

Database Tools for Evaluating Thermophysical Property Data

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Accurate thermophysical property data are essential for effective process and product design. In addition to providing a convenient compilation of available experimental data, most thermophysical property databases (TPD) also provide low level quality control checks. These are usually software-based, automatic checks to minimize transcription, data entry, unit-conversion, and magnitude errors that can be electronically trapped, using ranges of acceptable values, data-type checks, and relative comparisons. However, this presentation focuses on a much higher level of data evaluation used in the DIPPR® 801 TPD project, for pure chemicals. The purpose of the DIPPR® 801 database, is to provide “evaluated process design data.” Recommended values are provided for each property, based on high-level evaluations of the composite raw data. Although these evaluations require a substantial time investment, they significantly enhance the quality of the recommended values. The emphasis of the presentation will be on the valuable tools inherent in databases to achieve this higher-level evaluation and accuracy. For example, thermodynamic consistency requirements amongst the critical point, vapor pressure curve, enthalpy of vaporization, liquid density, and liquid and vapor heat capacities provide significant direction in defining the best values for these properties. Even more broadly, molecular structure-based trends in properties can be identified within the database and the properties of structurally-related compounds can be effectively used to discriminate amongst available datasets. In the DIPPR® database, recommended values may be estimated when no experimental data are available. In these cases, DIPPR® 801’s automated property prediction software can rapidly evaluate the effectiveness of different prediction methods in comparison with similar compounds and the database as a whole. This allows the accurate tailoring of prediction methods to specific types of compounds and molecular structures, with the result of enhanced accuracy of the recommended values. These and other high-level consistency tools will be illustrated.