Connections Between Green and Sustainable Chemistry, Systems Thinking and Existing Chemistry Curricula

ACS Green Chemistry Institute

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1 Project Philosophy

1.1 Project Aims

This ACS funded project is supporting the development of new curricular materials for undergraduate chemistry educators teaching general and organic chemistry. Materials will be designed to enable students to construct knowledge of core chemistry ideas through the lens of green and sustainable chemistry using a systems thinking approach. This approach to learning chemistry is still centered around foundational chemistry content (as is found in core chemistry curriculum), but opens the aperture to encourage students to be systems thinkers that relate chemistry concepts to real-world systems. The overarching goal for teaching through this lens is to empower students to use their knowledge of chemistry concepts and practices to create innovations that help solve grand sustainability challenges (e.g., The United Nations Sustainable Development Goals (UN SDGs)).

For the purpose of this project, it is important to delineate the differences and overlap between *green and sustainable chemistry* because not all *green chemistry* is *sustainable chemistry*. When the first 12 green chemistry principles were published, green chemistry was described by Anastas and Warner as:[1]

> "…a particular type of pollution prevention…an approach that provides a fundamental methodology for changing the intrinsic nature of a product or process so that it is inherently of less risk to human health and environment… Green chemistry involves the design and redesign of chemical syntheses and chemical products to prevent pollution and thereby solve environmental problems."

The 12 principles are therefore framed in a pollution prevention context to protect the environment and human health. While green chemistry thinking has evolved over time, the principles themselves remain a snapshot in history and were never intended to directly address sustainability or sustainable development. The 12 principles were a response to environmental concerns and seen as "…source reduction, the most desirable form of pollution prevention."[1] While sustainable chemistry encompasses green chemistry, sustainable chemistry goes well beyond in terms of its goals and objectives. Sustainable chemistry includes considerations of sustainable development, chemistry impacts over time (e.g., over periods of years, decades, centuries) and across geography (e.g., local and global considerations), as well as socioeconomic issues.

An example may be illustrative. One may wish to make a biodegradable chemical building block from biomass rather than petroleum. Let's say the chemical is vanillin and it is made by catalytically de-polymerizing lignin using an iridium catalyst. This example hits three of the green chemistry principles, but is it sustainable? While lignin can be obtained renewably, there is still a question of where it came from, if it was from crops that have been farmed using Conservation Agriculture practices to prevent losses of arable land and biodiversity, etc.[2] The organo-metallic catalyst is based on iridium and iridium is one of the rarest precious metals and in no way sustainably sourced; iridium mining has extensive environmental and social impacts.[3–5] Iridium may also require the use of some difficult to synthesize ligands and stoichiometric reagents or solvents which may or may not be green.[6] Vanillin itself is very biodegradable, and degrades into non-toxic products, so the molecule itself may be said to be green.[7] As this example illustrates, it is possible to label your approach as green chemistry without it being sustainable. *Green and sustainable chemistry* is a broader approach to practicing chemistry that uses green chemistry strategies in combination with life cycle thinking and systems thinking to recognize and minimize the net impacts of chemicals and chemical processes on people and the environment. Of note, "minimization of net impacts/maximization of benefits" is quite difficult and demanding. Inevitably some communities, animal species, locations, ecosystems, etc. will suffer an impact from any decision made; the goal is to equip students' with the skills to navigate such complexity and evaluate the consequences of their choices. Moreover, historically, industrialized communities have benefited most from chemistry innovations, while developing communities have had comparatively fewer benefits. Developing communities often have had their land's resources depleted and/or polluted, been forced to work in unsafe conditons, and faced many health impacts not borne by the developed world. This disparity must be at the forefront of scienists minds so they make more equitable and socially responsible decisions going forward.

Figure 1 shows how green chemistry, life cycle thinking, and systems thinking can relate to one another in the practice of sustainable chemistry. Green Chemistry and Engineering knowledge, skills and practices offer the core strategies by which environmental, health and safety impacts can be reduced and potentially eliminated for a given situation. They are summarized in the figure within the innermost lens. That lens is then broadened by considering the life cycle impacts of a chemical, material, or product. Using life cycle thinking a chemist can follow and evaluate the impacts generated by a chemical throughout its life cycle. This perspective can be further enriched by thinking about the systems in which a chemical interacts. This outermost systems thinking lens helps a chemist to see how chemicals interact in real-world societal, economic, and environmental systems. A systems thinking lens allows chemists to more holistically evaluate their choices by considering the impacts of a chemicals or processes in a specific situation, as opposed to assuming that a green solution can be broadly applied to be beneficial in different use scenarios. Thinking about life cycles and systems is complex and not taught in traditional chemistry courses though. Therefore, this document aims to help orient educators as to how these ways of thinking connect to existing resources and curricula, and how they can be implemented in lower division chemistry courses.

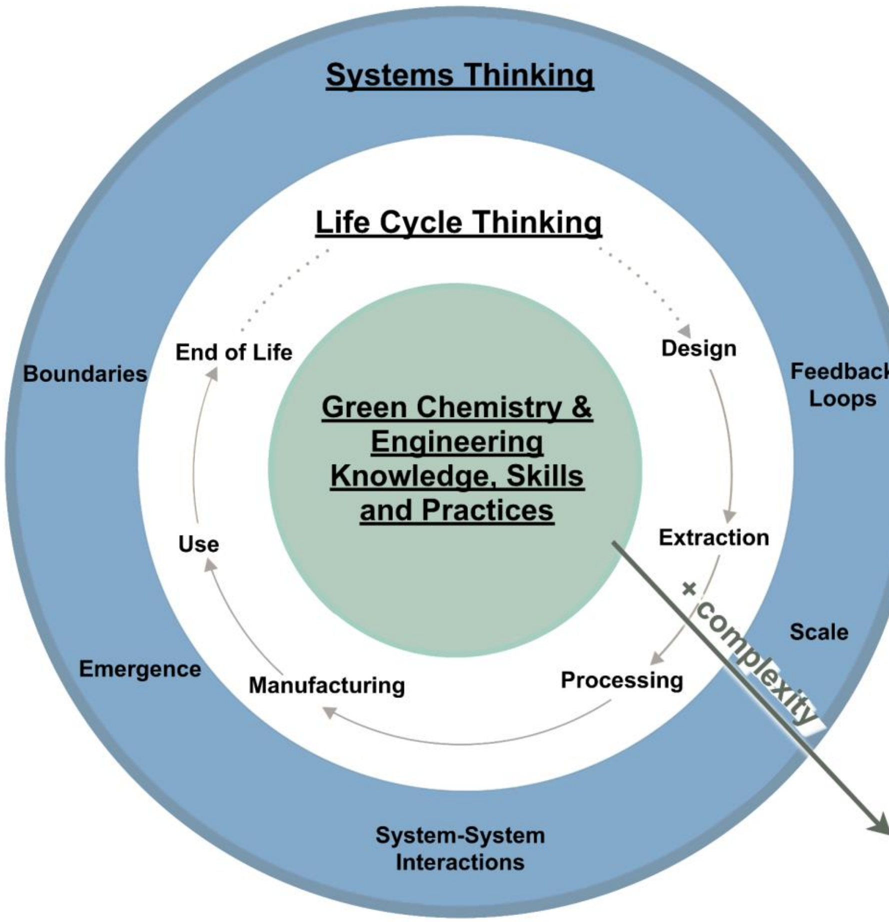

Figure 1. Multiple lenses for practicing green and sustainable chemistry. Green Chemistry & Engineering knowledge, skills and practices are the inner lens, with life cycle thinking broadening the perspective beyond those strategies, followed by systems thinking offering the most holistic and broad lens for practicing green and sustainable chemistry. Adapted from Ginzburg et al.[8]

The materials for this project will be developed as modules on specific foundational chemistry topics that can be related to grand sustainability challenges. While many green chemistry resources exist for instructional laboratory settings, in particular organic,[9,10] these modules will focus on creating holistic learning packages including, but not limited to, lecture notes, background readings, homework assignments, active learning activites, and assessment pieces. Modules will each cover a specific chemistry topic, with varying module format and length. More information on the module structure and requirements is provided in the rubric. The modules are intended to help students build a foundation for further developing the core competencies[11] they need in order to to practice greener and more sustainable chemistry. The green and sustainable chemistry core competencies are high-level skills that serve as a philosophical driver for the curricular materials developed throughout this project (see section 2.3 for more details on the core competencies).

