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The DIPPR® Databases[1]

G. H. Thomson[2]

The Design Institute for Physical Property Data® (DIPPR), one of the Sponsored Research groups of the American Institute of Chemical Engineers (AIChE), has been in existence for 15 years and has supported a total of 14 projects, some completed, some ongoing. Four of these projects are "database" projects for which the primary product is a database of carefully evaluated property data. These projects are Data Compilation; Evaluated Data on Mixtures; Environmental, Safety, and Health Data Compilation; and Diffusivities and Thermal Properties of Polymer Solutions. This paper lists the existing DIPPR projects; discusses DIPPR's structure and modes of dissemination of results; describes DIPPR's supporters and its unique characteristics; and finally, discusses the origin, nature, and content of the four database projects.

KEY WORDS: DIPPR; databases; thermodynamic properties; transport properties.

1. INTRODUCTION

DIPPR, the Design Institute for Physical Property Data, is one of the Sponsored Research groups of the American Institute of Chemical Engineers. DIPPR's mission is to supply its supporters with high-quality thermophysical and thermodynamic property data on compounds and mixtures of interest to them. To this end, DIPPR has supported data collection and measurement over the 15 years of its existence. The original emphasis was on common chemicals widely used in the chemical and petrochemical industries, but in the last 6 years DIPPR has broadened its scope to include data on polymers and their solutions as well as environmental, safety, and health data. Since these data are eventually disseminated to the public, they have been of benefit not only to DIPPR supporters, but also to science and engineering in general.

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[2] Consultant, 356 Fleetwood Drive, Bartlesville, Oklahoma 74006, U.S.A.

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This paper discusses the DIPPR projects, the dissemination of project results, DIPPR's structure, and its unique characteristics. The reasons for the creation of four database projects are noted, and the nature of each project is explained. The properties and substances treated in each project and the project output are described.

2. STRUCTURE

DIPPR is made up of a number of projects in which property data are collected, evaluated, correlated, predicted, and measured, together with a number of committees which oversee the work, maintain policies and procedures, arrange for dissemination of results, and perform various other administrative tasks.

2.1. Projects, Principal Investigators, and Steering Committees

The names and numbers of the currently active projects and one tentative project are listed in Table I. Several earlier projects have finished their work and closed. The Experimental Flammability Properties project did not receive enough support to start, although the current emphasis on safety, the OSHA Process Safety regulations, increasing emphasis on risk assessment, and the poor state of flammability data seemed to indicate that it would be received favorably. The projects fall into two general categories: projects in which the main activity is data collection and evaluation and those in which the main activity is experimental measurement. The first class will be called database projects. The day-to-day work is directed by the Principal Investigator (PI). The PI is responsible to the Project Steering Committee. That committee is made up of one Technical

Table I. Current DIPPR Projects

Data Compilation (801)
Experimental Data on Mixtures (805)
Pure Liquid Vapor Pressure Measurement (821)
Critical Properties of Pure Components (851)
Pure Component Ideal Gas Enthalpies of Formation (871)
Evaluated Data on Mixtures (882)
Environmental, Safety and Health Data Compilation (911)
Environmental, Safety and Health Data Prediction Manual (912)
Handbook of Diffusion and Thermal Properties of Polymer Solutions (922)
Data Prediction Methods (931)
Experimental Flammability Properties

Representative from each of the organizations which supports that particular project. The Steering Committee sets the direction and budget for the project, oversees the PI's work, and evaluates the project results. At present, six PIs are university faculty members, one works in a private laboratory, and one works in a Federal Government laboratory.

2.2. Other Officers and Committees

The various DIPPR activities are coordinated by the Technical Director. The Technical Committee is made up of the Technical Director, Associate Technical Director (if one has been appointed), and the Technical Representatives.

Each DIPPR supporting organization is also requested to appoint a Management Representative. Usually, it is the Management Representative who submits completed ballots indicating which projects his company will support.

The members of the Technical Executive Committee are the Technical Director, the Chairs of the Liaison, Publicity and Recruitment, Dissemination, and Steering Committees, and one or two Management Representatives. The Administrative Committee reports to AIChE Council and consists of up to seven Management Representatives, the Technical Director, and the Publicity and Recruitment Committee Chair.

