate the global warming caused by releasing 1 mol of methane by venting and by flaring. **Which is less harmful?**

The global warming potentials for CH_4 = 28 and CO_2 = 1, while those of O_2 and H_2O are negligible.

$$CH_4(g) + 2O_2(g) \rightarrow 2H_2O(g) + CO_2(g)$$

Answer:

(a) without flaring

$$m_{\text{methane}} = 1 \text{ mol} \times 16\frac{\text{g}}{\text{mol}} = 16 \text{ g}$$

$$I_{\text{GW}}(CH_4) = 16 \text{ g} \times 28 = 448 \text{ g of } CO_2 \text{ equivalents}$$

(b) with flaring

1 mol of CH_4 (g) gives 1 mol of CO_2(g)

$$m_{\text{carbon dioxide}} = 1 \text{ mol} \times 44\frac{\text{g}}{\text{mol}} = 44 \text{ g}$$

$$I_{\text{GW}}(CO_2) = 44 \text{ g} \times 1 = 44 \text{ g of } CO_2 \text{ equivalents}$$

Therefore, the global warming is lower if the methane is flared rather than vented.

Box 2. Ideal gas law sample problem

Question: Hydrochlorofluorocarbons are used as refrigerant gases, but sometimes they leak. Before it is turned on, an air conditioner with an internal volume of 70 L holds 8.0 atm of refrigerant gas at 20 °C. The refrigerant could be either CHF_2Cl or CH_3CFCl_2. Calculate the ozone depletion impact that would be caused by the accidental release of either refrigerant gas (their ozone depletion potentials are 0.055 and 0.11).

Which would be less harmful?

Answer: $PV = nRT$ or $PV = (m/M)RT$

(a) for CHF_2Cl

$$m_{CHF_2Cl} = \frac{MPV}{RT} = \frac{86.5 \text{ g/mol} \times 8.0 \text{ atm} \times 70 \text{ L}}{0.0821\frac{\text{L atm}}{\text{K mol}} \times 293 \text{ K}} = 2013 \text{ g}$$

$$I_{\text{OD}}(CHF_2Cl) = 2013 \text{ g} \times 0.055 = 110 \text{ g}$$

(b) for CH_3CFCl_2

$$m_{CHF_2Cl} = \frac{116.94 \text{ g/mol} \times 8.0 \text{ atm} \times 70 \text{ L}}{0.0821\frac{\text{L atm}}{\text{K mol}} \times 293 \text{ K}} = 2722 \text{ g}$$

$$I_{\text{OD}}(CH_3CFCl_2) = 2722 \text{ g} \times 0.11 = 300 \text{ g}$$

CHF_2Cl would be less harmful for ozone depletion.

challenge them to choose the greenest option from among them.

Questions such as those in boxes 1 and 2 can also be used by the instructor to encourage discussion and lateral thinking among students. After the question is answered, the students can be encouraged to think of alternative options not given in the question. What could be greener than venting and flaring of methane? What could be a greener way to cool a home without using refrigerant gases? Options that the students might come up with could include (a) capturing and using the methane, (b) using incineration or recycling of waste rather than landfilling, or (c) green roofs to cool buildings. Such discussion would help students to see that green chemistry is not limited to currently available options. Instructors could also discuss with students the limitations of this approach. For example, comparing two chemicals in terms of the harm they cause (as in Box 2) does not take into account the harm caused by their manufacture. The less harmful chemical might be made by a very harmful route, while the more harmful chemical might be made by a reasonably benign route. Other possible discussion questions are shown after each example question in the Supporting Information.

Resource for Impact-Based Metrics

The authors have created an educational resource to help educators integrate simple impact-based metrics into their classrooms (see Supporting Information). This resource is comprised of (1) example questions that add a green chemistry context for the first or second-year curriculum and (2) data tables and lists of external resources for 11 different impact potentials of common chemicals, along with the equations used to calculate the potentials and a calculator tool so that educators are not limited to the chemicals given. This resource outlines how to implement these questions into course lectures and tutorials and gives educators the resources to customize them as they see fit.

