High-Accuracy Equations of State – Continued Progress Through Art + Science

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Multi-parameter, fundamental equations of state (EOS) based on Helmholtz energy provide the most accurate description of fluid thermodynamic properties. The demand for such EOS is evident from the many literature citations, both to the papers describing a particular Helmholtz EOS and to database packages that implement these EOS for multiple fluids. The development of high-accuracy Helmholtz EOS is as much art as science and has been mastered by only a few; lengthy training is required for any new apprentice wanting to work in this field. As a result, long development times are the norm, and only a limited number of new EOS are published each year. Given the high demand from science and industry for additional fluids, the goal must be to make this high-level equation development more accessible so that high-accuracy EOS can be generated in a shorter time.

This leads to the provocative question: Where do we go from here? In this commentary, we point out possible solutions; while some may be naïve, we put them forward to stimulate discussion. One element will certainly be the transparent documentation of existing methods. Continued insights into the proper form of Helmholtz EOS (considering extrapolation behavior, proper representation of virials, ideal curves, etc.) will come from the EOS "masters" working with data sets of the highest quality. However, modern machine-learning approaches to regression analysis must also be considered. In addition, new approaches to planning measurement campaigns must also be pursued in experimental thermophysical property research. The "art" of EOS fitting has revealed that large quantities of experimental data are not required—instead, selected data with low measurement uncertainty have the highest information content for equation development. What is the optimum data set? Here, once again, mathematical methods, such as Optimal Experimental Design, can play an important role.