NIST/TRC Databases and Software Tools for Chemistry and Engineering

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The NIST Thermodynamic Research Center (NIST/TRC) is one of the oldest data research centers in the United States. For over 60 years of its history, TRC has produced a number of the periodical compilations and electronic databases that have become a major source of recommended data for scientific research and industrial process design, for both pure materials and mixtures.

The first software product implementing the dynamic data evaluation concept was developed – NIST ThermoData Engine (NIST Standard Reference Database 103). This concept requires the development of large electronic databases capable of storing essentially all 'raw' experimental data known to date with detailed descriptions of relevant metadata and uncertainties. The combination of these databases with expert software designed primarily to generate recommended data based on the available experimental data and their uncertainties leads to the possibility of producing data compilations automatically 'to order', forming a dynamic data infrastructure.

Recently, IUPAC Ionic Liquids Database, ILThermo - a free web research tool - has been developed. ILThermo allows users worldwide to access an up-to-date data collection from the publications on experimental studies of thermodynamic and transport properties of ionic liquids as well as binary and ternary mixtures containing ionic liquids.

Efficient and reliable data dissemination has been one of the drivers for the development of ThermoML - a new IUPAC XML-based standard format for data storage and exchange. NIST/TRC is currently partnering with five major journals to encourage authors to submit their data for validation as part of the publication process. As part of this cooperation, the Guided Data Capture software (GDC) has been developed guiding authors through the process of data submission. The functional features of the GDC as well as ThermoML archive publicly available from the NIST/TRC Web site will be demonstrated.

Amongst others, the following PC stand-alone databases will be demonstrated, also.

- NIST/TRC Table Database (NIST Standard Reference Database 85)
  This database, known as WinTable, is designed to retrieve and display recommended property values of pure compounds and is essentially the electronic version of the TRC Tables-Hydrocarbons and the TRC Tables-Non-Hydrocarbons which have been compiled by the Thermodynamics Research Center (TRC) for more than 50 years.
- NIST/TRC Vapor Pressure Database (NIST Standard Reference Database 87)
  The software calculates vapor pressures using the stored values of the parameters of the Antoine equation or the extended Antoine equation and displays tables for approximately 6,000 pure compounds.
- NIST/TRC Ideal Gas Database (NIST Standard Reference Database 88)
  This database provides information on the most important thermodynamic properties (heat capacities, entropies, enthalpies, Gibbs free energies and enthalpies and Gibbs free energies of formation) of organic and some other compounds in the ideal gas state. There is a total of more than 2000 compounds.