

Using the PPDS Dataexpert Software to Provide Thermodynamically Consistent Data for the Thermophysical Properties of Pure Compounds

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PPDS (The Physical Property Data Service) has been in existence for some 34 years and comprises a set of modular software packages that calculate the phase-equilibrium and thermodynamic and transport properties of pure fluids and their mixtures. The software demonstration will concentrate on the PPDS 'DataExpert' software package that utilizes known data on a pure compound with a bank of reliable estimation procedures to provide a complete set of thermophysical properties (thermodynamic and transport). The user-friendly package provides a complete audit trail of the methods and data used and associates the output parameters for each property with quality codes that encapsulate the uncertainty in the data so produced. The DataExpert software has access to the experimental data collections that have been developed by TRC (the Thermodynamics Research Center) which is now based at NIST and provides a seamless mechanism for the extraction of numerical data with associated uncertainties on a given compound.

The sequence of extracting the numeric data, validating it and putting it into a usable form will be demonstrated using this software tool. Powerful extraction, data screening and analysis software modules mean that the process engineer can pull out relevant data on a compound, review different data sets, and can analyze and predict data for properties. Flexible and easy-to-use options are available for the identification of components in the underlying TRC experimental data collections.

The final stored parametric data from a DataExpert run can be used by the main PPDS Thermoserver application to provide mixture properties and phase equilibria calculations which are so important for engineering design.