ACS Chemistry for Life®

Committee on Professional Training

Green Chemistry in the Curriculum

Context

Green chemistry principles provide bases for evaluating and designing new chemical products and processes that minimize adverse impacts on human and environmental health. Many undergraduate chemistry programs already implement green and sustainable chemistry concepts that have resulted in increased laboratory safety and decreased volume and toxicity of waste. This supplement suggests ways to integrate green chemistry strategies, concepts and practices throughout the chemistry curriculum. As a result, students develop the skills and vision that will enable them to contribute to a sustainable future through chemistry.

Conceptual Topics

Green chemistry leverages chemists' ability to design new beneficial/sustainable substances and processes while taking into account the interconnectedness with local and global systems. This approach, called **systems thinking**, is a problem-solving strategy that identifies and understands the key components of a system, in contrast to an isolated part, then investigates solutions based on the system interactions. Teaching a systems approach challenges students to apply scientific principles to solve real-world problems, demonstrates chemistry's role as an essential science in finding solutions, and prepares future scientists for the collaborative interdisciplinary work required. Integrating green chemistry into today's chemistry curriculum, and system thinking as we look to the future, can be accomplished by scaffolding in these **Conceptual Topics:**

- Continuing advances in chemistry research are integral to meeting society's essential needs of food, energy, and water in a sustainable path forward.
- Chemicals and chemical products provide many benefits to society; however, unintended consequences can negatively impact humankind and the earth. Green chemistry products and technologies have shown great potential for mitigating these impacts, some of which may disproportionately affect people of low socioeconomic status.
- The best approach to developing new chemical products and syntheses:
    - Is guided by the principles of green chemistry and life cycle thinking in order to minimize harm.
    - Employs molecular design for reduced hazards to the environment, health, and safety. It is a fundamental responsibility of chemists to design and synthesize safer chemicals.
    - Analyzes impacts throughout the lifecycle, from feedstock to end of final life using appropriate metrics.
    - Uses available knowledge and computational tools to design for function in concert with predicting hazards and environmental fate.
- Relationships between molecular structure and predicted properties such as metabolism, rates of chemical or biodegradation, and fate in the environment can be used for rational design of chemicals with reduced negative impact.
- Toxicology concepts expand a chemist's understanding of the relationship between structure and toxicity, and how exposure to chemicals, their degradation products and metabolites impact human and environmental health.

- Chemical risk is a function of hazard and exposure. In the past, risk management focused on strategies to reduce the exposure after it occurred. Incorporating green chemistry principles into risk management reduces the hazard before it occurs.
- Renewable feedstocks and alternative reaction media can be used to produce products with an improved sustainability profile.
- Increasing the efficiency and reducing energy requirements of synthesis, isolation, and purification operations can reduce the environmental impact of a process.

Practical Topics

Green chemistry can be used to illustrate many fundamental chemistry principles throughout the curriculum. Numerous opportunities exist to include experiments and demonstrations in addition to infusing green chemistry in lecture courses. A sampling of illustrative examples within each subdiscipline is described below.

General Chemistry

Illustrative examples include:

- The study of the periodic table can include the relative abundance and toxicity of elements and their uses in products such as electronics and cell phones.
- Balancing equations, stoichiometry, and classes of reactions can be used to contrast high and low atom economy and energy-efficient reactions, as well as metrics to assess the sustainability of a chemical product.
- Thermodynamics can provide a platform for discussing energy sources and current efforts to derive fuels from biomass and replace fossil fuels with renewable wind and solar energy.
- Laboratory experiments based on consumer products can emphasize the importance of science-based decisions in choosing safer products.
- Discussions of elements, ions, and chemical compounds can include chemical hazards and safety in the lab. For example, Cr^{3+} is relatively non-toxic whereas Cr^{6+} is a carcinogen.
- Physical properties such as polarity, solubility, and volatility can be discussed in the context of partitioning in the human body and the environment related to toxicity and transport.
- The study of the molecular shape and properties of gases such as CO_2, N_2O, CH_4 and O_3 can be tied to global warming potential.
- Teaching of skills such as number representations, graphing, and kinetic calculations can employ examples relating methods of assessing water quality, toxicity levels, and catalytic reactions.
- Life cycle thinking can be covered with topics such as the production of steel, renewable versus non-renewable polymers, and pharmaceuticals. A basic material and energy balance in the form of lists of inputs and outputs can be used to introduce the concept of life cycle inventory/assessment.
- Case studies can model the use of green chemistry and a systems thinking approach. Examples include the use of renewable soybeans in making foam mattresses or study of the Flint, Michigan water contamination event.

Analytical Chemistry

Illustrative examples include:

- The importance of accurate dose-effect relationships in evaluating the environmental and human health impacts of contaminants of emerging concern and their metabolites.
- The use of real-time and *in situ* analyses to improve the mass and energy efficiency of chemical production processes while reducing the amount and toxicity of waste.

