

Thermodata Engine: Critically Evaluated Data on Demand

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ThermoData Engine (TDE) is the first implementation of the Dynamic Data Evaluation concept, which allows immediate evaluation of thermophysical and thermochemical properties when the need occurs or when data become available. TDE contains a large database of experimental property data (called TDE-SOURCE) and provides completely automated evaluation of thermophysical properties using necessary assessments and predictions. Version 1.0 has been released that covers pure chemical compounds. Current development includes fitting equations of state (EOS), database updates via Internet, and the inclusion of binary mixture data. The upcoming version 2.0 database will provide users the possibility to build short Span-Wagner equations of state as well as certain other pure-compound equations of state, which can be used in process simulation. Quarterly database Web-updates will make the data evaluation on the user's end truly dynamic by providing newly published data every few months and allowing immediate reevaluation of the affected systems. Automated data evaluation for binary mixtures will be provided in version 3. The elements of version 3, which is currently under development, are used in the data entry process at the NIST Thermodynamics Research Center (TRC) for validation and checking of newly entered data under strict data quality assurance guidance.