As students work through modules they will come across a common theme that chemicals have both associated benefits and hazards, and evaluating these trade offs accurately requires considering the context of the function the chemical is being used for.[12,13] We aim to develop students' abilities to evaluate the relationships between chemicals, society, and ethics. Therefore, modules will be designed to help students grapple with the complexity of conducting chemistry in a way that balances societal benefits while preventing, reducing or mitigating damage to human health and the environment. Educators can convey key messages and have students demonstrate their ability to apply these messages to a specific problem. An example of a key message that can be directly relayed to students is:

> Chemicals improve human life in many ways. Examples are diverse, ranging from drugs that increase life expectancy, to the production of petrochemicals that sustain current modes of transportation. However, advances in chemical production have simultaneously led to consequences throughout the chemical life cycle. Critical and life-saving advances in pharmaceutical manufacturing may require hazardous chemicals and large volumes of solvents; the excreted drug metabolites and unused medications ultimately end up in soil and waterways where they can harm the ecosystem. Similarly, emissions associated with transportation have long contributed to a variety of adverse environmental impacts including climate change. As chemists, we must understand the implications of our choices and be aware that our decisions may adversely affect local and global systems. It is our ethical responsibility to carefully consider the full life cycle effects of our chemical products and processes. [14]

Educating chemistry students to understand molecular characteristics in terms of the functions they impart, and within the context of societal implications, will help prepare them to leverage their unique fundamental understanding of how to control matter. The goal is to equip students with the skills necessary to identify the connections between molecular characteristics and grand sustainability challenges. Additionally, teaching within a sustainability context helps chemistry students to pursue cutting edge research focused on furthering human society, preserving the earth's vital ecological systems, and bolstering economic well-being while still achieving traditional aims of advancing the science of chemistry.[15]

The grand sustainability challenges articulated in the 17 UN SDGs, adopted by the UN in 2015, will guide the selection of contextual examples for this project as much as possible. The ambitious goals, spanning a range of areas from economics to equality to resource availability, provide a framework for achieving peace and prosperity for people and the planet by 2030.[16] Chemists' foundational understanding of how to manipulate matter to achieve certain properties makes us critical players in advancing these goals, if we adopt appropriate priorities, approaches and practices.[14] Accordingly, the modules developed during this project are intended to use the SDGs to help identify grand challenges and place innovations in the context of the broader picture of global sustainable development. Modules will be designed to enforce the idea that chemistry, as the central science, is needed to support global sustainable development.

1.2 Project Methods

This section describes the green and sustainable chemistry skills and knowledge that students construct as they work through modules. More information on the educational philosophy, incremental benchmarks, and assumptions behind these methods can be found in a forthcoming document on our theory of change.

The modules are being created to engage students in green and sustainable science and engineering applications. We see this preparedness as being composed of three parts: knowledge, practices and applications (Figure 2). In the classroom, knowledge and practices are developed and refined, and portions of the applications are developed when possible, so students are well-equipped to implement more sustainable applications upon graduation. By iterating between knowledge and practices, students work towards better defining sustainability problems and sustainable solutions. It is worth noting that while the modules are intended for use in educating students from a range of disciplinary backgrounds and include the use of some engineering practices (e.g., solutions design), modules will be designed to align with the content traditionally covered in undergraduate general chemistry and organic chemistry curriculum.

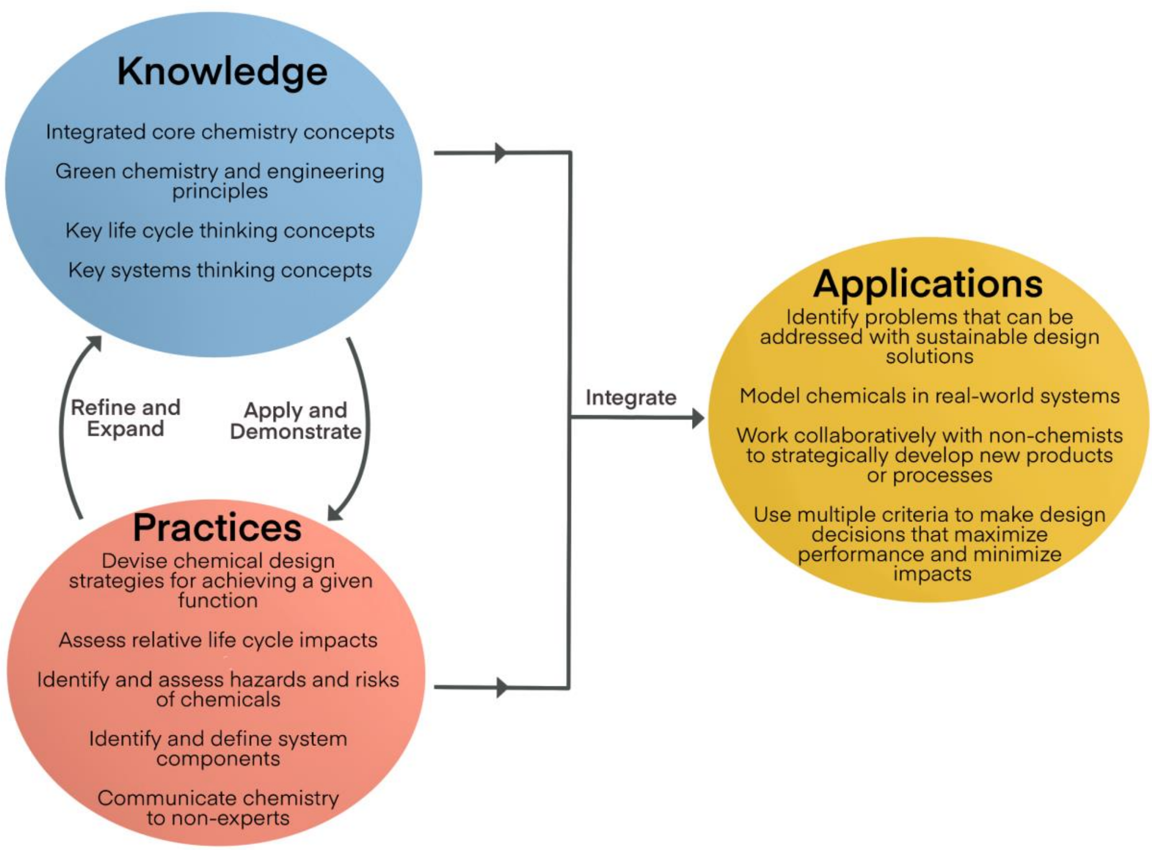

Figure 2. Pathway towards preparing chemistry students to engage in sustainable science and engineering applications.

Knowledge: The modules will be largely focused on knowledge and practice development. Knowledge is the information that an undergraduate chemistry major would graduate with if they were adequately prepared to take sustainable action. This knowledge is grounded in "integrated core chemistry concepts" meaning that students have to learn the same foundational chemistry concepts that they normally would, leveraging recent chemistry education transformation work (see section 2.2) to integrate those concepts. The other components of knowledge articulated in Figure 2 are specific to green and sustainable chemistry and not taught in traditional curricula. The reason that chemists need both the core chemistry foundation *and* an understanding of green and sustainable chemistry is that it isn't possible to develop green and sustainable chemistry without understanding how to manipulate matter from the atomic/molecular scale, considering the role of electronic interactions, structure, energetics, and equilibrium. Example targets for practicing green and sustainable chemistry include developing reactions that: are quantitative, rapidly progress to completion, require minimal additional reagents, solvents or complex processing steps, create no major by-products and minimal waste, and operate under mild conditions (room temperature and pressure). To do this as a matter of routine, following an undergraduate chemistry education, requires a chemist to consider the impacts of their choices on the environment, on human and ecosystem health, and on the proximate safety of humans and property, in addition to possessing a strong grasp on the fundamentals of chemistry.

Practices: These are the actions students perform in the classroom and laboratory that enable them to apply their knowledge. Herein, we used the practices published by the National Research Council[17] as inspiration for articulating specific practices necessary for green and sustainable chemistry. Both science *and* engineering practices have been included because addressing green and sustainable problems requires investigation/analysis as well as the ability to design solutions. The science and engineering practices have been described as the disaggregated, measurable components of inquiry,[18] therefore, practices provide a way for educators to articulate what they expect students to do with core knowledge and how it will be assessed. Of note, there are a number of green chemistry tools and metrics available;[19–25] students will gain experience working with some of these tools and constructing their knowledge of an individual tool's benefits and shortcomings. In particular, organic chemistry students will practice greener chemical selection using the solvent and reagent selection guides available on the ACS GCI Pharmaceutical Roundable website.

Applications: The applications listed in Figure 2 articulate what graduating students trained in green and sustainable chemistry should be able to perform; these are aligned with the skills outlined in Core Competency #3 (section 2.3). We envision applications as the intended outcomes of iterative and successive knowledge and practice-building cycles. When green and sustainable chemistry knowledge and practices are applied, chemists are positioned to design/innovate more sustainable solutions. Chemists need to be looking for opportunities to enact preventive measures, rather than the standard reactive measures that are often a consequence of inadequately anticipated impacts. Identifying innovation opportunities for sustainable development, regardless of whether something is currently considered a problem, is critically important. Doing this requires that chemists are able to model chemical systems beyond the lab bench. They have to be able to source the requisite information to construct systems-level models and anticipate how chemicals flow through a system. Using systems thinking requires making difficult and complex decisions about chemicals that consider multiple criteria and maximize the net benefit. Finally, chemists should be able to explain their thought process across disciplines and work alongside a range of stakeholders (e.g., toxicologists, biologists, engineers, public health experts, policy makers, etc.) to advance technologies using an interdisciplinary approach.

2 Moving Chemistry Content Towards Green & Sustainable Chemistry

2.1 Background

Science education research has shown that teaching foundational disciplinary concepts using rich and relevant contexts results in improvements in student addititudes, compared to that of conventional approaches, with comparable or better learning outcomes.[26,27] Teaching traditional chemistry concepts within a sustainable development context enables students to see that green chemistry is not a separate add-on to the core discipline, but instead, it is an application of those concepts. For example, ammonium nitrate's solubility leads to its extensive use in fertilizers and subsequent disruption of environmental nitrogen levels;[28] similarly, the chemical and structural properties of gases used in refrigeration can be used to explain their ozone-depleting and global warming potentials.[29] Placing foundational chemistry concepts in their relevant societal and environmental contexts makes lower-division chemistry courses more practical for students, many of whom will never go on to take upper-division chemistry courses because they are not chemistry majors.

