NIST ThermoData Engine Software for a Wide Range of Users

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The ThermoData Engine (TDE), developed by the NIST Thermodynamics Research Center, is software for validation, analysis, and representation with equations of thermophysical and thermochemical properties for pure compounds and mixtures needed by chemical engineers and researchers. Depending on the user's needs, TDE can provide a variety of functions at different levels of sophistication. Traditional functions include access to raw experimental data, reviewing data scatter, and automated property data evaluation involving literature (from the property database) and/or user's experimental data as well as predictions if necessary. The built-in database contains more than 6.3 million primary experimental property data values and is constantly amended with newly published and historical data as well as repeated data quality assessment with the use of additional information and methods. In addition to the tradition single-button one-system evaluation, TDE can be used for validation of new data, checking thermodynamic consistency of different properties, analysis of trends in compound series, comparison of models, validation of user's models (equations), and expert-mode refinement of models and special property calculations. All that functionality will be shown with examples illustrating application of TDE to solving several scientific and practical tasks.