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Editorial

Expectations for Manuscripts Contributing to the Field of Solvents in *ACS Sustainable Chemistry & Engineering*

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The editorial aims of *ACS Sustainable Chemistry & Engineering* (*ACS SCE*) are to report and promote excellence and innovation in the rapidly evolving field of sustainable chemistry and engineering. Evolution can be described as an observable change in a system resulting from that system being strained or placed under an unusual condition. As we publish this editorial, society and the chemicals industry are under tremendous pressure; there is an ever pressing need to deliver more sustainable materials that are produced by cleaner, more efficient processes that have a minimized impact upon our environment. This editorial focuses on the role of solvent selection and use in minimizing impacts on the environment and human health.

Solvents are omnipresent in chemical transformations. Solvents operate on the cellular level as water, in the extraction of plant-based essential oils as perhaps supercritical carbon dioxide, or as more traditional organic solvents that find application in the production of a vast and expanding group of ever-critical molecules, ranging from pharmaceuticals to agrochemicals, sanitizers, and polymers. As scientists and engineers, we often overlook the subtle roles that a solvent plays in any chemical reaction, including, for example, being transiently involved in catalytic turnover, driving the removal of reaction byproducts to ensure efficiency, and enabling dynamic separations.

Solvents enable reactions. They regulate energy transfer. Hot solvents provide activation where needed, and cold solvents can suppress exothermicity by sinking energy from the delicate molecular dance, therefore bringing control. Critically, solvents must be recovered or separated from the product of any reaction or process. This is often achieved via classical separation methods, such as filtering a solid product after precipitation or separating immiscible liquids based upon buoyancy and density. Above all else, separation is dependent upon knowledge of the physicochemical properties of the solvent itself and applying them judiciously to deliver effect.

Any molecule could, in principle, be a solvent; however, with just a few moments of reflective thought, we can all imagine many reasons why most molecules would definitely not be applied as solvents. Molecules might be too expensive, too high boiling, too volatile, too reactive, or have unacceptable noxious odors or high toxicity to humans or other organisms. The list goes on *ad infinitum*. Now, place upon this thought experiment the additional requirements that the solvent is also sustainable, such that all atoms are derived from renewable feedstocks, and the number of synthetic steps to make the solvent is small. Rapidly, the challenge of identifying the most appropriate solvent becomes clear and consuming.[1]

So, how can we possibly propose a defined scope for research for our journal in this field? In trying to address this question, we have considered a number of specific goals, or drivers, that we hope reflect the nature of defining research questions in the field of solvents research. We hope that these guidelines stimulate thought, discussion, and debate, so that each of us can perhaps reflect as practitioners what types of molecules should be considered as sustainable solvents. Indeed, as a community, we should perhaps reflect upon excellent examples that frame the application of solvents in industry where the considered codification of solvent properties, environmental impacts, and toxicity has led to a series of straightforward solvent selection guides[2] that empower the chemist to make "on the spot" choices which can strongly influence the environmental impacts of solvent use.

However, applying a rigorous selection route that underpins a *sensible* choice of solvent may not automatically render the work suitable for publication in *ACS Sustainable Chemistry & Engineering*. Our scope is defined by the necessity to present new insight that will empower readers to adapt and learn. Examples of similar transformations or processes where the only adaptation is the nature of the solvent medium applied will be considered out of scope, unless the use of the new solvent substantially improves the sustainability of the transformation or process.

Classical definitions of sustainability suggest the following: A product or process should respond to a need in society. Delivery of the product or process should not disproportionally impact our environment. The process that delivers the product should be economically viable. Satisfying this so-called "triple bottom line" is nontrivial. In the context of solvents, we could imagine triple bottom line performance criteria that are as follows: (i) The solvent must enable a reaction/process to function in high efficiency to deliver a product of need. (ii) The impact of the life cycle of the solvent upon the environment and ecology should be negligible. (iii) The

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economic costs of the solvent (which can be seen as a surrogate of invested energy) should also be small.

