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

NIST has developed a dynamic data evaluation system to help address shortcomings that have emerged with the current "static" and time-consuming methods of data collection and evaluation that involve highly skilled data experts. The NIST system uses expert system software, that leads to the ability to produce critically evaluated data "on demand" and "to order".

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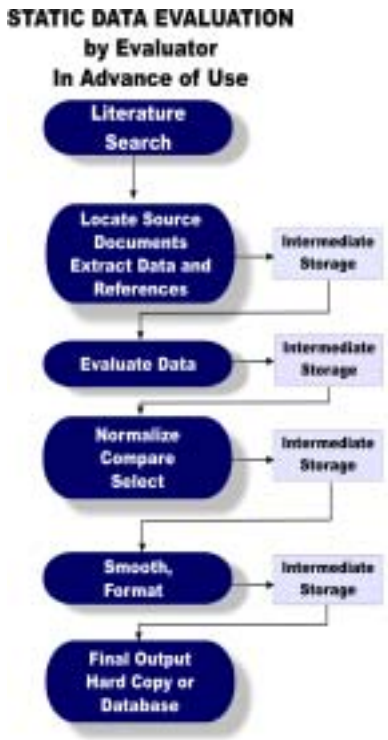
Traditionally, critical data evaluation is an extremely time- and resource-consuming process, which includes extensive use of labor in data collection, data mining, analysis, fitting, *etc*. Because of this, it must be performed far in advance of a need within an industrial or scientific application. In addition, it is quite common that by the time the critical data-evaluation process for a particular chemical system or property group is complete (sometimes after years of data evaluation projects involving highly skilled data experts), it must be reinitiated because significant new data have become available. 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 which need to be analyzed during the critical data evaluation process.

To address the weaknesses of 'static" evaluations, NIST developed the concept of a dynamic data evaluation system. This concept requires large electronic databases capable of storing essentially all experimental data known to date with detailed descriptions of relevant metadata and uncertainties. The combination of these electronic databases with expert-system software, designed to automatically generate recommended data based on available experimental data, leads to the ability to produce critically evaluated data dynamically or "to order" as shown in the schematic diagram. This concept contrasts sharply with static critical data evaluation, which must be initiated far in advance of a particular need.



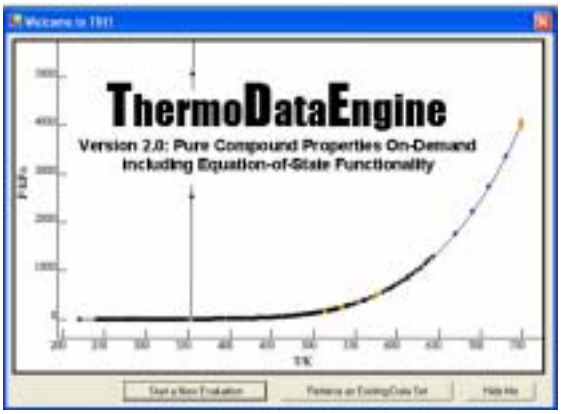
The dynamic data evaluation process dramatically reduces the effort and costs associated with anticipating future needs and keeping static evaluations current.

Critically evaluated data produced by the deployment of the dynamic data-evaluation concept can rigorously be characterized with their quality assessments. That, in turn, provides the ability to propagate reliable data-quality limits to all aspects of chemical process design. Implementation of the dynamic data evaluation concept consists of the solution of a number of major tasks: (1) design and development of a comprehensive database system structure based on the principles of physical chemistry and capable of supporting a large-scale data entry operation for the complete set of thermophysical, thermochemical, and transport properties for chemical systems including pure compounds, binary mixtures, ternary mixtures, and chemical reactions; (2) development of software tools for automation of the data-entry process with robust and internally-consistent mechanisms for automatic assessments of data uncertainty; (3) design and development of algorithms and software tools to assure quality control at all stages of data entry and analysis; (4) development of algorithms and computer codes to implement the stages of the dynamic data-evaluation concept; (5) 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 (6) development of procedures allowing

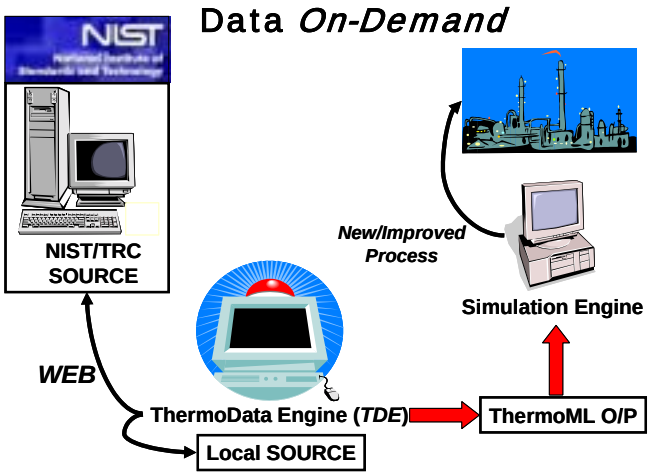
generation of output in a format suitable for application in major commercial simulation engines for chemical-process design.

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.

In FY05, version 2.0 was released *via* NIST Standard Reference Data Office (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 fitting, 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.' New version has two new principal features: (1) the ability to generate equations of state (EOS) on-demand depending on the data scenario (there are 4 types of EOS incorporated) and (2) provision for periodic updates of the local TDE-SOURCE database that "feeds" TDE via the Web.



NIST has reached an agreement with a number of industrial organizations about 'bundling' TDE, version 2.0, 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 (see figure 3) providing principally new opportunities of chemical process design on-demand. One example of such cooperation is a new technology incorporated in the 2006 version of the ASPEN PLUS™ process simulation engine developed as a result of the cooperative effort between NIST and Aspen Technology, Inc. In 2006 this technology has become available to 45,000 corporate users. It is currently planned to further expand this cooperation to other industrial and governmental organizations.



NIST plans to develop TDE 3.0 beta-version in FY07. This version will include incorporation expansion of TDE to critical data evaluation for binary mixtures as well thermodynamic properties of the formation reactions.

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