

DIPPR: Satisfying Industry Data Needs

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DIPPR, a Sponsored Research group of AIChE, has made a significant impact on the chemical process industries by improving thermodynamic and physical property data for process engineering. Participating organizations include chemical and petroleum producers, engineering contractors, software vendors, and government agencies. Projects are proposed and funded by interested DIPPR participants. By involvement of participants, guidance by project sponsors, annual accountability, and dissemination of project results, DIPPR has enjoyed continued success in satisfying industry data needs.

Introduction

The Design Institute for Physical Property Data (DIPPR) is an AIChE Sponsored Research group, active longer than any other such AIChE group. Since 1980 DIPPR has sponsored projects involving properties of pure chemicals, mixtures, and polymers important for chemical process engineering. The purpose of DIPPR is to satisfy industry needs for better data to meet new and more stringent requirements, such as those of energy conservation and environmental and safety regulations.

There are three types of DIPPR projects: database, correlation development, and measurement. Of the 17 DIPPR projects, seven have been completed and ten are currently active. DIPPR project results are used by a wide variety of firms, including chemical producers, equipment manufacturers, contractors, consultants, and software vendors in the chemical process industries.

A brief historical background is given, followed by a description of the unique characteristics of DIPPR and a discussion of DIPPR projects and their results.

Historical Background

In the mid-1970s, with widespread use of chemical process simulation, it became clear that better data were needed. Some companies were pooling resources in consortia such as the Thermodynamics Research Laboratory at Washington University and Fluid Properties Research, Inc. at Oklahoma State University. Government-sponsored efforts were underway in other parts of the world, including Germany (DECHEMA), United Kingdom (NEL, PPDS), and Japan (JUSE). There was no comprehensive data effort for the chemical industry in the United States. The efforts in other countries did not fully satisfy industry needs due to distance, minimal participation, and lack of access to source data.

A group of chemical engineering data specialists and researchers met in November 1975 to determine interest in launching a cooperative data effort supported by industry. Several discussions followed, regarding the selection of and arrangements with an appropriate umbrella organization. Finally, AIChE was approached and agreed immediately. DIPPR was then launched in November 1978 as the Design Institute for Physical Property Data of the

American Institute of Chemical Engineers. Project steering committees were organized and five projects were proposed. Over the next year more than 50 companies joined DIPPR, the proposed projects were balloted for funding, and contractors and principal investigators were selected for four funded projects. The first projects began in 1980.

Unique Characteristics of DIPPR

DIPPR participation and project funding are committed annually by a balloting procedure. Participants consider all current and proposed projects for the following year, and choose the projects they wish to sponsor, by committing funds. Those projects which receive adequate funding commitments are initiated or continued. The sponsors of each project appoint representatives to its Project Steering Committee. All DIPPR projects are reviewed regularly, at least annually, by the Steering Committees.

This annual accountability helps assure for each project that the Principal Investigator (PI) follows the direction of interest to the Project Steering Committee and gives both the PI and the Steering Committee the opportunity to suggest and to agree on changes in the direction of the project. The PI is able to bring potential problems to the attention of the Steering Committee as they arise, so solutions can be found and delays avoided.

DIPPR Participants are involved in several ways. Each Participant selects a Management Representative, a Technical Representative, and optionally, one or more Associate Technical Representatives. The Management Representatives participate in the administration of DIPPR and cast the ballots for project support. The Technical Representatives provide overall direction of the DIPPR technical effort, elect chairs of DIPPR standing committees and Project Steering Committees, approve projects and project budgets to be considered for funding, and ensure technical accomplishments and proper reporting of project results. Participants select new DIPPR projects through the annual balloting procedure.