Of course, upon first inspection, these "utopian" triple bottom line criteria seem insurmountable, and this may be true. However, they define a direction of travel and frame the nature of the manuscripts that we anticipate publishing in *ACS Sustainable Chemistry & Engineering*. These criteria set the pole star in the field of solvents-based research that all active scientists can see and move toward.

When considering appropriateness for publication, novelty is an important criterion, but it must not to be confused with uniqueness. One could argue that each time an experiment is performed it is under a unique set of conditions despite our best efforts to ensure reproducibility. If claimed novelty is limited to performance data that relate to an empirical change in raw material (perhaps a renewable), expansion of reaction scope, application of a new catalyst,[3] or screening of a different solvent (or class of solvents), then it is likely that the manuscript will fall out of scope.

It is the responsibility of the authors to present a convincing argument that an advance in green and sustainable chemistry has been achieved. The most likely outcome is that sustainable gains have not been accomplished in all three aspects of the adapted triple bottom line for solvents; however, intelligent application of sustainability metrics that enable evidenced comparisons to be made will certainly help to make the case.[4] While this can often lead to challenging and complex debate, we firmly believe that authors, with their first-hand knowledge of experimental design and expert opinion on the scientific landscape in which the new manuscript sits, are best placed to convince others of any sustainability advance.

While it is not possible to explicitly state which green solvent-based contributions fall within the scope of our journal, the aim of this editorial is *not* to outlaw any specific classes of solvents, e.g., room temperature ionic liquids, deep eutectics, supercritical fluids, gas expanded liquids, terpenes, and other renewable-based solvents, switchable media, or water. ***It is recognized that all classes of solvents can contribute to advances in the sustainability*** of a product or a process. We do, however, offer advice in this editorial on the types of manuscripts that are often considered as unsuitable for publication in *ACS SCE*.

Recognizing that a primary driver of sustainable chemistry and engineering is the opportunity to deliver impact at scale, the editors of *ACS SCE* believe that claims of improvements in sustainability, based upon solvent selection or manipulation, should be underpinned by the evaluation of the applicability of the solvent at scale. Truly sustainable solvents should be readily available and require minimal investment of energy during their isolation and/or preparation. *ACS SCE will not* consider publication of manuscripts based upon the small-scale application of newly acclaimed solvents unless viability for scale-up is considered. As guidance, we suggest that newly reported solvents that demand in excess of 10 steps/unit operations in their preparation from raw materials require either the demonstration of disruptive performance benefits or access to unique reaction outcomes that cannot be obtained using other solvent types.

ACS SCE will not consider publication of manuscripts that report the incremental variation of solvents and/or conditions to optimize well-studied processes in terms of productivity alone. Similarly, the empirical application of greener solvent media to the systematic extraction of natural products from niche biomass sources will be considered out of scope unless the manuscript includes fundamental new insights that have been learned during the design and execution of the study. In the absence of fully justified comparisons to current state-of-the-art processes, which are evidenced by appropriate metrics that explore efficiency in terms of energy resilience, atom efficiency, and evaluation of waste streams and other indirect impacts including to toxicology, manuscripts reporting incremental work will not be considered by our peer review process.

To summarize, we can imagine an infinitely large number of experiments that explore the impact of solvents on a wide range of processes, yet this does not mean that they are equal in terms of their scientific contribution. Solvents are an intrinsic component of most processes, and their impacts are significant. The search for cleaner, more sustainable solvents will always be an art of balancing tensions. The goal of solvents research should be the identification of the "most appropriate" solvent for any given process, and this may well be the solvent that is applied right now. As a community, we must not be afraid to acknowledge this. *ACS SCE* aims to publish high impact manuscripts that address all aspects of the adapted triple bottom line for solvents giving rise to robust, energetically sensible, and environmentally sustainable solutions. We hope that this editorial provokes thought and stimulates activity in the search and demonstration of appropriate solutions.

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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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