

Journal of Chemical & Engineering Data: An Update from the Editorial Team

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Accurate, precise, and reproducible thermophysical data have been, and will continue to be, pivotal for advancing the chemical sciences and addressing research needs with broad societal impact. High-quality thermophysical data enable, to name a few, energy-efficient and sustainable chemical production, capture of contaminants from air and water, and high-performance working fluids. For the past 65 years, *Journal of Chemical & Engineering Data* (JCED) has played a prominent role in the curation and dissemination of thermophysical data.

The beginning of 2021 marks a transition for JCED's Editorial Team, and in this first editorial of the year, we would like to thank Joan F. Brennecke (University of Texas at Austin) for her 10 years of dedicated service leading *Journal of Chemical & Engineering Data* as Editor-in-Chief. Under Joan's expert stewardship, the *Journal* has maintained its emphasis on high-quality thermophysical data in partnership with the NIST Thermodynamics Research Center, welcomed more contributions from molecular modeling and simulation, showcased the varied directions of thermophysical property research, and helped to celebrate the diversity of researchers in the field. The thermophysical properties community is fortunate to have Joan as one of its champions!

We would also like to express our sincere appreciation to outgoing Associate Editors Maaik Kroon (Khalifa University of Science and Technology) and Paul Mathias (Fluor Corporation) who, for many years, have shepherded innumerable manuscripts through the peer review process and provided valuable guidance to authors and reviewers.

Ilja Siepmann (University of Minnesota) transitions from Associate Editor (2015–2020) to the Editor-in-Chief role, while Ramesh Gardas (Indian Institute of Technology Madras), Ronny Pini (Imperial College London), and Cara Schwarz (Stellenbosch University) are welcomed to JCED's Editorial Team together with David Kofke (University at Buffalo), Gabriele Sadowski (TU Dortmund), and Jiangtao Wu (Xi'an Jiaotong University) (Figure 1).

Here, we would like to alert the reader to three updates as JCED begins 2021:

- (1) To elevate the thermophysical data field, JCED strongly encourages manuscripts that report on *consequential* (relevant, comprehensive, and robust) data and place these data into context by addressing what can be learned from differences and similarities to prior published data on related systems (see also updated *Journal Scope*).

- (2) The *Journal's* cover has a different look! We encourage JCED's authors to design eye-catching and informative cover art (for front and supplementary cover opportunities) that will help to change perceptions and contribute to the growth of the thermophysical data community.
- (3) The *Journal's* scope (<https://pubs.acs.org/page/jceaax/about.html>) has been updated with this first issue to be more explicit on the topical areas and on the scientific approaches that fall within JCED's scope.

SCOPE

Journal of Chemical & Engineering Data is a monthly journal devoted to the publication of data obtained from both experiment and computation, which are viewed as complementary. It is the only American Chemical Society journal primarily concerned with articles containing data on the phase behavior and the physical, thermodynamic, and transport properties of well-defined materials, including complex mixtures of known compositions. *Journal of Chemical & Engineering Data* encourages manuscripts that report on consequential (relevant, comprehensive, and robust) data and place these data into context by addressing what can be learned from differences and similarities to prior published data on related systems.

Topical areas considered in this *Journal* include vapor–liquid and supercritical fluid equilibria, liquid–liquid and vapor–liquid–liquid equilibria, solubility of solids, adsorption equilibria, gas hydrates, phase equilibria with amphiphiles, thermophysical properties including transport, and calorimetric properties.

While environmental and biological samples are of interest, their compositions must be known and reproducible. As a result, adsorption on natural product materials does not generally fit within the scope of *Journal of Chemical & Engineering Data*. While phase equilibria involving reaction and transport properties are of interest, reaction kinetics or adsorption kinetics do not generally fit within the scope of *Journal of Chemical & Engineering Data*.

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Figure 1. JCED Editorial Team from January 2021 (top left to bottom right): J. Ilja Siepmann (Editor-in-Chief), Ramesh L. Gardas (Associate Editor), David Kofke (Associate Editor), Ronny Pini (Associate Editor), Gabriele Sadowski (Associate Editor), Cara Schwarz (Associate Editor), and Jiangtao Wu (Associate Editor).

The scope of this *Journal* also includes phase behavior and thermophysical properties obtained from quantum chemistry, molecular simulation, and molecular mechanics calculations. The reported data must be an observable property in these calculations via a statistical-mechanical approach. As a result, calculations that relate a molecular property to thermophysical data via a correlation do not generally fit within the scope of *Journal of Chemical & Engineering Data*.

Reviews of experimental or computational techniques are encouraged, and these are not required to include new data.

Journal of Chemical & Engineering Data publishes Articles and Reviews. In addition, Comments and Additions and Corrections are published. The decision to publish a manuscript and the type it will appear as rests solely with the Editor.

We look forward to serving the thermophysical properties community with great enthusiasm.

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Notes

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