ACS Sustainable Chemistry & Engineering

Editorial

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Advancing the Use of Sustainability Metrics

Now in its third year, ACS Sustainable Chemistry and Engineering (ACS SCE) continues to receive high-quality manuscripts in the areas of green chemistry, green engineering, and the grand challenges for sustainability in chemistry and chemical engineering. This includes the development and demonstration of renewable feedstocks, fuels, and materials that are less toxic and more sustainable than their functional equivalents. It also includes the development and demonstration of alternative processes and products that are more resource-efficient (in terms of conserving energy and feedstock) and more sustainable compared to conventional chemical processes and products.

In presenting their findings, ACS SCE authors generally justify the contributions of their work to the sustainability of the chemical enterprise by qualitatively invoking the principles of green chemistry[1] and green engineering[2] or other principles of sustainability.[3] This approach is encouraged and acceptable. Ultimately, however, such qualitative approaches will be complemented by rigorous, semiquantitative and quantitative sustainability assessments. These may include life cycle analyses, toxicity assessments, or other indicators of sustainability. More quantitative approaches to sustainability assessments can also help identify the key features to be improved to make a process or product sustainable, providing valuable guidance to further process or product development.

Articles published in ACS SCE and other journals[4−10] have described and applied such quantitative sustainability assessments, and the editors wish to encourage more authors to consider utilizing *quantitative sustainability metrics* in their submitted work. Toward this end, we offer suggestions and helpful tools and resources that are simple to use and hopefully add more value to manuscripts.

GUIDELINES FOR INCORPORATING SUSTAINABILITY METRICS

At the outset, we want to make it clear that ACS SCE will continue to accept manuscripts for review, with or without the inclusion of quantitative sustainability metrics, as we do now. We also continue to welcome contributions that describe new approaches to quantifying sustainability or that are entirely focused on novel and rigorous quantitative sustainability assessments based on life cycle,[11−15] supply chain,[16−20] or other concepts.[21,22] The guidelines provided here are meant to help authors use quantitative metrics, in an evolving process, to demonstrate how their research contribution advances sustainable chemistry or engineering.

Because of the broad scope of research described in ACS SCE, ranging in scale from new nanomaterial development, to process synthesis and analyses of regional or global scale material flows, the types of metrics used by ACS SCE authors will take a variety of forms. These may range from evaluations of the properties of individual chemicals (e.g., toxicity, persistence in the environment, efficiency in material synthesis, or the extent of use of renewable materials) to assessment of a variety of impacts along a supply chain. Although there is great diversity in the use of metrics, some common principles are emerging and these common principles have been described by ACS SCE authors. For example, in the first issue of ACS SCE, Russell and Shiang[4] described the sustainability metrics and sustainability tools used by a multinational chemical manufacturer. In Volume 2, Giraud et al.[5] described results of a survey conducted by the American Chemical Society's Green Chemistry Institute on the commercial use of the principles of Green Chemistry and the metrics used to quantify progress in applying those principles. Multiple tools are now available to assist researchers in applying quantitative metrics. For example, the iSUSTAIN tool[23] is a freely available tool for quantifying progress in the application of the principles of Green Chemistry. The United States Environmental Protection Agency (EPA) has developed and made available online tools that can be used to assess the environmental fate, bioaccumulation, and toxicity of chemicals.[24] New computational methods for property estimation, relevant to sustainability assessments, are continuing to develop. Data for supply chains and individual process steps along supply chains are also becoming available. Commercial and public domain Life Cycle Assessment software tools such as *SimaPro*, *GaBi*, and *GREET*[25−27] can serve as a resource for authors seeking to benchmark their concepts with current supply chains.

On the basis of these considerations, some general guidelines for authors wishing to incorporate quantitative metrics are as follows:

- Whenever possible, place the contribution in the context of the life cycle or supply chain of the relevant product, process, or chemical function. Although a quantitative life cycle assessment will be beyond the scope of most manuscripts, framing the paper's contribution in the context of product and process life cycles will be a valuable addition.
- Cite or briefly describe relevant property data such as environmental persistence or toxicity.
- In describing chemical pathways or processes, consider using metrics such as those associated with the principles of green chemistry, such as atom economy, mass efficiency, E-factor, C efficiency, emission rates, or others.
- When using well established sustainability metrics (e.g., atom economy), detailed methodological descriptions are not necessary; however, if novel metrics are used, the method of their calculation should be described in the manuscript or Supporting Information.
- Authors who incorporate quantitative sustainability metrics are encouraged to highlight their results in the Graphical Abstract.

Recognizing that the field of quantitative sustainability assessments continues to evolve, these guidelines will be periodically reviewed and updated to reflect current trends.

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In closing, we want to reiterate that the current initiative is to encourage authors to assess more critically their work from a sustainability viewpoint via quantitative assessments. We hope that such efforts would not only serve to advance the field but also bring to light sustainability challenges that are nonobvious, and thereby guide process and product development.

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Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

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