These modules will use the UN SDGs as examples for laying the foundation of complex problems rooted in chemistry. Because the UN SDGs address complex issues involving science, equity, social justice, poverty, etc., taking a systems thinking approach when formulating solutions is imperative. It is important to differentiate here between context-based learning and a systems thinking approach. While both have an emphasis on contextualization, as noted by York and Orgill, that is the only characteristic they share.[30] A systems thinking approach focuses on a way of thinking about chemical phenomena. Systems thinking is focused on recognizing a whole system, including the interactions between parts, the behaviors of the system at large, and variables that affect system behavior. It is a tool or lens for thinking about problems or phenomena that change over time. To extend the above example of refrigerant chemicals, using a systems thinking approach, students can study the historical development of chlorofluorocarbons and see how scientific, societal, environmental and political systems have all influenced the different chemicals selected and their impacts.[29] This type of systems analysis helps students to understand not only the chemical interactions that cause chlorofluorocarbon's harm to the environment (i.e., bond interactions with UV-Vis light leading to free radical formation), but also the chemical properties that led to their use (inertness under conditions of use, easy compressibility, a large ΔH upon expansion that leads to efficient cooling). This approach allows students to first learn to recognize sytems within a broader context, then evaluate how chemical substitutions may alter function and impacts; the goal is to ultimately improve students' abilities to take sustainable action.

2.2 Current Chemistry Education Transformation Efforts

This project builds on current thinking in the chemistry education research space for developing chemistry curricula. Herein, we highlight key background information and resources that may be helpful for module developers. This is likely not a comprehensive list, and we welcome additional ideas and perspectives.

Anchoring Concepts Content Maps (ACCMs):[31] The Anchoring Concepts Content Maps (ACCMs) were developed by the ACS Examinations Institute as a means of mapping chemistry content across the foundational undergraduate chemistry courses, serving as an outcomes-based external metric for universities and as an assessment tool for aligning the ACS Examinations Institute standardized tests.[32,33] These documents outline the relevant content that could be covered in each of the six foundational chemistry courses (general, organic, inorganic, physical, analytical, and biochemistry). The ACCMs are centered around 10 big ideas, consistent throughout all foundational chemistry courses (e.g., kinetics and chemical reactions), and these big ideas are mapped to more granular content levels (4 levels total) for specific courses. These maps articulate the big ideas and enduring understandings that students should possess when they have finished the course. The general chemistry and organic chemistry maps have been iteratively revised by different groups of chemists over the past several years to incorporate green and sustainable chemistry concepts.[34] These green chemistry themed ACCMs demonstrate that green and sustainable chemistry concepts, knowledge, and examples can be integrated into the chemistry curriculum while adhering to foundational chemistry ideas. For this project, the ACCMs can be used to guide appropriate content selection for a given course and group multiple pieces of content together (typically from multiple big ideas) to get at one general or organic chemistry concept (e.g., teaching acid/base chemistry using content from big ideas V and VIII, chemical reactions and equilibrium). Therefore, modules developed in this project might touch more than one big idea. The maps are not meant to be curriculum and will not be used in this way, but rather they will be used a starting point for drawing connections between green and sustainable chemistry concepts and foundational chemistry ideas. The modules will begin to weave the core disciplinary ideas using green and sutainable chemistry examples and contexts into a modular curriculm format.

Transformed Chemistry Curricula: In 2012 The National Research Council published A Framework for K-12 Science Education,[17] this framework is the first step towards transformed science education standards in America. Building on two decades of research for defining science education knowledge and skills, this framework is designed to advance students' scientific profiency by emphasizing the overarching ideas and practices of science and engineering. This framework addresses the inadaquacies in current K-12 science education where graduates often lack the fundamental knowledge to be careful consumers of scientific information, engage in public discussions, or enter careers in science, engineering or technology. The approach taken to remedy these issues is to systematically organize scientific content across multiple years of school, changing the focus from wide-spanning discrete facts to more in-depth focus on how science is actually done. To do this, the framework proposes focusing on a limited number of disciplinary core ideas and crosscutting concepts, allowing students to integrate, build on and revise their knowledge over time. The committee recommends science education be structured to include three major dimensions:

- Scientific and engineering practices
- Crosscutting concepts that unify the study of science and engineering through their common application across fields
- Core ideas in four disciplinary areas: physical sciences; life sciences; earth and space sciences; and engineering, technology, and applications of science

Using this three-dimensional learning (3DL) approach, students actively engage in science and engineering practices and apply crosscutting concepts to deepen their understanding of each field's disciplinary core ideas.

Many of the K-12 science education shortcomings have also been reconignized at the university level and science professors have begun using this framework, or the research it was based upon, as inspiration for curricular transformation. Cooper and Klymkowsky created Chemistry, Life, the Universe and Everything (CLUE) to help undergraduate students develop a connected and coherent disciplinary understanding of chemistry.[35] CLUE transforms the undergraduate curriculum by changing the context and order in which general and organic chemistry content is taught.[36,37] CLUE developers adapted the 3DL framework approach specifically for chemistry (Box 1).[38] CLUE's components can serve as useful models for designing the sustainable chemistry modules envisioned for this project and can help connect chemistry knowledge to important skills. To avoid confusion, it is worth noting that although "systems and systems models" is a cross-cutting concept (see Box 1), this should not be conflated with systems thinking (explained in section 3). A recent paper by York and Orgill examined how the National Research Council's framework relates to systems thinking and concluded that a systems thinking approach includes aspects of all of the cross-cutting concepts.[30]

Box 1. Components of 3DL for chemistry developed by Underwood et al.[38]

(1) Core Ideas in Chemistry
   a. Electrostatic and Bonding Interactions
   b. Atomic/Molecular Structure and Properties
   c. Energy: Macroscopic, Atomic/Molecular, and Quantum Mechanical Energy Levels and Changes
   d. Change and Stability in Chemical Systems

(2) Scientific and Engineering Practices
   a. Asking Questions (for Science) and Defining Problems (for Engineering)
   b. Developing and Using Models
   c. Planning and Carrying Out Investigations
   d. Analyzing and Interpreting Data
   e. Using Mathematics and Computational Thinking
   f. Constructing Explanations (for Science) and Designing Solutions (for Engineering)
   g. Engaging in Argument from Evidence
   h. Obtaining, Evaluating and Communicating Information

(3) Cross-Cutting Concepts
   a. Patterns
   b. Cause and Effect: Mechanism and Explanation
   c. Scale, Proportion and Quantity
   d. Systems and System Models
   e. Energy and Matter: Flows, Cycles and Conservation
   f. Structure and Function
   g. Stability and Change

Even prior to the publication of the National Research Council's Framework chemistry educators had begun to discuss the shortcomings in current education including those mentioned above for K-12 science education, as well as challenges more specific to higher education, such as a disconnect between student's career goals and the course content. Talanquer and Pollard reformed the general chemistry curriculum at the University of Arizona using a framework they termed *chemical thinking*.[39] Chemical thinking emphasizes the application of mechanistic reasoning to build chemical rationales that support explanations, predictions, arguments, and decision-making in relevant contexts. Content, available freely online, is structured around issues in four critical areas: energy sources, environmental issues, life and medicine, and materials by design.[40] The Atoms First textbook, a free high-quality general chemistry textbook now in its second edition, introduces atomic and molecular structure much earlier than traditional curricula so that the atomic-focused theme is consistent and progresses logically throughout.[41] This has the additional benefit of delaying the introduction of stoichiometry, which the authors noted can be abstract and difficult for students to understand as they acclimate to the study of chemistry. Module developers for this project will likely find the readily accessible PDF of Atoms First to be useful a useful blueprint for organizing general chemistry content. Recently, McGill and colleagues at Emory Unviersity accomplished the impressive feat of implementing a new four-year undergraduate chemistry curriculum, termed *Chemistry Unbound*, that emphasizes core ideas and scientific practices by restructuring course content outside of historial course boundaries.[42] Students will progress through five foundation courses that all have the same core idea of atomic/molecular structure and properties. Chemistry Unbound starts students in a course on

Structure and Properties, where they first learn about atomic structure before progressing to the Principles of Reactivity, Advanced Reactivity, Macromolecules, and finally Light and Matter. The authors noted that data on the how the transformed curriculum affects student retention and success will be reported in forthcoming publications, as it becomes available. Course goals and learning objectives are provided in the supporting information of their publication. Finally, it is worth highlighting the recent ACS Symposium Series book chapter by Mio and Benvenuto from the University of Detroit Mercy.[43] This chapter urges educators to incorporate education on climate change into foundational chemistry coursework and provides numerous examples of how climate change chemistry connects to core concepts in general and organic chemistry courses, thus providing a useful starting point for module developers.

2.3 Green and Sustainable Chemistry Resources

Green and Sustainable Chemistry and Engineering Design Principles:[44] To understand this section, the reader should have the Design Principles for Sustainable and Green Chemistry and Engineering Booklet in front of them.

