

NIST ThermoData Engine (TDE) Software for a Wide Range of Applications: Current State and Development Opportunities

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ThermoData Engine (TDE), developed by the NIST Thermodynamics Research Center, is software for validation, analysis, and modeling of thermophysical and thermochemical properties for pure compounds and mixtures needed by chemical engineers and researchers. Depending on user's needs, TDE can provide a variety of functions at different levels of sophistication. Traditional functions include access to well-structured raw experimental data 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 property database currently contains more than 8.7 million primary experimental property data values (for approximately 29,000 pure compounds, 79,000 binary mixtures, 25,000 ternary mixtures, and 8,200 chemical reactions) and about 5,600 enthalpies of formation from high-level quantum-chemical calculations. The database is constantly amended with newly published and historical data. A continuous data quality assessment with the use of additional information and methods is performed in the database. TDE provides access to NIST REFPROP models and supports several equations of state for pure compounds (original and modified volume-translated Peng-Robinson, Sanchez-Lacombe, PC-SAFT, and Span-Wagner EOS). For mixtures, users can access predictive models such as COSMO-SAC and various versions of UNIFAC or fit several activity-coefficient models (NRTL, UNIQUAC, Wilson, and Redlich-Kister models). The present version also allows analysis of trends in compound series and comparison of different models.

Public version 10.4.5 of the TDE software will be shown on examples covering different TDE features. Potential new functionalities (checking thermodynamic consistency of different properties, validation of user's models and equations, expert-mode refinement of models and special property calculations, stepwise evaluation, additional models and equations, and wider comparison capabilities) illustrating application of TDE to solving several advanced scientific and practical tasks will also be demonstrated.