■ UPPER-YEAR ACTIVITY: AN LCA PRIMER

We propose a new class activity for upper-year chemistry courses to introduce impact-based metrics and LCA.[18] In designing the activity, we drew on the teaching models of scaffolding and problem-based learning.[20] In small groups, students worked through an exercise to determine which of three possible synthetic routes was the "greenest." The problem-based learning approach was drawn from research on implementing systems thinking into chemistry education since assessing the scope of LCA similarly requires setting boundary conditions and multivariate reasoning.[17,21,22] In our activity, two routes were selected to have relatively similar impact indices when compared using LCA, and the third was obviously the worst overall. This feature meant that students would need to engage in conversation and multivariate reasoning to reach an answer. LCA requires reasoning and decision-making without a definite "correct" answer regarding the greenest option. To assist students through the LCA process, our approach to designing the activity relied on scaffolding. Assessment scaffolding can help learners understand the process of problem-solving and can also help manage many variables.[20] Our activity supports students through the process of first building an inventory of data masses and calculating impact indices for a single metric (Figure 1, top), then combining these metrics to make a final decision (Figure 1, bottom). Throughout the process, students are encouraged to verbalize their reasoning through peer teaching and discussion.

Activity Details

In our implementation (see Supporting Information), we used a situation that gave students a choice between three different routes for the synthesis of 1 kg of 1-hexylfluoride (Table 1). Route 1 was the greenest (meaning lowest relative index value) on 3/5 metrics: Human Inhalation Toxicity, Global Warming

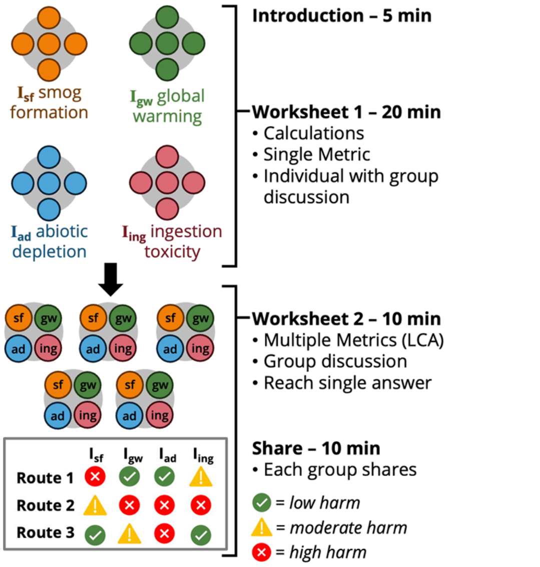

Figure 1. Proposed timeline for this type of activity in a 50 min class period with 5 min of buffer time. Students first separate into 3–6 groups (4 groups shown here) to discuss and calculate single metrics for each route. Then, students form new groups to discuss multiple metrics and build a table to compare routes for their relative harm on all metrics.

Table 1. Impact Indices for Three Routes to Synthesize 1-Hexylfluoride in the Activity[a]

route	I_{sf} (smog formation)	I_{gw} (global warming)	I_{ad} (abiotic depletion)	I_{inh} (inhalation toxicity)[b]	I_{ing} (ingestion toxicity)[b]
1	16	9.4	1.0×10^{-4}	9.4	2.2×10^{5}
2	48	116	3.0×10^{-2}	96	2.1×10^{8}
3	11	27	9.6×10^{-1}	27	1.4×10^{2}

[a]Indices are calculated using information from the published procedure for each route, scaled to 1 kg, and using assumptions on mass emitted (see the Supporting Information). [b]Human toxicity.

Potential, and Abiotic Depletion Potential. Route 2 was poor for all metrics, having the highest indices (except for abiotic depletion, which was moderate) and thus greater potential for harm. Route 3 was the greenest on 2/5 metrics: Human Ingestion Toxicity and Smog Formation Potential.

The LCA Primer activity followed the structure outlined in Figure 1 and involved two main phases performed consecutively in the same class period:

Single Metric Task (Worksheet 1). Students in a class are appropriately split into 3–6 groups, depending on class size. Each group is assigned an impact-based metric and a worksheet. The details of these metrics can be covered in a class-wide introduction by the educator or through the worksheet. The class is then given a scenario that involves choosing the greenest synthetic route for a chemical product out of three options:

"Your team has been hired as consultants by a chemical engineering firm that is trying to decide on a greener process for the synthesis of 1-hexylfluoride (also called 1-fluorohexane). Below are the three routes they are considering. Each route was scaled to produce 1 kg of product, as outlined in its Life Cycle Inventory Table. Use your knowledge of impact-based metrics to determine the greenest synthesis."

In their groups, students are tasked to calculate the indices of their metric for each route based on the provided impact potentials. Students should work together but also record the results on their individual worksheets.