There have been 48 published principles of green chemistry and engineering, spanning four publications since 1998, and in 2019, another 12 were published for chemistry and the circular economy.[45] For a majority of those in the green chemistry community, it is generally true that only 12 principles are ever considered. The 48 principles of green chemistry and engineering, if viewed as a collection and not in isolation from each other, begin to help chemists to think more holistically about the implications of selecting elements, molecules, chemicals, and materials for reactions across the life cycle of products. To help chemists see these associations, the ACS GCI published The Design Principles for Sustainable and Green Chemistry and Engineering Booklet. This booklet organizes the principles by different areas of interest and themes. The collection of principles is grouped into three overarching areas of interest: maximize resource efficiency, eliminate and minimize hazards and pollution, and design systems holistically/use life cycle thinking. Within these three general areas of interest, the principles may be placed into one of four identified themes: design, measurement, efficiency and sustainability.

Organizing the principles in this way helps to illustrate several important ideas about green and sustainable chemistry. First, it is only when one considers all of the principles at one time that one can begin to see a few ideas in the principles that may link to sustainability. For example, ideas about sustainability are more evident in two of the areas: resource efficiency and systems and life cycle thinking. It is worth noting that these sustainability ideas are associated most clearly with the green *engineering* principles, not chemistry principles. Second, grouping these principles together makes clear that for green and sustainable chemistry to be successful, it is impossible to decouple chemistry and engineering practices and habits of mind. Finally, these principles are only a beginning, they don't contain all the necessary elements to make chemistry more sustainable, but they are a good place to begin.

Green and Sustainable Chemistry Core Competencies:[11] A group of green chemistry experts developed a set of core competencies that describe the skills and knowledge chemistry graduates should achieve in order to practice green and sustainable chemistry. The three overarching competencies are summarized below:

- Competency 1: Graduates will be able to design and/or select chemicals that improve product and sustainability performance from a life cycle and systems perspective.
- Competency 2: Graduates will understand that chemicals and materials are prepared through transformations of raw materials via synthetic pathways and be able to design and/or select chemical syntheses that are highly efficient, take advantage of alternative feedstocks, and generate the least amount of waste.
- Competency 3: Graduates will understand how chemicals can be used/integrated into products to achieve the best benefit to customers while minimizing life cycle sustainability impacts

Like the principles of green chemistry and engineering, the core competencies are highly aspirational, which presents a challenge in developing curricular resources that will enable students to attain these competencies. However, the modules need to be designed to move students towards these competencies without the expectation that they will be able to achieve full competency by the end of their undergraduate chemistry experience. As much as possible we will work to develop level appropriate performance expecations that measure a student's progress towards these competencies.

Connections Between Chemical Safety and Green and Sustainable Chemistry:

A survey was conducted in 2015 and again in 2020 by the ACS GCI to assess educator's preparedness to teach green and sustainable chemistry.[11]

Table 1. Survey results from a question where educators were asked to indicate the importance of teaching chemical hazards and exposure. Chemical hazards and exposure were defined here as "Identifying environmental, safety and health hazards, as well as potential sources of exposure. Selection and design of chemicals that are less hazardous alternatives to known chemicals and products"

	Survey Year	
	2015	2020
Essential	84%	68%
Important, but not essential	15%	30%
Not important	1%	2%
Number of Respondents	358	986

As can be seen in Table 1, in both cases these surveys found that a significant proportion of chemistry educators believe it is essential for students to learn about chemical safety. Chemical safety can be understood in multiple ways, but the two most prominent are protecting people and protecting physical infrastructure; i.e., labs, equipment, buildings, etc. Chemical safety is historically less identified with protecting the environment.

Given the importance of safety, it is worth highlighting the overlap between hazard and risk identification, assessment, mitigation and management processes and practicing green and sustainable chemistry. Green and sustainable chemistry focuses on the effects of chemicals on human health, safety, and the environment. Therefore, choosing safer chemicals and processes is aligned with the goals of both green chemistry and safety. Teaching chemical safety, and green and sustainable chemistry, should encourage a chemist to evaluate hazard and understand exposure to assess risk, minimizing it as much as possible. Where it's not possible to eliminate or substitute, proper safety controls must be in place. The practice of green and sustainable chemistry, if rigorously, comprehensively, and systemically practiced should always result in a safer, greener, more sustainable approach to practicing chemistry. This should be the result if one assesses and minimizes the potential impacts while optimizing the benefits across multiple categories. To illustrate this, a new solvent that inventors claim to be green, say an organic solvent that is bio-based and non-volatile or an ionic liquid that is non-volatile, may in fact have a variety of health (human and environmental), safety, and environmental impacts that renders it, on balance, less safe and green than an existing solvent. In this regard, effective personal protective equipment is a last resort for protecting human health, not the primary method for preventing exposure and potential harm. Green and sustainable chemistry methods aim to design for risk prevention, mitigation and minimization.

While green chemistry concepts and approaches give chemists helpful strategies to reduce hazards through careful selection of safer reagents, to truly design a procedure with the least risk, a systems thinking approach that considers the experimental system as a whole is required. In addition to the hazards presented by the chemicals themselves, factors such as lab conditions, scale, concentration, temperature, pressure, etc. all influence desirable safety outcomes.[46] These parameters (i.e., the system) are important for students to become familiar with considering as they evaluate hazards and exposure to determine risk. The ability for students to accurately assess a system and the risks presented, and then make decisions based upon their assessment, is increasingly being valued and built into teaching lab curriculum.

3 Systems Thinking for Chemistry Education

3.1 Background

For chemists to address sustainability opportunities and challenges it is necessary to consider the broader, systems-level impacts of how chemistry is practiced. Systems thinking helps chemists explore the implications of making and breaking chemical bonds, not only in a flask at a molecular scale, but also at the macroscopic scale to explore how those molecules interact with and affect people, the economy and the environment. These interactions can be studied from extraction to end of life (or ideally new use as we shift towards a circular economy). Integrating systems thinking into the chemical design and evaluation process illuminates areas where intervention will effect large changes. In December of 2019, *The Journal of Chemical Education* released a special issue on systems thinking and green chemistry that can be referenced for further reading about the motivations for introducing systems thinking into chemistry education.[47]

Giving students the training to practice systems thinking can benefit their professional development, whether or not they go on to be professional chemists. Systems thinkers recognize the complex interconnectivity of chemistry with other disciplines; they are habitually anticipating feedback loops and are able to identify multiple causal factors that could influence a single observation or outcome. This ability to anticipate outcomes is critical for developing students that are comfortable making chemical decisions where the best choice must be selected in the face of uncertainty, trade-offs, and imperfect data. While traditional chemistry typically operates using closed systems, at small scales, with tight boundaries (e.g., considering the reaction vessel on a benchtop), performing sustainable chemistry requires examination of open systems that are part of societal and planetary systems at much larger scales. By expanding a chemistry system's boundaries to consider the environmental, economic, and societal implications, students are able to recognize and navigate the complexity and importance of systems.

Figure 3 outlines the concepts and process that systems thinkers use to define a chemical system. First, a chemist must decide what scale is of interest (e.g., the cellular level, a single organism, or an entire community). More details on scale are provided below in Table 2. Setting the boundaries will determine what system elements and connections are being examined within the set scale, and the hierarchies show the arrangement of these elements into subsystems. Subsystems have components that are strongly connected to one another and balanced to serve the larger system goals. Constraints limit the elements that can be included in the system and they can be intentionally added to increase system benefits, such as with safety requirements and energy restrictions, or they can be practical challenges related to things such as project geography, budgets and timelines. After narrowing down the system to a reasonable size for analysis (through defining the scale, boundaries, hierarchies and constraints), the elements (also known as components) are what is left for studying. They can be nouns (e.g., fossil fuels) or clauses (e.g., burning fossil fuels) that describe a subject, process or effect. Once the elements are outlined, identifying their interactions with one another is key to understanding system structure and process. There are a number of ways that elements can interact and influence system behavior. They can have time- or distance-dependent interactions (e.g., acute vs. chronic biological effects), interfacial phenomena (e.g., sodium potassium pumps), loops (e.g., permafrost thawing feedback loops), or emergent properties (e.g., organs). More information about the meaning of these terms can be found in Donella Meadows seminal book on Systems Thinking.[48]

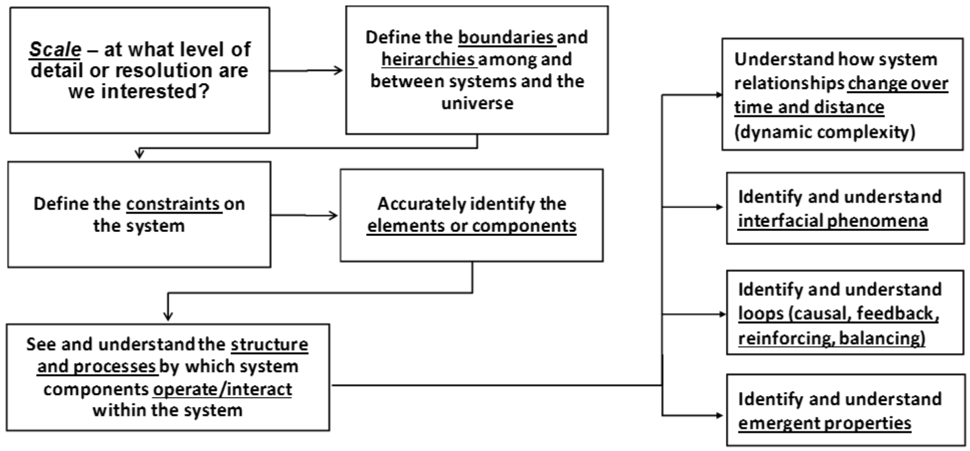

Figure 3. Process for defining a chemistry-specific system from [Constable et al.](#)[49]

Traditional chemistry curricula operate at two scales, the macroscopic scale relating to what is happening in the lab and the molecular scale at which the chemistry is occurring.[49] However, the reality is that the same chemicals in a beaker are engaged in systems at scales beyond just those two. Figure 4 shows some of the potentially important considerations at different scales for a benchtop reaction. Reaction parameters such as the reactants, catalyst, heat and solvents impact sustainability at the beaker scale, and oftentimes that is all that is considered when a greener reaction is developed. Expanding the scale, the laboratory in which the reaction is taking place can be considered. What are the energy impacts of the fume hoods? Do the chemists need personal protective equipment to reduce or eliminate exposure, and if so, do they have the understanding to select the appropriate equipment? How much waste is being generated from the reactions being performed? At the community scale, the impacts of having chemical laboratories can be considered. Are they generating pollution? Are they bringing in local employment? Whether these labs are academic or industrial will have an effect on the makeup of the community population. Finally, the impacts of that same reaction at the international scale can highlight some critical information about a reaction. Was the catalyst mined using unethical labor practices? How abundant are the materials used? What are the transportation impacts?

