Fifty Years of Reference Data

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The year 2021 marks the 50th year of publication for the Journal of Physical and Chemical Reference Data (JPCRD). JPCRD is a joint effort between the National Institute of Standards and Technology (NIST, which prior to 1988 was the National Bureau of Standards, NBS) and the American Institute of Physics (AIP). Today, NIST provides editorial expertise while the publication process is ably handled by AIP Publishing.

We are privileged to have an Editorial in this issue from David Lide, the founding Editor of JPCRD. Dr. Lide became the head of the NBS Standard Reference Data program in 1969 and quickly recognized that a more visible dissemination outlet was needed than the government-printed reports then being issued by NBS. This led to the launch of JPCRD, which began with Vol. 1 in 1972. David Lide shepherded JPCRD for its first two decades, retiring from the Editorship in 1993. He has continued to make significant contributions to the field of reference data since that time, most notably as Editor for many years of the CRC Handbook of Chemistry and Physics and as Secretary General and President of the Committee on Data for Science and Technology (CODATA) of the International Council of Scientific Unions.

Jean Gallagher was Editor from 1993 until her death in 1996. Malcolm Chase then served for over a decade, including for several years after his official retirement from NIST. The present Editors took the reins in 2008. During these years, we have been supported by management in the NIST Standard Reference Data office, including Robert Watters and now Adam Morey. In the years before manuscripts were processed electronically, other NIST staff provided invaluable clerical support; the last person in that role was Diane Decker. We also benefit from an Editorial Board, which currently has 8 members, some within NIST and some outside, representing a wide range of specialties and data contexts. The staff of AIP Publishing continues to be essential to the success of the journal.

The first paper in JPCRD was a 116-page (!) critical evaluation of data for binary diffusion coefficients of dilute gases, which has been cited approximately 700 times. Comprehensive, impactful articles have continued to be a feature of the Journal; the most cited paper (with over 7000 citations) is a 1988 chemical kinetics paper that reviewed rate constants for hydrated electrons, hydrogen atoms, and hydroxyl radicals in aqueous solution, and the next two spots on the list (with over 2500 citations each) belong to standard reference equations of state for the important fluids carbon dioxide and water. Our list of most downloaded articles since 2017 is similar, with an appearance also from the article reporting the periodic CODATA adjustment of recommended values for fundamental physical constants (we expect to publish the next CODATA article in 2021).

Formal and informal connections to ongoing data evaluation and standards efforts have provided much journal content. Since 1998, JPCRD has cooperated with the International Union of Pure and Applied Chemistry (IUPAC) to publish the IUPAC-NIST Solubility Data Series, resulting in about 75 publications during that period. A short overview of the IUPAC-NIST Solubility Data Series was provided in 2010. JPCRD has also been the venue of choice for most of the standard thermophysical property formulations developed by the International Association for the Properties of Water and Steam (IAPWS). Another major field has been evaluated gas-phase kinetic data for both atmospheric and combustion chemistry. Over the years, JPCRD has published about 35 of these evaluations by international committees, and the top 10 articles have each received on average 1007 citations. A citation half-life on the order of 30 years in many cases attests to the long-term value of these articles. JPCRD has also published about 100 articles with thermochemical data and a similar number with atomic energy levels (and related data). The latter set of articles has fed data into the internationally employed NIST Atomic Spectra Database (NIST Standard Reference Database 78).

The scope of JPCRD is unique among journals and is sometimes a source of confusion. The domain of science covered is, as the name
suggests, physics and chemistry, broadly defined to include areas such as materials science, atmospheric science, and biochemistry. However, within this broad domain, most original experimental and theoretical work is outside our scope because it does not produce “reference data.” For purposes of the Journal, reference data are not merely “good data”; the phrase refers to critical evaluation of all available information, producing recommendations for the best available data in a particular area (say, the viscosity of toluene or the rovibrational spectrum of water), preferably with uncertainty analysis. These recommendations might be in the form of a correlation or in the form of discrete recommended values, as appropriate to the area evaluated.

In 2018, the Scope was expanded to include Review Articles, which might describe and document a reference database, review the data situation in a particular field, provide an overview of a series of JPCRD articles, review reference-quality measurement techniques, or review data evaluation methods. The first paper published in this new category was a review of reference values and correlations for the viscosity and thermal conductivity of important pure fluids. For Vol. 50, we have commissioned several special “50th anniversary reviews,” representing some of the key areas that have contributed content to JPCRD over the years.

The scope was expanded slightly further in 2019. We now publish selected experimental or theoretical results if they are the state of the art for the property measured or calculated, have thorough uncertainty analysis, and have significant application outside their immediate context, for example, as a reference for calibrations. An example is a painstaking measurement of the Gross Calorific Value of methane, which is an important reference in the natural gas industry. As we look to the future, we would highlight two trends. The first is that, in order to be useful in the 21st century, data should preferably be online rather than on printed pages (or simple PDF files). We are exploring ways to make electronic data associated with our articles more available and discoverable, and also continue to offer JPCRD as a vehicle for publishing articles that document electronic databases maintained elsewhere.

The second trend is related. As more data appear online, scientists and engineers looking for “data” are likely to turn to a search engine and use whatever number comes up first in a free source. As in many other areas, the quality of what is available on the internet varies widely, and the non-expert may not be able to assess the reliability of information. In this new world where high-quality data may be drowned out by a flood of mediocre data (and values from estimation techniques that are often applied outside their ranges of validity), critical data evaluation by experts is more important than ever. We hope JPCRD can continue to be a place where scientists and engineers can turn to be guided to data that are well-documented and of the best available quality—in other words, reference data.

References