Multivariate Peer Discussion Task (Worksheet 2). Subsequently, students move into new teams composed of one member from each of the previous groups. In this way, each team has one "expert" (for the scope of this activity) in each impact-based metric. Teams are given the same case but are now asked to consider all available impact-based metrics and compile their data into an LCA table (Table 2). Then, they must deliberate as a team to determine what they believe is the greenest option given the situation. The activity is structured to allow "experts" to peer-teach what they learned and explain their reasoning to the rest of the team, helping to solidify the concepts.

Table 2. Results from Worksheets 1 and 2

stage	task	count
worksheet 1 (Single metric) individual[a], n = 27	calculations completed correctly	24/27
	identified greenest route from a single metric	16/27
worksheet 2 (multivariate) groups, n = 5	identified greenest route from multiple metrics	5/5
	supported conclusions with reasoning	5/5
	changed choice given additional context	4/5[b]

[a]Students worked in groups with other students assigned to the same metric but were meant to fill out their worksheets individually. [b]Four groups reconsidered another option with a lower human ingestion toxicity index.

To extend the discussion, teams are also asked a question that places the case into a different context. In our example situation described above, it is revealed that the chemical plant that would be synthesizing 1-hexylfluoride is located on the banks of a river used for swimming and fishing. Given this new information, students must explain if they would change their answer and justify this choice. Each team submits their LCA table and their final verdict to the educator.

The learning objectives for this activity (if done with 5 different impact metrics) are

1. Students can confidently describe the following impact-based metrics and their relation to green chemistry principles, including safety, waste production, and the environment:
   (a) human inhalation toxicity
   (b) human ingestion toxicity
   (c) smog formation
   (d) global warming
   (e) abiotic depletion
2. Students can use data to calculate the potential and index of a reaction or process.
3. Students can use impact-based metrics to compare and contrast different processes and decide which process is greenest based on those metrics.
4. Students can rationalize how different contexts might influence which process is greener when considering different impact-based metrics.

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Implementation of the LCA Primer

The LCA Primer activity was piloted in a third-year undergraduate course on Environmental and Green Chemistry at Queen's University in Kingston, Ontario, Canada. It was carried out after students were introduced to the fundamentals of impact-based metrics but before learning how to do LCA. A total of 27 students participated in the activity in teams of roughly five for each phase. The entirety of this intervention was conducted in one 50 min class period. This included time spent on pre- and postsurveys to assess educational effectiveness. Students completed a survey at the beginning and end of class, each asking them to rate their confidence in their ability to execute each learning objective. Additionally, the worksheets that students completed were evaluated as evidence of learning. All surveys and worksheets were submitted anonymously as approved by our General Research Ethics Board.

RESULTS AND DISCUSSION

This section outlines the results of our implementation of the LCA Primer activity in an upper-year chemistry course and discusses student perceptions and teacher reflections on the activity.

Impact Metric	Total Index per Metric (kg)		
	Route 1	Route 2	Route 3
Human Inhalation Toxicity	9.423 *	95.72	27.18
Human Ingestion Toxicity	2.2×10^5	2.10×10^8	136.76 *
Smog Formation Potential	16.36	47.53	11.25 *
Global Warming Potential	9.381 *	116.36	26.57
Abiotic depletion potential	1.0215×10^{-4} *	0.03056	0.963

Figure 2. Example of one group's LCA table in Worksheet 2.

Student Work

The worksheets that the students completed in both stages of the activity were evaluated for (1) performing correct calculations and using the appropriate values, (2) providing a reasonable answer in their identification of the greenest route, and (3) drawing on learned concepts about impact-based metrics and LCA to justify their conclusions. We found that students were able to demonstrate that they could perform the calculations correctly, use those data to reasonably identify the greenest option, and use the concepts they learned in the activity to justify their conclusions (Table 2).

Multivariate reasoning from peer discussions was evident in the students' answers to Worksheet 2. All five groups (each with an "expert" on one impact-based metric) explained on this worksheet that Route 1 had the lowest impact for three out of five evaluated metrics and chose to make a trade-off for its high smog formation potential and human ingestion toxicity (Figure 2). When presented with the new information that the chemical plant producing 1-hexylfluoride would be near a lake used for swimming and fishing, four groups changed their choice to Route 3. Three of the groups identified the need for low human ingestion toxicity to reduce the risk to human health and the environment, and one did not provide any justification. One of these groups noted "if the plant is well maintained and not careless, route 3 should not be as important as route 1." Only one group kept their choice to Route 1, stating that it did not have the highest human ingestion toxicity index, and they did not think the trade-off