Participants that support a project financially become the project sponsors. Their involvement becomes more direct in determining the project type and scope, selecting the PI, and guiding the project. All DIPPR projects start with a list of properties to be included and chemicals to be studied. The properties may be changed by agreement

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Table 1. Summary of DIPPR Projects

no.	project name	principal investigator	status
801	Data Compilation	T. E. Daubert, Penn State	ongoing
802	Data Prediction Manual	R. P. Danner, Penn State	completed 1991
804	Acetic Acid-Water PVT and VLE Measurements	G. M. Wilson, Wiltec	completed 1981
805	Experimental Data on Mixtures	Various	ongoing
811	Electrolyte Phase Equilibria	M. Rafal, OLI	completed 1984
821	Pure Liquid Vapor Pressure Measurements	W. V. Steele, NIPER	ongoing
832	Pure Component Organic Acid Latent Heat of Vaporization and PVT Measurements	G. M. Wilson, Wiltec	completed 1985
851	Critical Properties of Pure Compounds	L. Wilson, Wiltec	ongoing
861	Aqueous Electrolyte Solution Database	D. Smith-McGowan, D. E. Newmann, NIST	completed 1989
871	Determination of Pure Component Ideal Gas Heat of Formation	W. V. Steele, NIPER	ongoing
881	Handbook of Polymer Solution Thermodynamics	R. P. Danner, Penn State	completed 1993
882	Evaluated Data on Mixtures	K. N. Marsh, Texas A&M	completed 1996
911	ESH Data Compilation	M. E. Mullins, T. N. Rogers, Michigan Tech	ongoing
912	ESH Data Prediction Manual	M. E. Mullins, T. N. Rogers, Michigan Tech	completed 1996
922	Handbook of Diffusivities and Thermal Properties of Polymer Solutions	J. M. Caruthers, Purdue	completed 1996
931	Data Prediction Methods	P. C. Jurs, Penn State	ongoing
961	Handbook of Polymer Miscibility and Interfacial Energy Properties	T. Lodge, U. Minnesota	starting 1996

between the PI and the Steering Committee. The chemicals may be selected and prioritized. The project sponsors also advise on many other aspects of the project, such as project policies and procedures, data sources, correlation and prediction methods, experimental methods, data qualification methods, data processing, use of computers and electronic communications, and review and dissemination of project results.

The mechanisms of project selection and funding assure that DIPPR projects will be of appropriate scope. *Appropriate* here applies to selection of chemicals and properties to be studied, level of accuracy and coverage, use of estimated values, and time span. The chemicals and properties covered are selected by the project sponsors, and so are definitely of interest to industry, the audience DIPPR seeks to serve.

DIPPR is interested in a practical level of accuracy and coverage. For example, the initial emphasis of the Data Compilation project was to obtain data adequate for engineering purposes quickly. As experience was gained, the emphasis shifted to more accurate and consistent data and more complete coverage. However, coverage focuses on properties important for process or environmental engineering, so the DIPPR effort does not include such information as complete thermodynamic surfaces (which have been developed for major chemicals) or NMR spectra.

For database projects, if experimental data are not available for a given property of a chemical, estimated values will be used if possible. Source data and estimates of accuracy are provided, so process engineers can judge the adequacy of the data for a given purpose. Project investigators with data evaluation experience can usually provide better estimates than process or environmental engineers in the field.

While some DIPPR projects are completed within two to four years and others continue much longer or indefinitely, some deliverables are usually required at least once a year, to justify continued funding and to keep the project direction consistent with sponsor expectations.

DIPPR Projects

DIPPR projects are summarized in Table 1. All DIPPR projects are identified by a name and a three-digit project number. The first two digits indicate the year the project began. The three types of DIPPR projects—database, correlation development, and measurement—will be discussed. The different types of projects complement each other in satisfying industry needs. Projects of different types in a given technology area will be described together in some cases, and some projects include more than one of these types to some extent.

Database Projects

The objective of DIPPR database projects is to develop a compilation or database of critically evaluated data for specified properties of industrially important chemicals or mixtures. The database projects are Data Compilation (Project 801), Aqueous Electrolyte Solution Database (861), Evaluated Data on Mixtures (882), and Environmental, Safety and Health (ESH) Data Compilation (911).

Data Compilation (801). The Data Compilation project began in 1980 and has been active since then at the Chemical Engineering Department at The Pennsylvania State University under the leadership of T. E. Daubert and R. P. Danner. The project seeks to organize and make available a convenient compilation of reliable property data on industrially important chemical compounds and mixtures. Its objective is to satisfy industry needs for more accurate and complete thermodynamic and physical property data for process engineering. The Data Compilation also serves as a repository of measured data from other DIPPR projects. The Data Compilation now includes 29 property constants and 15 temperature-dependent properties for 1508 compounds in its most recent public release (Daubert et al., 1996a, 1996b; STN, 1996). The Data Compilation is also available through several commercial software and process simulation vendors. The properties are listed in Table 2.