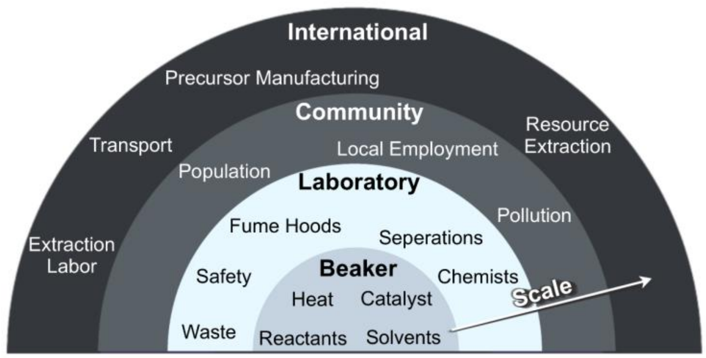

Figure 4. Example topics that can be considered when examining a benchtop chemical reaction at various scales.

Table 2 provides examples of different scales for potential areas of chemistry-related focus. To demonstrate the importance of considering scale during chemical decision making, let's imagine policy makers wanted to explore the implications of banning the use of certain classes of flame retardants from soft foams that are used in furniture. The policy makers may start by examining the toxicology reports of a series of flame retarding molecules, but interpreting this data requires knowing the right questions to ask and who to ask them to. Are the data sets comparable between molecules? Are they relevant to human health (e.g., on a similar enough scale)? If the data are sufficient to where a toxicologist feels confident ranking the toxicity of the molecules, simply banning the most toxic molecules may not yield the intended result. There is still the potential for unanticipated impacts at larger scales like the environment. Other relevant questions might include how prevalent are retardants used in public seating? Do the policy makers' communities have a high prevalence of smokers? Will furniture covers have any fire resistant properties? If certain flame-resistant fibers will be promoted, what are their impacts? Of course, it is not practical to consider details at all scales before making chemical-related decisions, but it is indeed necessary to acknowledge that a practical solution at one scale may be detrimental at another. It is also worth noting that in this hypothetical scenario, the policy makers' approach to the problem could be improved. Instead of asking whether or not to restrict/ban the use of flame retardants in soft foams, they might instead ask what function are these flame retardants serving, and how else might that same function be achieved? More details on designing for function can be found in section 3.4.

Table 2. Common areas of focus when thinking about chemical systems.

Potential Areas of Focus	Chemistry	Environment	Safety	Health	Human/ Social/ Organizational
Increasing Scale (bottom row to top row)		Earth Systems	International	International	
	Earth Systems	Eco-systems	Nation	Nation	Earth Systems
	Supply Chains	Regional	Region	Region	International
	Process	Local	State	State	Nation
	Route	Mesocosms	Community	Community	Region
	Laboratory	Plants and animals	Building	Single organism level	State
	Self-assembly	Cells	Work space	System (e.g., endocrine, nervous)	Community/ work/ organizational
	Physical / Physico-chemical Properties	Molecules	Human and Environmental Organism	Organ	Family and Friends
	Molecules		Physical Properties	Cells	Person
	Atoms		Molecules	Molecule	
	Sub-atomic Particles		Atoms		

3.2 Visualizing Systems

Systems-thinking visualization tools can help define the interconnections within a complex system, highlight the components and scales of interest, and establish boundaries. These visualizations provide a way for students and educators to articulate and assess a system and break out of traditional linear cause-and-effect thinking. The visualizations are most appropriately used as tools for: instructors to construct themselves as aids in their planning of curricular materials or as tools for students to construct as a way of understanding/describing a system.

It is helpful to start a visualization by defining a system's purpose, then deciding on the scale and connections that are important. The purpose of the visualization will determine the complexity necessary; in lower division chemistry courses it is most likely the case that the purpose is for students to become familiar with these diagrams, so encouraging students to keep them simple and approachable is key. One strategy for doing this is minimizing the number of subsystems and connections examined, while acknowledging that many others exist. Preventing cognitive overload likely requires students to practice creating their own systems visualizations, adding connections incrementally, rather than interpreting previously generated diagrams in all of their complexity. Below we will briefly describe three types of systems visualizations that are most likely to be relevant for lower-division chemistry courses. For more specific examples applied to chemical systems and additional types of systems visualizations, we recommend the manuscript by Aubrecht et al.[50]

System-oriented concept map extension tool

A system-oriented concept map extension (SOCME) tool is like concept maps traditionally found in education in that it shows elements and their interconnectedness, but it is extended to include specific systems thinking features. SOCME tools are useful for organizing system elements into subsystems that interact with one another. They illustrate how subsystem interactions achieve a system's purpose. The defining characteristics of SOCME tools are their emphasis on system boundaries and multiply-connected subsystems. When constructing a SOCME one must consider the boundary setting and its appropriateness for a given issue. Effective boundary drawing is key for highlighting the important scale and connections of interest. Additionally, the choice of which subsystems to include must balance the need for understanding complexity with course appropriateness.

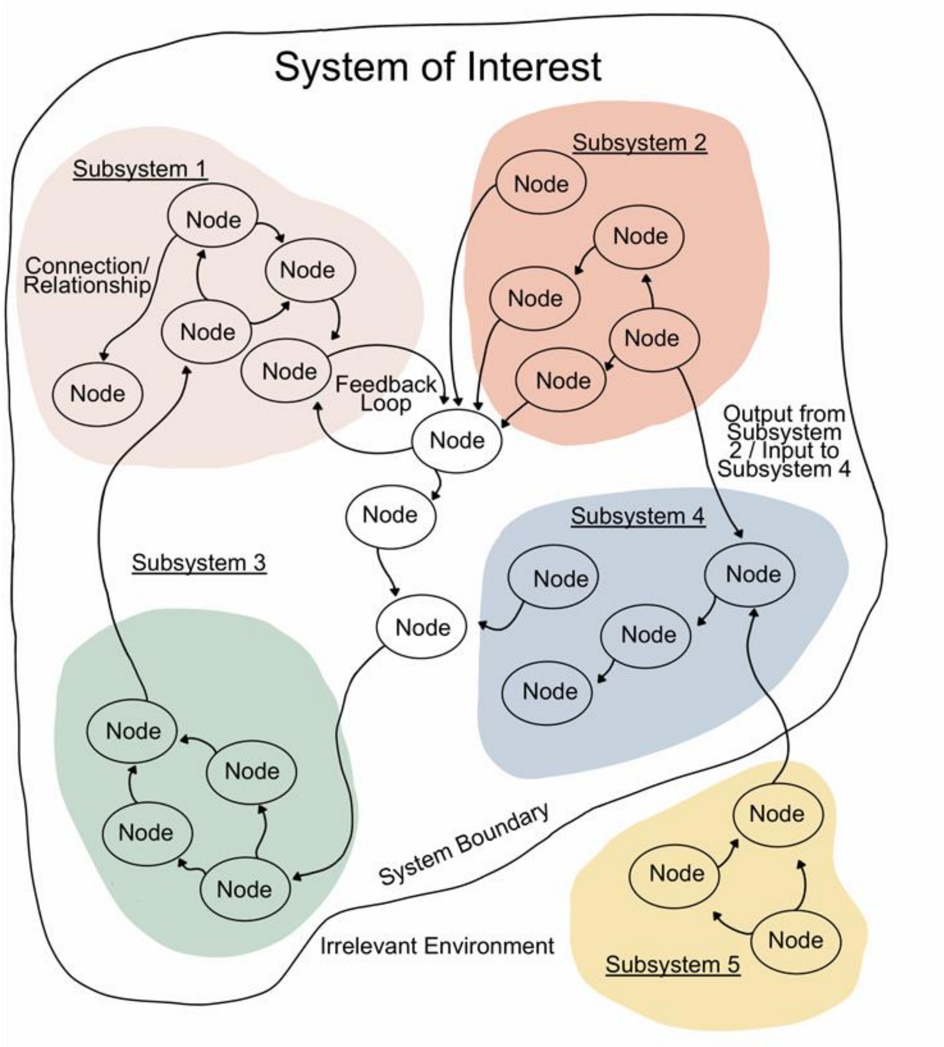

Figure 5. General structure of a SOCME. Note that connections between nodes can be extensive but here they are minimized for simplicity Also, in practice the boundary is likely implicit and subsystem 5 would not be shown.

