



Integration of NIST Chemical Property Database in aspenONE[®] Engineering

An Executive Summary

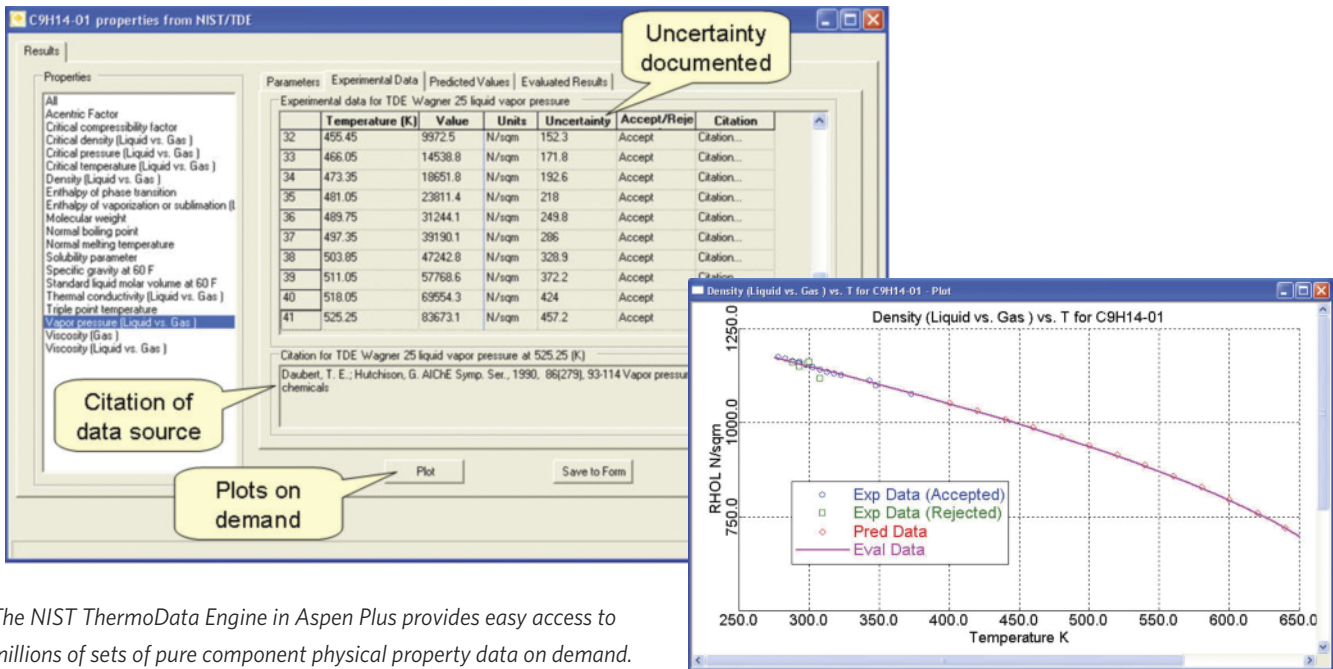
On July 20, 2009, Aspen Technology Inc. and the US National Institute of Standards and Technology (NIST) jointly received an *R&D 100* award for their collaborative development to include NIST data and technology in aspenONE Engineering V2006.5.

Winning an R&D 100 Award demonstrates a mark of excellence known to industry, government, and academia that the product is one of the most innovative ideas of the year. Since 1963, the R&D 100 Awards have honored such revolutionary technologies as the fax machine (1975), the liquid crystal display (1980), HDTV (1998), and others.

The winners of the R&D 100 Award are selected by an independent panel of judges based on the business, technical, and societal impact of the products released to the market over the past year.

AspenTech and NIST have been collaborating to incorporate several technologies and the world's most comprehensive physical property database into Aspen Properties®, the shared property component used within aspenONE Engineering, notably within Aspen Plus®, Aspen HYSYS®, and AspenTech's Exchanger Design and Rating products.

aspenONE Engineering V2006.5 includes two major features jointly developed with NIST. The NIST SOURCE database includes pure component physical property data for over 17,000 organic species. The uncertainty and sources (technical citations) of all the data are fully documented and viewable within the software. In addition, the software includes the NIST ThermoData Engine (NIST TDE), an expert system for evaluating, estimating, fitting, and validating pure component data. The NIST TDE provides customers with direct access to experimental property data and critically evaluated properties of a very wide range of compounds. The expert system applies the laws of thermodynamics to ensure all the estimated data and model parameters are accurate and self-consistent.



The NIST ThermoData Engine in Aspen Plus provides easy access to millions of sets of pure component physical property data on demand. The uncertainty and source of every data point is fully documented. The experimental data can be plotted against model predictions with a single mouse click, making it easy to validate the quality of the model.

These features save process engineers weeks or even months of effort in collecting, estimating, fitting, and validating the pure component property data that underlie their process and equipment design models. Further, the system captures thermodynamics expertise and puts it at the fingertips of a wider range of engineers and scientists. Within a matter of minutes, an engineer can evaluate and visually validate the quality of key model predictions, such as component vapor pressure or density, against a wealth of experimental and estimated property data. The software also benefits thermodynamics experts by providing quick and easy access to experimental data, which experts can use to fine-tune their models to particular ranges of operating conditions found in their processes.

Further improvements were made in aspenONE V7. The pure component database was extended to 18,840 species. The workflow of the NIST TDE was improved to make it even more flexible. In addition, aspenONE V7 includes the NIST reference fluid property (RefProp), an extremely accurate set of models and data for common refrigerants, gases, and heat transfer fluids. These features expand the applications of NIST TDE to include the modeling of the utility side of the process and to accurately design, size, and rate utility-to-process heat exchangers. As a result, chemical process companies can realize the following benefits:

- Increase in engineering productivity
- Faster and more accurate analysis of data
- Ability to design new processes to support emerging technologies
- Reduced capital and operating costs

Looking ahead, AspenTech and NIST plan to continue collaborating to bring further value to our mutual customers. We expect to continue updating and improving the NIST pure component databases to keep them current. We are also planning to expand the NIST TDE within aspenONE from pure component data to binary mixture and phase equilibrium data. This will save customers additional months of effort in the process of collecting, fitting, and validating phase equilibrium predictions to support their process and equipment design models.

For more information on the value of this collaborative solution for chemical process engineers, please read the white paper, *The Benefits of NIST ThermoData Engine in aspenONE® Engineering*, by visiting the [AspenTech support website](http://support.aspentech.com). (Please note: You need a user name and password to view this white paper. If you do not have an AspenTech web support account, you may register for one at <http://support.aspentech.com>.)

||||||| About AspenTech

AspenTech is a leading supplier of software that optimizes process manufacturing—including oil and gas, petroleum, chemicals, pharmaceuticals and other industries that manufacture and produce products from a chemical process. With integrated aspenONE solutions, process manufacturers can implement best practices for optimizing their engineering, manufacturing and supply chain operations. As a result, AspenTech customers are better able to increase capacity, improve margins, reduce costs and become more energy efficient. To see how the world's leading process manufacturers rely on AspenTech to achieve their operational excellence goals, visit www.aspentech.com.



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