Table 2. Properties in the Data Compilation (Project 801)

Property Constants	
formula	enthalpy of formation, std. state, 298.15 K
common name	Gibbs energy of formation, std. state, 298.15 K
CAS name	absolute entropy, std. state, 298.15 K
IUPAC name	298.15 K
CAS registry number	enthalpy of fusion at melting point
structure	standard enthalpy of combustion, 298.15 K
synonyms	acentric factor
molecular weight	radius of gyration
critical temperature	solubility parameter, 298.15 K
critical pressure	298.15 K
critical volume	dipole moment
critical compressibility factor	Van der Waals volume
melting point, 1 atm	Van der Waals area
triple point temperature	refractive index
triple point pressure	flash point
normal boiling point	lower flammability limit
liquid molar volume, 298.15 K	upper flammability limit
enthalpy of formation, ideal gas, 298.15 K	autoignition temperature
Gibbs energy of formation, ideal gas, 298.15 K	
absolute entropy, ideal gas, 298.15 K	
Temperature Dependent Properties	
solid density	second virial coefficient
liquid density	liquid viscosity
sublimation pressure	vapor viscosity
vapor pressure	solid thermal conductivity
enthalpy of vaporization	liquid thermal conductivity
solid heat capacity	vapor thermal conductivity
liquid heat capacity	surface tension
ideal gas heat capacity	

Table 3. Properties in the Evaluated Data on Mixtures Database (Project 882)

Information Included	
mixture identification	
reference	
source of sample	
component names, formulas, and CAS registry numbers	
source of sample assessment	
imprecision and inaccuracy in independent variables	
imprecision and inaccuracy in measured variables	
final purity	
method of determining purity	
purification method	
table of data values	
plot of the data	
Properties Included	
critical properties	
density	
diffusion coefficient	
solubility	
surface tension	
thermal conductivity	
viscosity	

Evaluated Data on Mixtures (882). The aim of the Evaluated Data on Mixtures project is to develop a computer-searchable database containing evaluated experimental data on selected properties of mixtures. This database should be useful not only for the data themselves, but also for testing models of mixture behavior. Under the guidance of K. N. Marsh at the Thermodynamics Research Center at Texas A&M University since 1988, two of the planned four volumes of tables have been published (Gammmon *et al.*, 1993, 1994). The database has also been made available in computer form (Dong *et al.*, 1995). A total of about 2040 mixture/property tables will eventually be published. The properties included are listed in Table 3.

Environmental, Safety and Health Data (911, 912). The ESH Data Compilation and ESH Data Prediction Manual projects began in 1991 with M. E. Mullins and T.

N. Rogers in the Chemical Engineering Department at Michigan Technological University as project investigators. The ESH Data Compilation project goal is to develop a database of chemicals which are regulated by the government or which are important to the chemical industry and to society at large for environmental, safety, and health concerns. The properties are listed in Table 4. The first public release is scheduled for November 1996. The chemicals are taken from the 1990 Clean Air Act Amendments, the OSHA Process Safety Management list, the EPA Risk Management Program, and chemicals of special interest to project sponsors. The database now contains approximately 45 000 data values for 490 chemicals.

The purpose of the ESH Data Prediction Manual project is to develop and select estimation methods for properties needed for the ESH Data Compilation. A computer program has been developed for property estimation and retrieval. The project will be merged into the ESH Data Compilation project in 1997.

Correlation Development Projects

These projects have the objective to develop or recommend correlations for specific properties. The projects include the Data Prediction Manual (Project 802), Data Prediction Methods (931), Electrolyte Phase Equilibria (811), Polymer Solution Thermodynamics (881), Handbook of Diffusivities and Thermal Properties for Polymer Solutions (922), Handbook of Polymer Miscibility and Interfacial Energy Properties (961), and Environmental, Safety and Health (ESH) Data Prediction Manual (912).

