

Dynamic Data Evaluation: First Experiences and New Developments

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ThermoData Engine (TDE), implementing the concept of Dynamic Data Evaluation for thermophysical and thermochemical properties, has been extended for state-change and equilibrium properties of chemical reactions. Directly measured reaction properties are used to demonstrate the consistency of pure-compound data or to derive previously unknown properties for a particular reaction participant. Practical experience in the use of Dynamic Data Evaluation (DDE) has yielded certain conclusions about its application and further development. It has become evident that DDE tools should be immediately applied to all newly obtained data in order to reveal inconsistencies with existing data and models. This approach can identify errors before publication or use. DDE has proved to be useful in planning of experiments as a source of information about existing data, gaps in data, and inconsistencies. Having a dynamic nature, DDE requires tracing previous evaluations in order to detect and analyze large changes in the results due to new data or prediction methods. Compound-by-compound evaluations with DDE may give inconsistent results for families of similar compounds due to specific low data quality or different prediction method used. Consequently, it is apparent that implementation of consistent multi-compound evaluation and development of globally consistent property prediction methods is essential. Development and implementation of the new tools and property evaluation methods will be discussed.