The DIPPR 801 Gold Standard Systems Approach to Critical Evaluation of Thermophysical Property Data

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Accurate, pure-chemical, thermophysical property data are an essential component of designing and optimizing chemical processes, but the literature is filled with conflicting information and incorrect values. Using inaccurate data can be expensive. For example, an error of 10% in liquid heat capacity can results in thousands of dollars in unanticipated heating costs annually for a single medium-sized heat exchanger. To combat inconsistent literature, the DIPPR database uses a *systems* approach to evaluate the data from all available sources and triangulate on the best values. This approach applies over one hundred constraints—including inter-property relationships, expected trends between related chemicals, and chemical similarities and differences—to produce higher accuracy than could be achieved using only individual points or an evaluation approach which applies only a few consistency checks. Once the constraints are simultaneously satisfied for all properties, experts manually review the compound prior to addition to the database as a final quality check. This presentation will explain the systems approach to critical evaluation in more detail, and how this fits into DIPPR's mission to be the gold standard database in terms of both accuracy and completeness. Efforts to continuously improve the database, by developing new prediction methods and reevaluation of compounds already found in the database, will also be explained using two examples. The first is a description of a new method to predict liquid heat capacities from heat of vaporization, ideal gas heat capacity, and liquid vapor pressure using thermodynamic integration along the liquid-vapor saturation curve of a compound. The second is a recent reevaluation of the properties of the 1,*n*-alkanediol family of compounds. Taken as a whole, the results show the robustness of the systems approach to data evaluation, and how it provides insights into thermophysical property data that cannot be obtained using simpler methods.