Data Prediction (802, 931). The Data Prediction Manual project began in 1980 along with the Data Compilation project, also under R. P. Danner and T. E. Daubert at The Pennsylvania State University. The two projects were coordinated closely, each complementing the other, under the same Project Steering Committee. The purpose of the Data Prediction Manual project was to evaluate and recommend methods for predicting properties important for process engineering. The Data Prediction Manual was published (Danner *et al.*, 1987), as well as a supplement for organometallic compounds (Myers *et al.*, 1991) and a handbook for vapor-liquid equilibrium (Gess *et al.*, 1991). The project was then complete.

The Data Prediction Methods project began in 1993 as a successor to the Data Prediction Manual project, but focusing on new methods for predicting physical and thermodynamic properties using molecular descriptors as correlating parameters. P. C. Jurs in the Chemistry Department at The Pennsylvania State University is the PI. Prediction methods for normal boiling point and autoignition temperature have been developed, and software to implement the methods has been made available to the project sponsors.

Electrolyte Solutions (811, 861). The Electrolyte Phase Equilibria project developed methods for correlating and predicting the behavior of aqueous electrolytes. J. F. Zemaitis at Chem Solve, Inc. and M. Rafal at OLI Systems, Inc. were the PIs for this project, which lasted from 1981 to 1984. The principal result was a comprehensive handbook (Zemaitis *et al.*, 1986).

Building on the Electrolyte Phase Equilibria project, the Aqueous Electrolyte Solution Database project compiled data and included software for data access and retrieval from personal computers. The project work was done at the National Institute of Standards and Technology by D. Smith-McGowan and D. E. Neumann from 1986 to 1989. The database was published (Neumann, 1994).

Table 4. Properties in the ESH Data Compilation (Project 911)

General Physical Properties	
molecular weight	molecular diffusivity in water, 298.15 K
liquid density, 298.15 K	surface tension, 298.15 K
solubility in water, 298.15 K	heat of formation, ideal gas, 298.15 K
solubility of water in chemical, 298.15 K	critical temperature
melting point	critical pressure
normal boiling point	critical volume
vapor pressure, 298.15 K	heat of vaporization, 298.15 K
molecular diffusivity in air, 298.15 K	heat of vaporization at normal boiling point
Temperature Dependent Properties	
liquid density	liquid thermal conductivity
vapor pressure	vapor thermal conductivity
liquid viscosity	liquid heat capacity
vapor viscosity	ideal gas heat capacity
surface tension	heat of vaporization
Oxygen Demand Parameters	
biochemical oxygen demand (BOD)	theoretical oxygen demand (carbonaceous)
chemical oxygen demand (COD)	theoretical oxygen demand (combined)
Partitioning Parameters	
octanol/water partition coefficient	organic carbon/water partition coefficient
soil/water partition coefficient	bioconcentration factor
Vapor-Liquid Equilibrium Parameters	
activity coefficient in water	Henry's law constant for water mixtures
activity coefficient of water in chemical	
Fire and Explosion Parameters	
lower flammability limit in air	autoignition temperature
upper flammability limit in air	heat of combustion
flash point	
Sensory, Health, and Toxicity Impact Parameters	
aquatic toxicity	human toxicity

Table 5. Properties in the Polymer Solution Databases (Projects 881, 922)

Polymer Solution Thermodynamics
polymer pressure-volume-temperature data
finite concentration vapor-liquid equilibria
infinite dilution vapor-liquid equilibria
binary liquid-liquid equilibria
ternary liquid-liquid equilibria
Polymer Solution Diffusivities and Thermal Properties
diffusivity of solvent into polymer
diffusivity of polymer into solvent
thermal conductivity
heat capacity
density
enthalpy of polymerization
coefficient of thermal expansion

Polymer Solutions (881, 922, 961). The Handbook of Polymer Solution Thermodynamics project began in 1988 with R. P. Danner at The Pennsylvania State University as PI. Its purposes were to provide an evaluated depository of data, evaluate and extend models for polymers in both organic and aqueous solvents, develop improved models, and provide a standard source of results in both handbook and database form. The purposes were accomplished with the publication of the Handbook with accompanying software (Danner *et al.*, 1993). This project was followed by the Handbook of Diffusivities and Thermal Properties for Polymer Solutions, 1992-1996, with J. M. Caruthers at Purdue University, for which the technical work is complete and the Handbook and software are in preparation. The properties included in the databases accompanying both handbooks are given in Table 5. A new project, the Handbook of Polymer Miscibility and Interfacial Energy Properties, is to begin in 1996 with T. Lodge at the University of Minnesota.