2.3. Dissemination

The DIPPR bylaws require the dissemination of project results. These are, of course, immediately available to the supporters of the projects. Project output becomes available to the public one year after acceptance by the project Steering Committee. AIChE distributed project results in hard copy as part of its Symposium Series and more recently as the new DIPPR Data Series. The National Institute of Standards and Technology (NIST) distributes the Data Compilation on computer tape and diskettes. It is also available online through Chemical Abstracts Services' STN and in hard copy from Taylor and Francis. Technical Database Services, Inc., sells the Data Compilation with data retrieval software as a computer program. The tables created by the Evaluated Data on Mixtures Project may be obtained in hard copy from AIChE and, in the form of a relational database, from the Thermodynamics Research Center at Texas A & M University. Electronic products are planned for the other database projects, but details have not been finalized. Among the electronic options which have been considered for future distribution are online ditribution, computer tape and

diskettes, "floppy books," CD-ROM, and multimedia CD-ROM. Distribution on CD-ROM is planned.

2.4. Supporters

DIPPR supporters are mostly chemical and petroleum companies, contract engineering firms, and vendors of process simulation software, but also include the National Institute of Standards and Technology (NIST) and the National Institute for Petroleum and Energy Research (NIPER). The Departments of Energy (DoE) and Agriculture (DoA), the National Science Foundation (NSF), and NIST have provided grants. DoE matched DIPPR funding for one project for a number of years. It appears that DoE will match funding for two projects under a Cooperative Research and Development Agreement (CRADA) beginning in 1995.

3. CHARACTERISTICS OF DIPPR AND ITS PROJECTS

DIPPR emphasizes frequent communication between Project Steering Committees and project investigators. These frequent meetings help to ensure that the Steering Committee members, in their role as representatives of the project supporters, clearly understand the status of the project, are made aware of any special problems impeding the progress of the project, and can communicate to the PI any modifications needed in the scope or direction of the project. Most Steering Committees also formalize the review process in some way to ensure a careful, thorough review of the project's products.

Because DIPPR supporters are generally interested in near-term use of project output, DIPPR projects tend to be applied rather than theoretical. Thus, the chemicals included in the projects are usually those suggested by the supporters. However, some, such as the potential "oxygenates" for gasoline and the "new" refrigerants, are important to major groups of supporters. The projects also emphasize "appropriate" quality. Although it would be desirable to have a complete, consistent thermodynamic surface for every compound, this level of detail is not appropriate for DIPPR; neither, however, are the crudely calculated and estimated values scattered through the literature and in various handbooks. Supplying data for, and developing, estimation methods also have a high priority because we will never have good experimental data on all the substances of interest.

The leverage of shared funding and the interactions among DIPPR supporters also contribute significantly to DIPPR's success. Use of DIPPR projects to obtain data for longer-range and more basic projects permits the supporter's staff to concentrate on high-priority, short-term work.

DIPPR projects also supply a reservoir of carefully measured or carefully evaluated data to meet future needs of the supporters, industry, and the scientific and engineering communities.

3.1. Database Projects

Since data collection, evaluation, and correlation are parts of several DIPPR projects, it is somewhat difficult to specify which constitute "database" projects. The four projects which fit this classification most

Table II. Compound Constants in DIPPR Data Compilation (Project 801)

Formula
Common name
CAS name
IUPAC name
CAS registry number
Structure
Synonyms
Molecular weight
Critical temperature
Critical pressure
Critical volume
Critical compressibility factor
Melting point
Triple point temperature
Triple point pressure
Normal boiling point
Molar volume, 298.15 K
Ideal gas enthalpy of formation, 298.15 K
Ideal gas Gibbs energy of formation, 298.15 K
Ideal gas entropy, 298.15 K
Enthalpy of fusion at melting point
Net enthalpy of combustion, 298.15 K
Acentric factor
Radius of gyration
Solubility parameter
Dipole moment
Van der Waals volume
Van der Waals area
Refractive index
Flash point
Lower flammability limit
Upper flammability limit
Autoignition temperature

clearly are Data Compilation; Evaluated Data on Mixtures; Environmental, Safety and Health Data Compilation; and Polymer Solution Diffusivities and Thermal Properties. Each is discussed below.