A general SOCME structure is shown in Figure 5. SOCMEs illustrate relationships between factors that influence a system using arrows and nodes. The nodes contain system elements and the direction of the arrows indicates cause and effect relationships between elements. These connections are useful for predicting how changes in one factor will influence others. Elements are organized into subsystems, with arrows going in any appropriate direction(s). Subsystems can show multidisciplinary or multicultural perspectives, in addition to chemical connections such as intended use and energy inputs.[27] Much of the value of a SOCME is in the inclusion of multiple subsystems, which make it evident that a chemical's intended use is only one subsystem, within a system with much broader implications (subsystems). See Figure 6 below for an example of this.

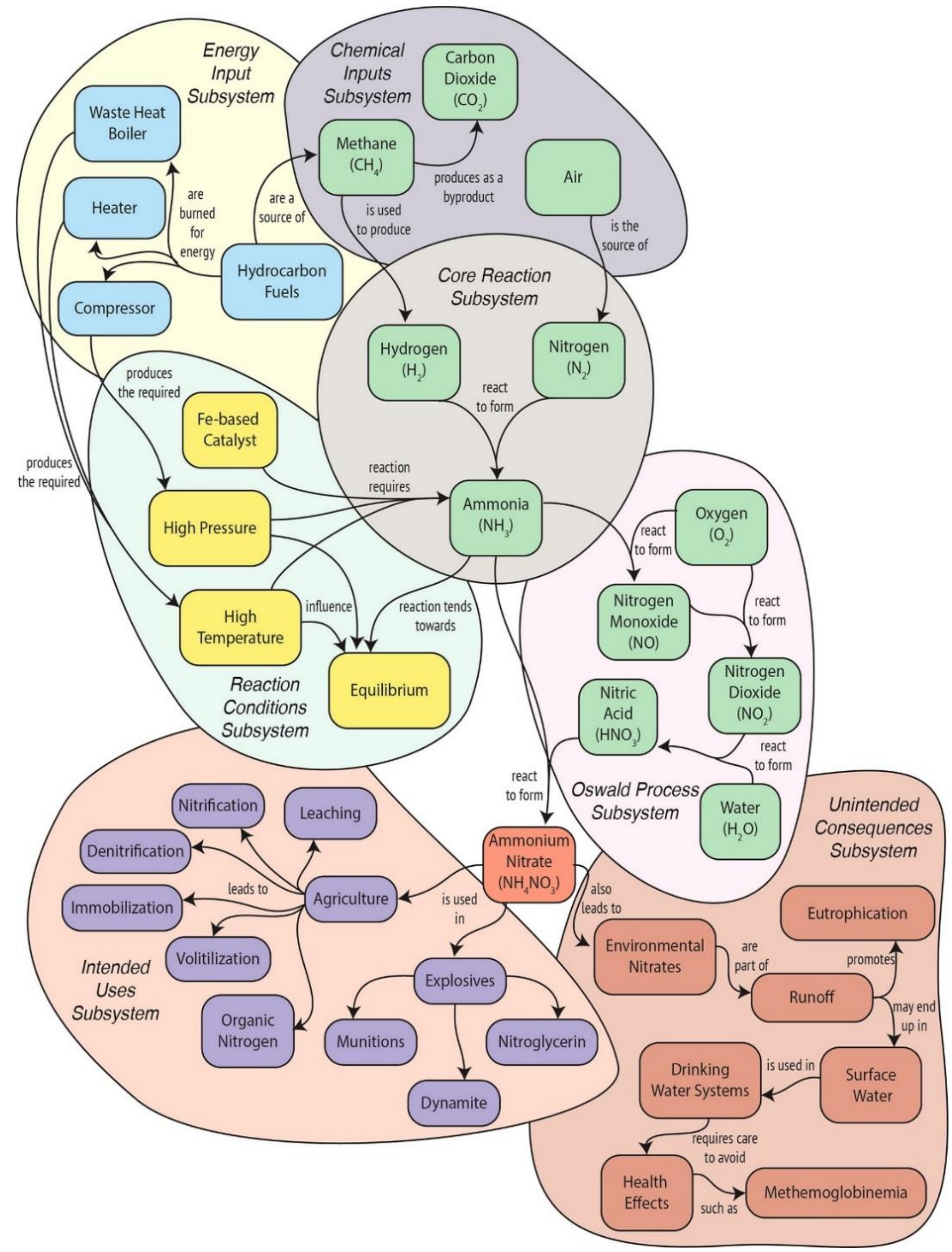

Figure 6. An example SOCME for the Haber-Bosch reaction from Mahaffy et al.[28]

Figure 6 shows how a SOCME may look when constructed around a chemistry process, in this case, the Haber-Bosch process. Although mentioned in most general chemistry textbooks, the process is usually only taught to provide an isolated contextual fact surrounding equilibrium concepts and calculations. This is a missed opportunity to connect vital real-world chemistry systems to general chemistry content. The Haber-Bosch process allows the world to mass-produce crop fertilizers, thus sutaining the global food supply. This production of reactive nitrogen is critical, but not without consequence. Constructing a SOCME visualization that shows the chemical inputs, energy inputs, reaction conditions, outputs and unintended consequences allows students to see the relevance of this chemistry and develop analytical skills to ask questions surrounding sustainable practices. In Mahaffy et al.'s manuscript they discuss the various subsystem impacts and how this SOCME can stimulate student questions such as "is this reaction good for agriculture, for mining/construction, for the environment, for the wellbeing of the planet?". In addition, the authors present an alternative version of this SOCME that emphasizes different subsystems, thus highlighting the fact that systems visualizations depend upon the question being asked and the boundary, scale, etc.

Systemigrams

A systemigram can be thought of as containing much of the same information and visual representation as SOCME but more specifically applied. They are used to depict information in a specific order, like that of a story, and are therefore most helpful as visual aids for a long and complex prose narrative. Systemigram designs demand a flow from upper left to lower right (see "input node" and "output node" in Figure 7). Like a SOCME, systemigrams still have nodes and connections between them, but here nodes are specifically expected to be nouns and connections are verbs. Because the ordered flow is the main emphasis of a systemigram, the subsystems and boundaries are of less focus than in SOCME. The pre-determined flow of systemigrams does make divergent discoveries unlikely, but they are quite efficient at information representation.

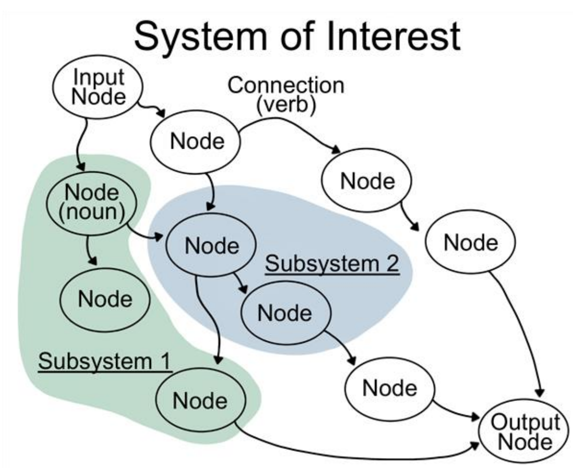

Figure 7. General structure of a systemigram.

Causal Loop Diagrams

Causal loop diagrams (CLD) help to identify specific processes that contribute to a particular trend over time, i.e., feedback loops. They are most useful when used in tandem with graphs depicting behavior over time. The power of CLDs is that they explicitly show feedback loops; the drawback is that they are not quantitative and can thus be misleading when not supplemented with quantitative visualizations.

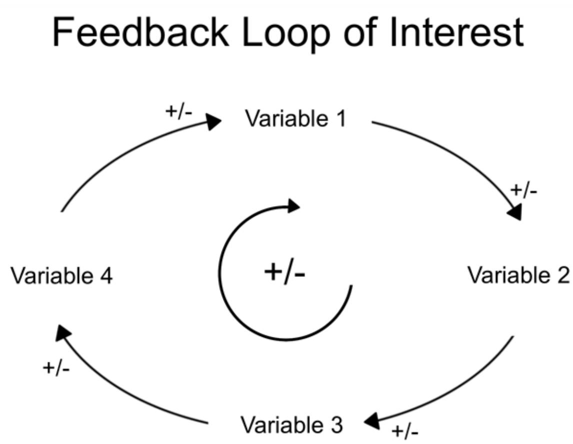

Figure 8. General structure of a CLD.

As shown in Figure 8, linkages are connected using +/- signs to show how one factor influences another. A (+) indicates that a change in one factor causes an effect on another factor in the same direction. A (-) relationship means that a change in one factor causes an effect on another factor in the opposite direction. The sign on the inner circle describes if the CLD is reinforcing (+) or balancing (-). A reinforcing loop means that if one variable has a perturbation, it will continue to trend in the same direction the second time through the loop. In contrast, a balancing loop means that if the variable is perturbed it will show the opposite directional trend the second time through the loop. An odd number of CLD links with opposite signs will be yield a balancing loop.

