Integration of Data and Models in the ThermoData Engine Software

Vladimir Diky[1, S, C], J. Richard Elliott[2], David Parkhurst[3], D. Kirk Nordstrom[4] and Ala Bazyleva[1]

[1]*NIST, Boulder, CO, U.S.A.*
[2]*University of Akron, Akron, OH, U.S.A.*
[3]*ObjectiveGeochemistry, LLC, Lakewood, CO, U.S.A.*
[4]*U.S. Geological Survey, Denver, CO, U.S.A.*
diky@nist.gov

Studies of thermophysical properties of substances and materials have a long history and continue to expand due to new applications and new methods for old applications. In many cases, properties are needed for entirely new compounds as evidenced by recent work on ionic liquids and metal organic frameworks. The scope of conceivable compounds and properties of interest often exceeds the ability to experimentally measure all properties, necessitating correlation and prediction methods. Each research specialty is typically focused on a narrow range of materials, methods, and models, but both practitioners and researchers need to access an increasing range of data and models. How can one data interface provide current and rigorous models of so much specialized and evolving expertise? To provide a better service, the ability to use externally developed mathematical models has been added to TRC/NIST ThermoData Engine (TDE) software [1].

TDE combines a computation engine, database of experimental data, and a user interface to access the data, provide model-parameter fitting and analysis of model-data consistency. Traditionally, adding support of a model to TDE required re-implementation of that model in the C++ programming language. An exception was NIST REFPROP [2], which is provided by its developers as a dynamically linked library (DLL) with an application programming interface (API) specific to REFPROP. Expanding on the REFPROP approach, the next step of TDE development is the development of a unified API to access external components implementing mathematical models for thermophysical properties, including equations of state (EOS) for pure compounds and mixtures and activity-coefficient models for mixtures. The API includes the capability to query for available property data for compounds and mixtures and methods to call models to calculate properties. If calculation of derived properties (such as vapor pressure or solubility) is supported, it is directly called; otherwise, calculations based on fugacity or activity coefficients are done by TDE. Model parameter fitting to the data available to TDE can also be done. This technique was successfully applied to the modeling package related to the 6th edition of "The Properties of Gases and Liquids" (PGL) [3] and to the United States Geological Survey's PHREEQC program for aqueous electrolyte solutions [4]. Similar DLLs can be created and run by TDE users without participation of the TDE developers. Publicly available and proprietary data in formats not supported by TDE can be accessed using import/export filters also implemented as DLLs. These developments should save experts' time and facilitate collaboration in the development of models for thermophysical properties. To illustrate how this capability can be shared broadly, examples are described of the necessary handshaking codes to implement the models for PGL and PHREEQC.

References

1. Vladimir Diky, Robert D. Chirico, Michael Frenkel, Ala Bazyleva, Joe W. Magee, Eugene Paulechka, Andrei Kazakov, Eric W. Lemmon, Chris D. Muzny, Alexander Y. Smolyanitsky, Scott Townsend, and Kenneth Kroenlein. NIST ThermoData Engine, NIST Standard Reference Database 103a/103b, version 10.4.5. NIST, Standard Reference Data Program: Gaithersburg, MD, 2023.
2. REFPROP. NIST Standard Reference Database 23. https://www.nist.gov/srd/refprop
3. J. Richard Elliott, Vladimir Diky, Thomas A. Knotts IV, W. Vincent Wilding. *The Properties of Gases and Liquids*, Sixth Edition. McGraw-Hill: NY, USA. (2023)
4. PHREEQC. https://www.usgs.gov/software/phreeqc-version-3