ThermoData Engine: New Generation Expert System for Thermodynamic Data Critical Evaluation

Traditionally, critical data evaluation is an extremely time- and resource-consuming process, which includes extensive labor in data collection, data mining, analysis, fitting, etc. Because of this, it must be performed far in advance of a need within an industrial or scientific application. This type of slow and inflexible critical data evaluation can be defined as 'static.' These shortcomings have become magnified dramatically within the last 5 to 10 years due to the significant increase in the rate of publication of experimental and predicted thermodynamic data. This new information ideally needs to be considered to assure the robustness of the values recommended from a critical evaluation. To address the weaknesses of 'static" evaluations, the concept of a dynamic data evaluation system was developed at the Thermodynamics Research Center (now NIST's TRC Group).

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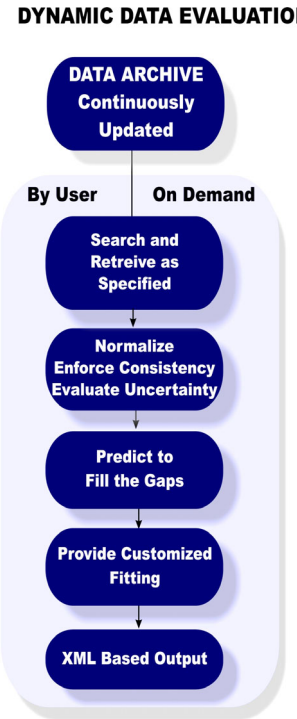
A dynamic data evaluation system requires large electronic databases containing essentially all experimental data known to date with detailed descriptions of relevant metadata and uncertainties; these are characteristics of the NIST/TRC SOURCE database.

The combination of electronic databases with expert-system software, designed to automatically generate recommended values, leads to the ability to produce critically evaluated data dynamically or "to order", in sharp contrast to conventional static evaluations.



The dynamic data evaluation process dramatically reduces the effort and costs associated with anticipating future needs and keeping evaluations current. In addition, critically evaluated data produced by expert-system software can rigorously be characterized with uncertainty assessments; as a result, changes in input data uncertainties, either real or hypothesized, can be readily propagated to the final values. This, in turn, provides the ability to assess the impact of data-quality limits on all aspects of chemical process design.

The key characteristics of SOURCE that support "Dynamic Data Evaluation" are: (1) it is comprehensive and current; (2) the data are consistent with the applicable physical laws and subject to numerous quality control steps; and (3) the data uncertainties are assigned on the basis of robust and internally consistent algorithms. The key elements for creation of the expert evaluation system are: (1) development of algorithms and computer codes to capture the science in the "art" of data evaluation; (2) development of algorithms to implement, target, and apply prediction methods depending on the nature of the chemical system and property, including automatic chemical structure recognition mechanisms; and (3) development of procedures allowing generation of output for the occasional user (including graphical representations) and in a format suitable for both common desk top application as well as for major commercial chemical-process design simulators. The key functionalities are illustrated in the figure.

The ThermoData Engine (TDE) software incorporates all major stages of the concept implementation including data retrieval, grouping, normalization, sorting, consistency enforcement, fitting, and prediction. The SOURCE data system is used in conjunction with TDE as the comprehensive storage facility for experimental thermophysical and thermochemical property data. In addition the NIST/TRC Ideal Gas Database is used as a source of thermodynamic property data in the ideal-gas state.

NIST recently released Version 1.0 NIST Standard Reference Database 103.

This version is limited to thermodynamic properties of pure compounds. The software architecture emphasizes enforcement of consistency between related properties (including those obtained from predictions), assumes an imperfect source of original data, provides for flexibility in selection of default data models depending on the particular data scenario, incorporates a large variety of models for secondary fit-

ting, and allows saving of critically evaluated data in the ThermoML format. The latter assures compatibility of the TDE software with any engineering application equipped with a ThermoML software "reader".

NIST has reached an agreement with a number of industrial organizations about "bundling" TDE, version 1.0, to their chemical process engineering software, so that TDE would serve as a source of critically evaluated thermophysical property data for pure compounds in the "bundled" products. We plan to further expand this cooperation to other industrial and governmental organizations.

Future Plans

TDE 2.0 beta-version will be developed in FY06. This version will include incorporation of the computational tools for generating equations of state such as the 12-parameter Helmholtz equation, the PC-SAFT equation, and the Peng-Robinson equation on demand, depending on the data "scenario". It will also contain a capability of updating the TDE-SOURCE database using recently developed Web-Oracle dissemination infrastructure. Longer-term plans include expansion of TDE to critical data evaluation for binary mixtures.

References

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