3.3 Using Systems Thinking to Understand how Chemists can Help Solve Global Problems

Designing molecules, synthetic pathways, processes, and products involves many decisions that interact, perturb and otherwise affect existing systems. Where a chemical comes from, the impacts of the process in which it is used, and the final fate of the chemical all have consequences on the environment, the economy, and society. It is important that students learn to understand, navigate and manage this inherent complexity and make design decisions that avoid adverse outcomes.[49] For chemists in particular, their decisions inherently affect the system structure and flow. A chemist, when modifying, optimizing, reproducing, or scaling a reaction, converts a linear reaction pathway into a system with feedback loops. Therefore, much of the onus is on the chemist to adjust the system to produce positive/sustainable outcomes. Students can learn this through the examination of real-world systems.

The SDGs provide a high level starting point of global problems with complex systems. For example, by beginning with one of the SDGs, responsible production and consumption, we can think about framing waste and pollution as a consequence of chemistry decisions made upstream during production, rather than as a downstream effect to be managed. This framing provides insight into how chemists can address the challenge in meaningful ways.

Table 3 presents examples of broad chemistry connections to seven SDGs with a strong chemistry component. These example chemistry connections were selected because of their relevance to general or organic chemistry curricula. A general chemistry module that starts with the need to end hunger and achieve food security (SDG #2) can introduce the importance of ammonia production to food security while using the Haber–Bosch process to have students practice equilibrium mathematics and explain equilibrium concepts. Afterwards, students could follow transformations of ammonia throughout an agricultural system and gain experience predicting and balancing reactions while learning about a real-world system. This exercise can help students learn that while the chemist is responsible for efficiently making ammonia, forming relationships with other scientists is critical for managing associated impacts such as disrupted soil nitrogen levels, loss of ammonia into air, runoff of nitrates into waterways, and other gaseous pollution. Developing multidisciplinary partnerships and planning for the product life cycle is critical to achieving the most sustainable outcomes.

As another example, we can consider the range of scientists needed throughout the life cycle of a hypothetical grid-scale energy storage system that uses low-cost and energy-dense batteries (addressing SDG #7): Physical/computational chemists to predict efficient and low-cost materials; materials scientists and electrochemists to develop the battery components and integrate the cell; chemical engineers to implement the battery at scale and manufacture it; environmental scientists to assess the impact on the land; electrical engineers to design the infrastructure and install the grid; and a combination of scientists (e.g., chemists, environmental scientists, toxicologists) to recycle the materials and remediate the land at the end of use. Using the SDGs and relevant materials/chemicals (e.g., ammonia, batteries, etc.) gives opportunities for students to learn foundational chemistry concepts while appreciating grand sustainability challenges and the importance of interdisciplinary work.

Table 3. Chemistry Connections to the SDGs

Priority SDGs for Chemistry	**Example Chemistry Connections**
Goal 2: Zero hunger	• NH_3 production • Active food packaging • Phosphate recovery and reuse
Goal 3: Good health and well-being	• Targeted drug delivery • Extended drug release • Drug bioavailability • Rational molecular design
Goal 6: Clean water and sanitation	• Desalination/treatment technologies • Removal of metal impurities

Goal 7: Affordable and clean energy	• Renewable energy production from earth abundant materials • Materials for waste heat/cooling utilization • Energy storage devices
Goal 9: Industries, innovation & infrastructure	• Phase change materials • Low/no VOC materials • Indoor air quality • Low CO_2 composites for heavy construction (cements, etc.)
Goal 12: Responsible production and consumption	• Circular economy • Feedstock changes
Goal 13: Climate Action	• Low energy catalytic reactions • Direct utilization of CO_2 • Low energy conversion of CO_2 • Alternative separations technologies

3.4 Using a Systems Thinking Framework for Sustainable Chemical Design

Once a system's landscape is mapped, often with the aid of visualizations, chemists can consider intervention strategies. This is the stage at which chemists have iterated between sustainable chemistry knowledge and practices (refer to Figure 2) and are now prepared to apply their skills. When an area for chemistry innovation has been identified, there are multiple ways to define the desired solution. Oftentimes this solution is defined to be the inverse of the problem: Reef-safe sunscreens, paraben-free cosmetics, BPA-free bottles, etc. This type of definition is limiting because it misses opportunities to intentionally develop a product or process with an improved performance while solving the problem. Worse yet, it can lead to regrettable substitutions when a molecule may be replaced by a less effective one, resulting in increased impacts at the necessary concentration for use. A better way to define the solution has been described by Tickner et al. as *designing for function*.[13] Using this approach, the chemist works backwards from a given function (e.g., antimicrobial properties, UV-absorber, etc.) to ask how and why a chemical is used, and how else that same function can be achieved. By designing with the chemical's function in mind, a chemist can examine how specific structural or physiochemical properties affect the product or process impacts and performance. This approach also highlights the importance of working alongside toxicologists who can describe how certain chemical properties relate to biological impacts, thereby increasing the potential for making safer chemicals. By taking a creative approach to defining what the solution to a problem should be, chemists aren't limited to merely finding drop-in substitutions, but can be galvanized into designing functional equivalents with improved performance and reduced impacts.

The following section walks through a systems thinking chemical design framework to show how one uses the concepts described in this document to actually design solutions. The goal is to provide a detailed example of how foundational chemistry concepts can be used by an expert to understand, mitigate, and possibly solve sustainability challenges. This example is meant to demonstrate how one can use a combination of green chemistry, life cycle thinking, and systems thinking strategies to develop sustainable solutions. It is not intended to suggest that all solutions presented below are of equal ease of adoption or performance. Those considerations are beyond the scope of this thought exercise. Additionally, this extended example on textile chemistry is beyond the scope of many lower-division courses, but portions can certainly be adopted or used as inspiration. Section 3.6 provides a general template for adopting this exercise into an assignment.

Improving textile sustainability

The textile industry needs major reform to address issues of substantial energy usage and massive amounts of water consumption leading to significant wastewater generation;[51] these issues are being compounded by population growth and the emergence of "fast fashion". There are many ideas about effecting sustainable changes, but inevitably some solutions will have a higher net benefit than others.

Opening question: What societal and consumer preferences should be considered for assessing the practicality of a textile innovation? *Considering the industry trends and constraints (e.g., technical, economic, regulatory) that will influence choices made.*

- Production costs must be reasonably low to produce garments that consumers will pay for
    - "Fast fashion" is still prevalent and reinforces low-cost pressure on brands
    - "Sustainable fashion" is a rising consumer concern and may be valued enough in niche markets to warrant higher costs
- Emergence of digitization has created a resale and rental market for clothing
    - Durability is being increasingly valued by consumers
    - Designing for longevity means avoiding fashion designs that have typical fast product cycles (i.e., "trendy")
- Consumers have a rising interest in functional textiles (e.g., odor prevention, durable water and stain resistance, UV-protection, etc.)
- Clothing should be easily cleaned or cleaned with a minimal amount of resources – water, detergents, stain removers (enzymes), energy (heating, drying, compression/recompression, etc.)

Assessing the current system landscape: What is the status quo? What are some of the biggest sustainability challenges for textiles production right now? *Identifying the system, boundaries, and leverage points of interest. Systems visualization tools are helpful here.*