- The use of: direct analysis (involving no sample preparation), miniaturized and/or assisted extractions, lower solvent volumes and less toxic solvents, and energy efficient methods to reduce the environmental impacts of analysis methods.
- The importance of analytical characterization of the composition, molecular mass, metal content, and stability of polymers in completing a life cycle assessment of these materials.

Biochemistry

Illustrative examples include:

- The differences between essential versus excessive chemical species. Iron in hemoglobin – necessary. Iron in vitamins – potentially toxic. Iron in the environment – hazardous under some conditions.
- Local and systemic toxicities caused by disturbances in the normal redox state of cells. Redox regulation may dictate enzyme activity.
- Use of synthetic biology to manipulate the sequence of chemical reactions/transformations that occur within the cell in the hope of producing a different outcome.
- Use of biosynthetic pathways and enzymatic (biopolymer) transformations to streamline syntheses of beneficial molecules occurring in water at 37^{o}C.
- Compare features of natural polyamides and polyesters to commercial materials made from non-renewable sources.
- The potential use of predictive toxicology based on key molecular initiating events (MIEs) and higher-level mechanisms of action to develop adverse outcome pathways (AOPs) to supplant conventional *in vivo* testing.
- The importance of a wide range of chemical and environmental exposures in driving epigenetic changes that can alter the physical structure of DNA and prevent genes from being expressed.

Inorganic Chemistry

Illustrative examples include:

- The classification of some metals and metalloids as critical or endangered due to geological abundance, geopolitical, and/or economic factors.
- Environmental impacts of ore extraction and processing.
- Evaluation of synthetic efficiency through the application of appropriate metrics (cost, atom efficiency, nature of the catalysts).
- Design of catalysts that are recyclable or recoverable and/or use earth abundant metals.
- The influence of speciation, particle size, particle morphology, and chemical similarity on the bioavailability and toxicity of metals in the environment.
- Metals can be both physiologically necessary and toxic depending upon the dose. Organismal mechanisms for the binding, transport, storage and excretion of metals to maintain beneficial concentrations.
- Centrality of inorganic materials to renewable energy technologies such as batteries, photovoltaics, thermoelectrics, and materials for artificial photosynthesis.
- The design of unique mechanically stable hybrid materials using biomimetic polymer/inorganic materials.
- Examination of the benefits and drawbacks of nanomaterials. Synthesis and utilization of nanomaterials in a more sustainable and environmentally benign manner.

Organic Chemistry

Illustrative examples include:

- Emphasize the importance of side products, catalysts and solvents when teaching reactions and mechanisms. Balancing organic chemical reactions and illustrating mechanisms as balanced elemental equations can improve conceptual understanding of reactivity, efficiency and production of waste by-products.
- The importance of chemical structure and particular functional groups on the function of a molecule, its toxicity and environmental impact.
- The importance of solvent selection or solvent-free systems in reducing waste and the hazards associated with a chemical process.
- The role of catalysts and bio-inspired chemistry in designing more efficient multistep syntheses to minimize the number of steps, use of protecting groups, and waste production while improving chemoselectivity, regioselectivity and stereoselectivity.
- Assessment of reaction efficiency through metrics of reagent costs, reaction selectivity, product yield and atom economy.
- Introduced the Environmental factor (e-factor) and Process Mass Intensity (PMI) for evaluating the material efficiency and environmental impact of a synthetic process.
- The use of green chemistry technologies to reduce the impacts of producing, using and disposing synthetic polymers through renewable monomer feedstocks and well-designed end of life fate (biodegradation, mechanical recycling, and chemical recycling).
- Relevant molecular mechanisms (i.e., S_N2, S_N2, acylation, Schiff Base formation, Michael Addition and S_NAr) explain how certain organic compounds can affect human health and the environment.
- Use a systems-thinking (defining the problem, identifying key system components, investigating solutions based on the system interactions) case study to examine the unintended consequences of an organic chemical (e.g., diesel fuel, Bisphenol A, thalidomide, DDT, brominated flame retardants, methyl isocyanate).
- Introduce the concept of Molecular Design: the application of green chemistry principles to optimize synthetic pathways and product design with minimum toxicity and maximum material/energy efficiency.

Physical Chemistry

Illustrative examples include:

- Use of boiling points, heat capacities, vapor pressure and explosivity limits in evaluating the environmental, health and safety outcomes of chemicals and chemical processes.
- Use of Gibbs free energy, enthalpy, and entropy to compare and contrast the efficiency of synthesizing compounds via covalent bond-forming methods versus supramolecular strategies involving non-covalent interactions.
- Use of thermodynamics and kinetics in understanding environmentally important reactions and improving the efficiency of chemical and/or bio-chemical reactions.
- Importance of chemical potential, partitioning and phase behavior in understanding human and environmental health impacts of chemicals, environmental fate and effects of chemicals, and chemical process sustainability.
- Application of computational and spectroscopic techniques to green chemistry-related concepts: designing environmentally friendly reaction conditions, polymerization kinetics, toxicity evaluation, and the study of gas phase molecules and solids present in the environment.

