ThermoML Based New Data Delivery Process and its Impact on Publication Data Quality

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ThermoML is the new XML-based IUPAC standard for storage and exchange of experimental, predicted, and critically-evaluated thermophysical and thermochemical property data. In September 2002 the Editorial Board of the Journal of Chemical and Engineering Data in cooperation with NIST/TRC (NIST Thermodynamics Research Center), established a policy for submission and dissemination of experimental data with use of Guided Data Capture software (GDC) and ThermoML at its core. Following the peer-review process, authors are requested to download and use GDC to capture experimental property data accepted for publication. The output file from GDC is submitted directly to NIST/TRC, and after additional consistency tests, the files are converted into ThermoML format. Upon publication of the manuscript, ThermoML files are posted on the public domain TRC Web site for unrestricted access. This process is now established for four additional journals; The Journal of Chemical Thermodynamics, Fluid Phase Equilibria, Thermochimica Acta, and the International Journal of Thermophysics. The data delivery process will be described with particular emphasis on present and potential impacts on data quality. Present methods of data quality determination will be described. New, freely available, software tools for easy conversion of property data into ThermoML format and conversion of ThermoML formatted files into simple spreadsheet format will also be described.