

Global Submission and Validation of Experimental Thermodynamic Data using Guided Data Capture (GDC) Software

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New procedures for global submission and dissemination of experimental thermodynamic data published in the Journal of Chemical and Engineering Data has been developed in cooperation between the Journal and the Thermodynamics Research Center at NIST (NIST/TRC). To implement these procedures, Guided Data Capture software (GDC) has been developed at NIST/TRC. The software is freely available for download from the Internet. The experimental data including numerical values, uncertainty estimates, and metadata descriptions are captured with a strictly hierarchical system based upon rigorous application of the thermodynamic constraints of the Gibbs phase rule with full traceability to source documents. The scope of GDC spans essentially all experimentally determined thermodynamic and transport property data (more than 120 properties) for pure compounds, two- and three-component mixtures, and chemical reactions (including change-of-state and equilibrium). The focus at present is molecular compounds. Although properties determined by direct experimental measurement are emphasized in its application, GDC also covers key derived properties such as azeotropic properties, Henry's Law constants, virial coefficients (for pure compounds and mixtures), activities and activity coefficients, fugacities and fugacity coefficients, and properties derived from high-precision adiabatic heat-capacity calorimetry, such as standard entropies. Features of the software will be described with particular emphasis on the underlying scientific principles and their role in ensuring complete and accurate specification of the data captured.