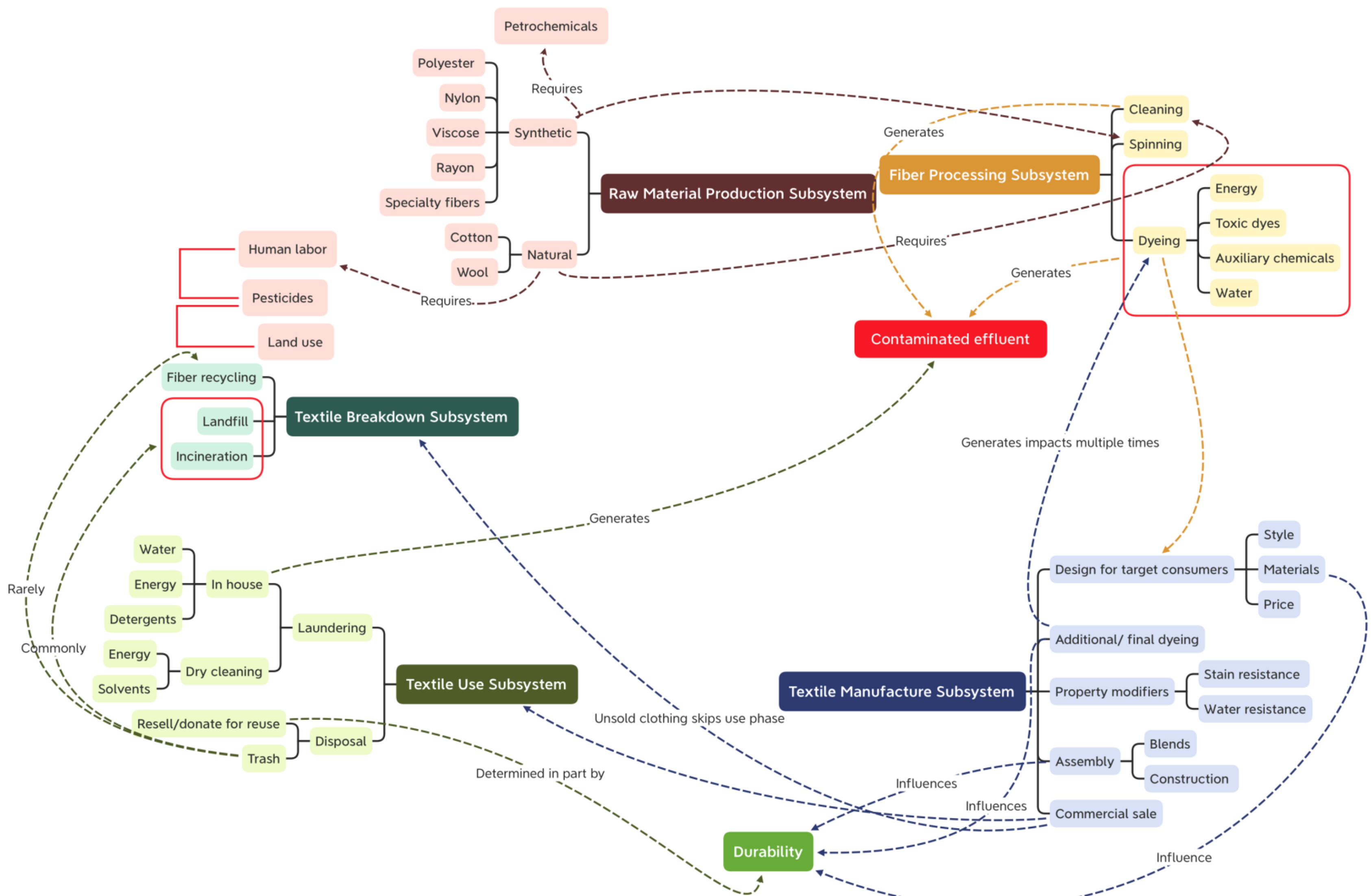

Figure 9. SOCME for textiles.

Selected overarching goal: Improve sustainability of coloring textiles. *There are clear challenges related to the production of textiles that chemistry innovation can address. We could have selected raw material production or textile recycling challenges, but those are more heavily reliant on collaborations with engineers, agricultural experts, and sociologists, so we are focusing on dyes for this example. Certainly though, these interdisciplinary challenges highlight the need for multi-disciplinary collaboration to address sustainability issues.*

Solution-design question: <u>What is the most chemically- and energy-efficient method to impart color to a cotton fiber such that the overall process produces less hazardous waste?</u> *Specific question about reducing chemical impacts that works backwards from molecular features that yield a given function (imparting color).*

Developing an answer for the above question is the crux of the challenge. Box 2 describes a series of questions that chemists can ask to use a systems thinking framework for designing solutions.

Box 2. Chemistry strategies for approaching the solution-design question.

1. What are the chemical properties/nature of the cotton fiber?
    a. What functional groups are available for adhering the dye to the fiber?
2. What functionality would be required in the dye molecule to ensure a thermodynamically and kinetically favorable reaction?
    a. Are there more efficient methods to promote reactivity?
        i. Electrochemical
        ii. Photochemical
        iii. Supercritical or other high-pressure solvent systems
        iv. Enzymes
3. What chemical structure would be required (what kind of chromophore) to ensure the desired color?
    a. What functional group would be in the chromophore-containing center?
        i. EWD or EDG substituents?
    b. Does color have to come from transitions in conjugated organic compounds or would other ways of generating color be practical as well?
        i. Electronic transitions in inorganic particles
        ii. Light dispersion and scattering (structural color)
4. What molecular functionality, topology, geometry would you need to ensure minimal or no toxicity?
    a. Does nature make this color in a non-toxic way? How?
5. What kinds of auxiliary products (dispersing agents, pH modifiers, surfactants, reductants, etc.) would be required to facilitate the reaction between the dye and the fiber and/or facilitate downstream processing?
    a. Are there potential alternatives with lower EHS hazards and associated risks?
    b. Could these be avoided by changing the dyeing process?
        i. Supercritical dyeing
        ii. Inkjet printing
6. At the end-of-useful life of the textile, how could the dye be removed chemically or physically without much waste?

Communicating Design Guidelines and Solutions: *Let's say that after asking questions, like those in Box 2, and iterating on potential solutions, that a decision is made to pursue a more efficient dyeing process by designing a new dye carrier molecule.*

Guidelines for designing a greener and more sustainable dyeing carrier molecule.

- Hydrophobic carriers usually interact with polyester fibers through pi-pi interactions, so an effective carrier should have an aromatic ring in its structure to promote interactions between the fiber and the carrier.

- The carrier should be smaller in size than the dye molecules to readily diffuse into the fiber; this diffusion is also affected by solubility of the carrier so it should have a Hoy solubility parameter similar to that of polyester and a minimized water solubility limit.[52]

- Carriers are often toxic and persistent, they should be free of halogens that often yield environmental persistence and have their risk assessed based upon the expected exposure to workers and the environment.

Describe design guidelines using descriptive underlying chemistry and scientific ideas that allow others to understand how to use disciplinary concepts to design their own sustainable solutions. Guidelines should help other chemists to think about the tools a chemist has to work with to design a solution that maximizes benefits and minimizes impacts; tools include the modification of conditions such as concentration, temperature, pressure and knowledge of relevant chemical properties such as solubility and structural binding motifs.

3.5 Developing Education Materials to Teach Sustainable Chemical Design

As can be seen by the complexity and breadth of knowledge necessary to answer the questions in Box 2, there is no simple way to think in systems. Practicing green and sustainable chemistry requires a strong grasp of chemistry fundamentals in addition to the skillset necessary to minimize chemical impacts. While never simple, the complexity can be managed by defining specific questions and goals (in the classroom these should be commensurate with student experience level). This example had a fairly broad boundary, which led to a lofty goal of imparting color into cotton textiles with minimal harm; certainly, setting a narrower system boundary would be appropriate for lower-division students. As an example, students could be instructed to only examine the fiber dyeing process and determine a more sustainable strategy for achieving the same function that a specific auxiliary agent does. That would still require understanding of the dye reaction chemistry, chemical purpose of the auxiliary agent, and impacts of the dyeing process, but would have contained the scope to be more manageable for undergraduates.

Taking inspiration from the thought exercise above, below is an example of a general template that could be used, in part or in full, to guide students through a sustainable chemical design assignment.

1. **Posing an opening question:** What is the intended area of focus for this innovation? What should it do? What problem does it address?
2. **Identifying constraints:** Describe some of the relevant constraints (e.g., technical, economic, regulatory) that will influence the success of the chemical product.
3. **Assessing the current system landscape:** Construct a systems visualization to show the status quo, making sure to identify relevent boundaries and subsystems. What are some of the biggest sustainability challenges in this system? What sustainability impacts would a chemist be well-equipped to solve?
4. **Selecting an overarching goal:** Looking at the answers to question 3, specifically identify what systemic impacts this innovation can address, and where it may create new impacts.
5. **Beginning solution-design:** What chemistry is responsible for this innovation being able to perform its function?
6. **Describing chemistry strategies for approaching solution-design:** Draw the relevant molecular structures and annotate those structures to indicate interactions between molecules/atoms and describe what is happening. Use literature to predict the energetics of the underlying chemistry and methods to promote reactivity. Explain any constraints on this design.
7. **Communicating design guidelines:** Describe the general design guidelines that would allow another chemist to arrive at a solution similar to yours. Describe the underlying chemistry and scientific ideas. What conditions (e.g., concentration, temperature, pressure) or chemical properties are important for your design? What are the major benefits of your design and what are the anticipated impacts?

3.6 Conclusion and Future Directions

In summary, designing for sustainability requires a strong understanding of chemistry fundamentals as well as experience with systems thinking. The aim of this curriculum development project is to provide educational materials that can prepare students to develop those skills simultaneously during their first two years of chemistry in higher education. For too long green chemistry has been viewed as separate from the discipline of chemistry, and it is time we maximize the benefit of lower-level chemistry coursework by preparing the next generation of students to use their basic chemistry education to address sustainability challenges.

The modules developed from this project will be an important step towards preparing students to take action towards more sustainable practices. When looking at biological or Earth systems over long generational timelines, the effects of persistent or abundant chemicals remain nebulous. Long-term damage to these systems, in the forms of epigenetic changes and climate change, respectively, will likely be irreversible. Thus, it should be a top priority for scientists to develop more methods for assessing and mitigating these types of long-term impacts. Elucidating generational chemical effects will require far more interdisciplinary collaboration than is currently being practiced. What is really needed to understand the outcomes of chemicals are structured networks of subject matter experts (e.g., chemists, biologists, public health officials, toxicologists, ecologists, etc.) who regularly interface and share results across fields. Furthermore, efforts towards addressing issues of environmental justice require this same type of generational, multi-disciplinary analysis because many of the impacts associated with chemical injustices are legacy issues with deeply intertwined systemic effects.

Curriculum transformation efforts like this one will continue to influence the way science is conducted. While long-term outcomes typically remain elusive for new chemicals, teaching students approaches that minimize risk in the face of scientific uncertainty can help preclude unintended consequences and regrettable substitutions. With so many advances in technology over the past few decades there are more opportunities than ever for understanding and designing chemicals. Chemists can now use powerful tools and strategies such as computational modeling and rational design, nanoscale imaging, and automated high-throughput screening to innovate with more intention and speed than ever before. With these tools in hand, chemists are well-equipped to design new chemicals and processes that address global sustainability issues in need of immediate attention. It is the responsibility of educators to prepare and inspire the next generation of scientists to work towards solving these issues.

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