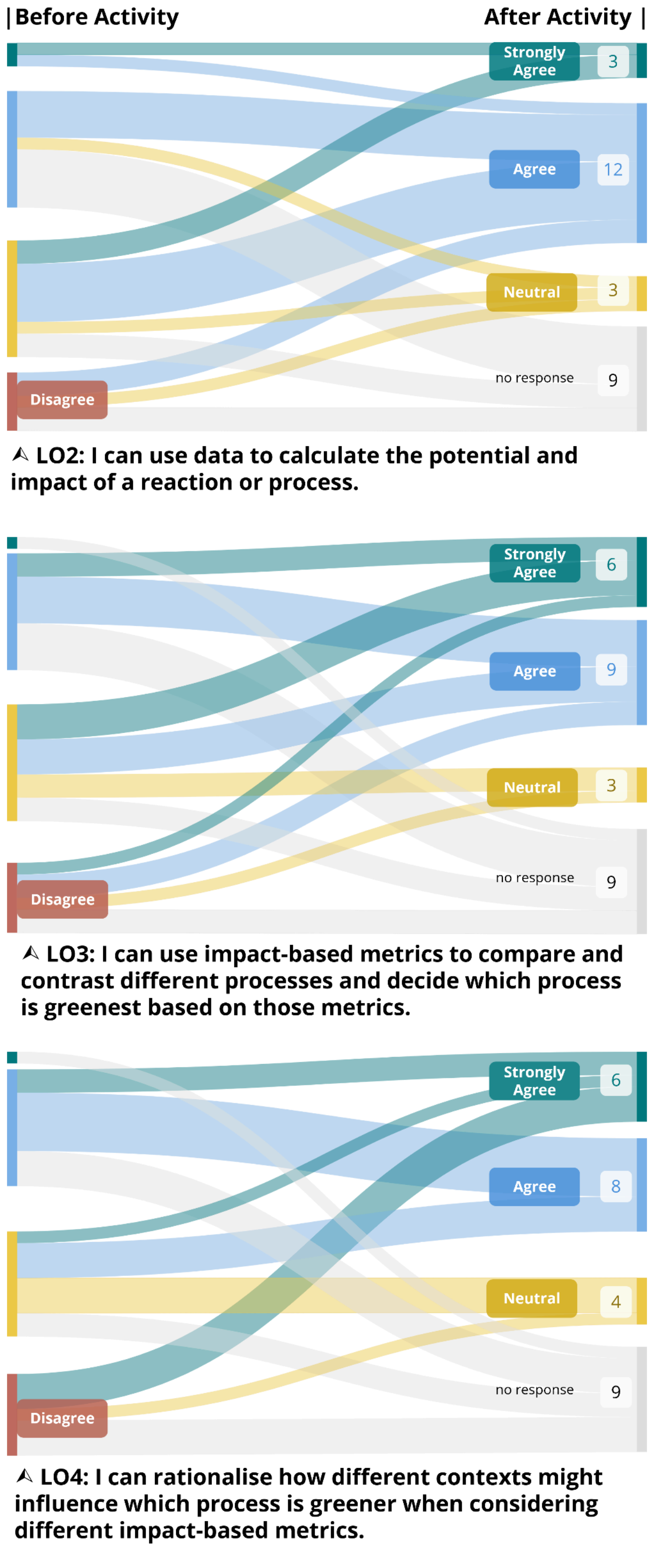

Figure 3. Comparison of students' self-reported confidence before (n = 27) and after (n = 18) the exercise in the learning objectives (LO2, LO3, and LO4) of the activity. Nine students chose not to complete or missed the second page of the postsurvey which had these LO rating questions.