Measurement Projects

Experimental measurements of properties of specific chemicals or mixtures may be made for a variety of

reasons: sponsor request, determination of values for key compounds or homologous series, development or improvement of property correlations, and provision of values to DIPPR database or correlation development projects. Measurement projects include Experimental Data on Mixtures (Project 805), Pure Liquid Vapor Pressure Measurements (821), Critical Properties of Pure Compounds (851), Determination of Pure Component Ideal Gas Heat of Formation (871), Acetic Acid-Water PVT and VLE Measurements (804), and Pure Component Organic Acid Latent Heat of Vaporization and PVT Measurements (832). Results of these projects have been published (Benson *et al.*, 1985; Black, 1987; Shih *et al.*, 1989; Selover, 1990; Cunningham *et al.*, 1990, 1991, 1994). Beginning in 1996, DIPPR experimental results are expected to be submitted to *J. Chem. Eng. Data* for publication.

Experimental Data on Mixtures (805). This project is directed at obtaining vapor-liquid equilibrium, liquid-liquid equilibrium, and solubility data on systems of important industrial chemicals and on systems selected to augment predictive techniques for phase equilibria from molecular structures. Instead of having a single PI, several investigators worldwide are involved, according to their capabilities and interests. The scope of the project each year is finalized by the Steering Committee in response to proposals received after a list of potential systems is distributed to potential investigators. Each investigator makes the desired measurements on specified mixtures. The project began in 1980, and measurements have been made on over 280 systems.

Pure Liquid Vapor Pressure Measurements (821). This project makes accurate measurements of vapor pressure over a wide range of temperatures. Measurements on more than 110 compounds have been made since 1982. Since 1991, the PI for this project has been W. V. Steele of the National Institute for Petroleum and Energy Research (NIPER), Bartlesville, OK, and the scope of the project has been expanded to include measurements of vapor and

liquid heat capacities, liquid density, and critical temperature and density. Critical pressure, enthalpy of vaporization, acentric factor, and solubility parameter are derived.

Critical Properties of Pure Compounds (851). The critical point (critical temperature, pressure, and volume) of pure compounds is experimentally determined in this project. The focus is on key compounds for which reliable data are lacking, by using new, rapid measurement methods, since many such compounds are unstable at their critical temperature. The critical point is important for correlating the behavior of pure compounds and is used in many estimation methods. This project began in 1985, and measurements have been made on over 110 compounds. The current PI is L. Wilson at Wiltec, Inc., Provo, UT.

Determination of Pure Component Ideal Gas Heat of Formation (871). In this project, highly accurate enthalpies of combustion and ancillary data on solid and liquid organic compounds are measured to enable ideal gas enthalpies of formation to be computed. The ancillary data include two-phase heat capacities, vapor pressures, triple points, and enthalpies of fusion when needed to convert condensed state values to ideal gas heats of formation. The PI is W. V. Steele at NIPER. Heats of combustion have been measured for over 72 compounds since this project began in 1987.

Measurements on Specific Chemicals (804, 832). Two DIPPR measurement projects of limited scope have been completed: Acetic Acid-Water PVT and VLE Measurements, 1980–1981; and Pure Component Organic Acid Latent Heat of Vaporization and PVT Measurements, 1983–1985. The PI for both projects was G. M. Wilson at Wiltec.

Conclusions

DIPPR has conducted successful physical property data projects since 1980 for the chemical process industries. The unique characteristics of DIPPR include industry involvement, short-term accountability, and a wide variety of projects. By focusing on satisfying industry needs while maintaining high standards of quality, DIPPR has produced significant results of lasting value.

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