

The Contribution of Dr. Randolph Wilhoit to Databases, Data Evaluation, and Expert Systems for Thermophysical Property Data for Organic Compounds

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Dr Randolph (Randy) Wilhoit was the primary instigator of the Thermodynamics Research Center's current approach to data evaluation. In 1983 he realized that the methods in use to evaluate data were archaic and extremely labor intensive. Many data evaluation projects had been financed by Government, Industrial Consortia, and Industry. The problem was that much of the data was stored on cards and when the project was completed generally much of the collected experimental data was thrown out and that "stored electronically" was often stored in undocumented formats on outdated storage media and could not be used. He proposed the development of an archival relational database that could be queried in diverse ways that would include, as well as the original experimental data, relevant metadata, such as the source and purity of the material, purification method, measurement method, and uncertainties in all the measured variables in sufficient detail that there would be no need to revisit the original literature. This formed the basis of the present TRC/NIST SOURCE relational database. To populate the database he worked within a CODATA (Committee on Data for Science and Technology) Taskgroup to develop COSTAT as a standard for the exchange of thermophysical property data. The practical implementation of COSTAT was hindered primarily because of software limitations at that time. COSTAT formed the basis for the recent IUPAC standard for thermophysical property data exchange, ThermoML.

Randy's vision in developing both the SOURCE database and COSTAT was to provide an archival database where authors and data evaluators could deposit original experimental data and the resulting database would form the basis of an on-demand dynamic data evaluation system. The vision has now been implemented in the development at TRC of a unique expert system, ThermoData Engine (TDE). The talk will provide a more detailed exposition of the extraordinary contributions made by Randy Wilhoit to the advancement of thermophysical property data evaluation.