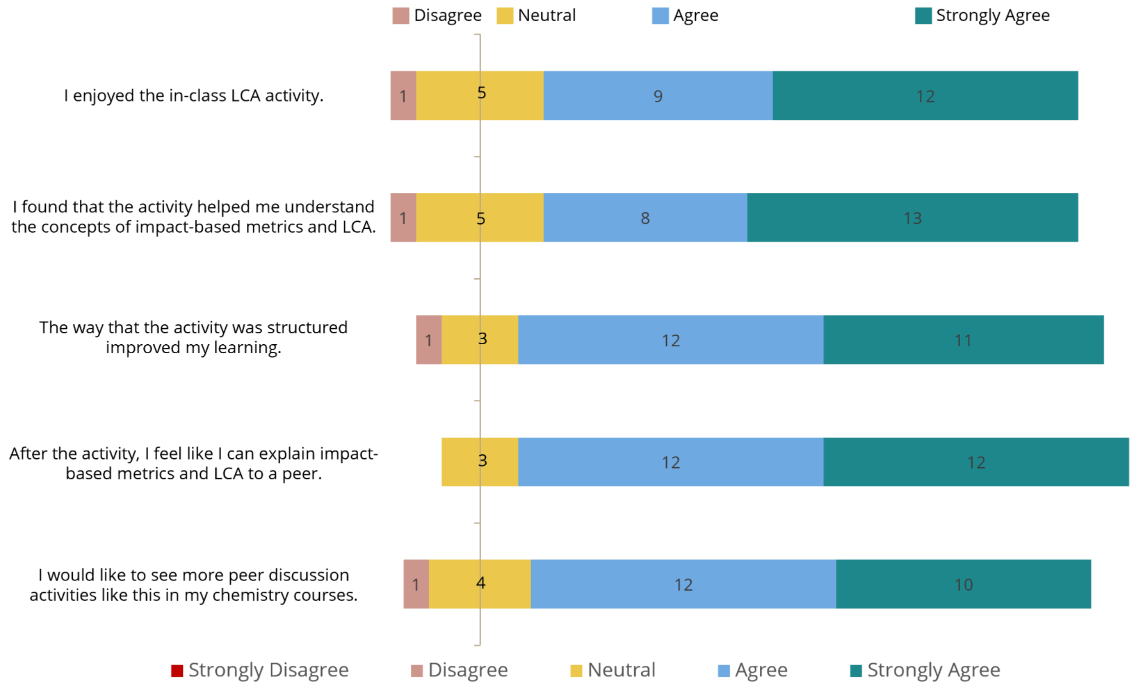

Figure 4. Students (N = 27) reported on the value they saw in the activity on the postsurvey.

with inhalation toxicity, global warming potential, or abiotic depletion was worthwhile.

Student Perceptions

The pre- and postsurveys included the learning objectives of the exercise and asked students to self-report their confidence with each learning objective. There is a noticeable increase in "agree" and "strongly agree" responses between the pre- and postsurvey results, although 9 of the 27 students chose not to complete or missed this second page of the postsurvey. For learning outcome #1 (LO1), which asked students to rate the statement "I can confidently describe the following impact-based metrics and their relation to green chemistry principles, including safety, waste production, and the environment" for each of the five impact-based metrics, which we combined for a total of 136 responses. We saw a notable increase in responses of strongly agree (13% from 5%) and a decrease in disagree (0.1% from 29%) for LO1. The pre- and postsurvey ratings for LO2, LO3, and LO4 for each participant (N = 27) are compared in Figure 3. These data suggest that students generally felt more confident after the activity, which supports the effectiveness of the exercise as an educational tool.

The postsurvey also asked about students' enjoyment of the activity. The results suggest that the activity was a valuable learning tool to most students, who generally reported favoring the activity, as shown in Figure 4.

Teacher Reflections

The data collected suggests that students better understood impact-based metrics and LCA and found the activity helpful to their learning. In addition to the students' results, the activity's facilitation was straightforward. The facilitator could visit between groups to answer questions and judge how quickly the students completed the worksheets. The total activity, from when students received the presurveys to when they submitted their postsurveys, took 48 min. These results suggest that the activity is effective in its goal. Students learned critical green chemistry concepts from the activity, and additionally, it can be easily implemented by an educator in a 50 min class period.

Delimitations

This activity was only conducted once and implemented in a green chemistry class. While the students had not yet learned about LCA or performed any calculations with impact-based metrics, the fact that they were enrolled in an elective green chemistry course suggests an interest in the concepts and material of the course. In showing pre- and postsurvey results, we make no quantitative claims of statistical significance.

CONCLUSIONS

The presence of green chemistry in the undergraduate curriculum is essential in preparing future chemists to create greener alternatives and combat climate change; however, integrating it can be challenging due to time and resources. We hope the resources provided herein (Supporting Information) will be helpful for educators wishing to provide their students with a meaningful introduction and a strong foundation for green chemistry. The first-year questions accomplish this by modifying existing types of questions to give them a green aspect, rather than displacing other content, and only require addition of impact potentials (catalogued in the Supporting Information). The upper-year activity provides an approachable introduction to the complex and time-consuming process of LCA, and our implementation found that students enjoyed and learned from the exercise.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.3c01217.

Educator Resource: Example Problems with Answers and Possible Discussion Questions (PDF)

LCA primer activity instructions and worksheets (PDF)

Educator Resource: LCA Potentials (XLSX)

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Notes

The authors declare no competing financial interest.

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