References and Resources

ACS Green Chemistry Institute. https://www.acs.org/content/acs/en/greenchemistry.html. Accessed July 2017.

ACS GCI Pharmaceutical Roundtable Process Mass Intensity (PMI) Calculator. https://www.acs.org/content/acs/en/greenchemistry/research-innovation/tools-for-green-chemistry.html. Accessed August 2017.

ACS Division of Organic Chemistry *Green Organic Chemistry Resources*. https://www.organicdivision.org/greenchemistry/. Accessed July 2017.

Anastas, P. J.; Warner, J. C. *Green Chemistry: Theory and Practice*; Oxford University Publishing: New York, 1998.

Anastas, P.; Eghbali, N. Green chemistry: principles and practice. *Chem. Soc. Rev.* **2010**, *39*, 301-312. (DOI: 10.1039/b918763b)

Andraos, J.; Dicks, A. P. Green chemistry teaching in higher education: a review of effective practices. *Chem. Educ. Res. Pract.* **2012**, *13*, 69–79. (DOI: 10.1039/C1RP90065J)

Beyond Benign. http://www.beyondbenign.org/. Accessed July 2017.

Burmeister, M.; Rauch, F.; Eilks, I. Education for sustainable development (ESD) and chemistry education. *Chem. Educ. Res. Pract.* **2012**, *13*, 59–68. (DOI: 10.1039/C1RP90060A)

Collins, T. J. Review of the twenty-three year evolution of the first university course in green chemistry: teaching future leaders how to create sustainable societies. *J. Clean. Prod.* **2017**, *140*, 93-110. (DOI: 10.1016/j.jclepro.2015.06.136)

Coish, P.; Brooks, B.W.; Gallagher, E.P.; Kavanagh, T.J.; Voutchkova-Kostal, A.; Zimmerman, J.B.; and Anastas, P.T. Current Status and Future Challenges in Molecular Design for Reduced Hazard. *ACS Sustainable Chem. Eng*., **2016**, *4* (11), 5900–5906. (DOI: 10.1021/acssuschemeng.6b02089)

de la Guaria, M; Garrigues, S., Eds. *Handbook of Green Analytical Chemistry*; John Wiley & Sons, Ltd, Chichester, UK, 2012.

Doxsee, K. M.; Hutchison, J. E. *Green Organic Chemistry: Strategies, Tools, and Laboratory Experiments*; Brooks/Cole, Cengage Learning. 2004

EPA Green Chemistry. https://www.epa.gov/greenchemistry. Accessed July 2017.

EPA (Presidential) Green Chemistry Challenge Winners. https://www.epa.gov/greenchemistry/presidential-green-chemistry-challenge-winners. Accessed July 2017.

Greener Education Materials for Chemists. (GEMs) http://greenchem.uoregon.edu/gems.html. Accessed July 2017.

Graedel, T. E.; Harper, E. M.; Nassar, N. T.; Nuss, P.; Reck, B. K. Criticality of metals and metalloids. *Proc. Natl. Acad. Sci. USA* **2015**, *112*, 4257-4262. (DOI: 10.1073/pnas.1500415112)

Jiménez-González, C.; Constable, D. J. C. *Green Chemistry and Engineering: A Practical Design Approach*; John Wiley & Sons, Inc. 2011.

Lasker, G.A.; Mellor, K.E.; Mullins, M.L.; Nesmith, S.M.; and Simcox, N.J. Social and Environmental Justice in the Chemistry Classroom. *J. Chem. Educ*. 2017, *94*, 983−987 (DOI: 10.1021/acs.jchemed.6b00968) http://pubs.acs.org/doi/pdfplus/10.1021/acs.jchemed.6b00968. Accessed August 2017.

Matlin, S. A.; Mehta, G.; Hopf, H.; Krief, A. One-world chemistry and systems thinking. *Nat. Chem.* **2016**, *8*, 393-398. (DOI: 10.1038/nchem.2498)

Meadows, D. H. *Thinking in Systems: A Primer*; Chelsea Green: White River Junction, VT, 2008.

Middlecamp, C. H.; Jorgensen, A. D., Eds. *Sustainability in the Chemistry Curriculum*; ACS Symposium Series 1087, American Chemical Society: Washington, DC, 2011.

Rational Molecular Design for Reduced Toxicity (ACS) https://www.acs.org/content/acs/en/greenchemistry/research-innovation/research-topics/rational-molecular-design-for-reduced-toxicity.html. Accessed July 2017.

Roesky, H. W.; Kennepohl, D. K., Eds. *Experiments in Green and Sustainable Chemistry*; Wiley VCH: Weinheim, 2009.

Zhu, Y. Q.; Romain, C.; Williams, C. K. Sustainable polymers from renewable resources. *Nature* **2016**, *540*, 354-362. doi:10.1038/nature2100.

Approved March 2018