3.2. Data Compilation (Project 801)

The rationale for this project was the lack of reliable physical and thermodynamic property data for use in process engineering in the late 1970s. With carefully evaluated data on 1509 compounds available to supporters, the DIPPR Data Compilation is one of the most comprehensive collections of evaluated data available. This compilation consists of a Source File, which contains the actual data, quality codes, and keys to notes and references; and Notes and References Files, which contain the actual text of the notes and references. A Policies and Procedures Manual documents such items as calculational procedures and temperature ranges. Quality codes specify whether the data are experimental and give the project staff's estimate of their accuracy. All of these files are computer-readable. The properties covered are given in Tables II and III. The Data Compilation has also been designated as the repository for the results from DIPPR experimental projects. The Principal Investigator for this project is T. E. Daubert at Pennsylvania State University.

Table III. Temperature-Dependent Properties in DIPPR Data Compilation (Project 801)

Solid density
Liquid density
Vapor pressure
Enthalpy of vaporization
Solid heat capacity
Liquid heat capacity
Ideal gas heat capacity
Second virial coefficient
Liquid viscosity
Vapor viscosity
Liquid thermal conductivity
Vapor thermal conductivity
Surface tension

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

Mixture identifiers
Reference
Source of sample
Table of data values
Component names, formulas, and CAS registry numbers
Source of sample assessment (unknown, given in the paper, etc.)
Imprecision and inaccuracy in independent variables (temperature, pressure, etc.)
Imprecision and inaccuracy in measured variables
Properties: critical properties, density, diffusion coefficient, solubility, surface tension, thermal conductivity, and viscosity
Final purity
Method of determining purity
Purification method
Plot of the data

3.3. Evaluated Data on Mixtures (Project 882)

The large amount of published physical property data on mixtures makes it difficult to find specific data and to judge its quality. The objective of this project is to supply evaluations of published mixture data and make them readily available in hard and electronic copy. This compilation should be quite useful for testing models of mixture properties. In addition to the actual property values, the tables give references, components, conditions of measurement, information on sample purity, estimates of the imprecisions and inaccuracies in the variables, and graphs of the data. The content of the database is summarized in Table IV. The Principal Investigator for this project is K. N. Marsh at Texas A&M University.

3.4. Environmental, Safety, and Health Data Compilation (Project 911)

A few years ago it took an environmental engineer considerably longer to find the data needed for a calculation than to make the calculation. The purpose of this compilation is to supply carefully evaluated data for these calculations. It is also hoped that the data will be accepted by governmental agencies for calculations and simulations. The compilation is a relational database, which contains a Values Table which points to a Chemical Number Table, a Properties Table, and an Article Number Table. The Chemical Number Table contains the chemical identifiers, the Properties Table contains the actual property values and quality codes, and the Article Number Table contains the references. The Policies and Procedures Manual is a separate file. The properties covered are listed in Tables V and

Table V. Properties in the Environmental, Safety, and Health Data Compilation Database (Project 911)

General physical properties
Molecular weight
Liquid density
Solubility in water
Melting point
Normal boiling point
Vapor pressure at 25°C
Molecular diffusivity in air
Molecular diffusivity in water
Surface tension
Liquid thermal conductivity
Vapor thermal conductivity
Heat of formation
Critical temperature
Critical pressure
Critical volume
Temperature-dependent properties
Liquid density
Vapor pressure
Vapor viscosity
Liquid viscosity
Surface tension
Liquid heat capacity
Vapor heat capacity
Heat of vaporization

VI. Current government regulatory activities suggest that this project will be needed for many years. The Principal Investigators are M. E. Mullins and T. N. Rogers at Michigan Technological University.

3.5. Handbook of Polymer Solution Diffusivities and Thermal Properties (Project 922)

This project succeeded the Handbook of Polymer Solution Thermodynamics project. In both cases the intention was to collect in one place evaluated data and models for polymers and their solutions for use in modeling processing operations. The Principal Investigator, J. M. Carruthers of Purdue University, has already developed an interesting model for the *PVT* properties of polymers, but since DIPPR projects results remain proprietary for one year, the model has not yet been published. Properties in this database are listed in Table VII.

Table VI. More Properties in the Environmental, Safety, and Health Data Compilation Database (Project 911)

Partitioning parameters
Octanol/water partition coefficient
Organic carbon/water partition coefficient
Soil/water partition coefficient
Bioconcentration factor
Oxygen demand parameters
Biochemical oxygen demand
Theoretical oxygen demand (carbonaceous)
Chemical oxygen demand
Theoretical oxygen demand (combined)
Vapor-liquid equilibrium parameters
Activity coefficient of chemical in water
Aqueous Henry's law constant
Activity coefficient of water in chemical
Fire and explosion parameters
Lower flammability limit in air
Flash point
Autoignition temperature
Upper flammability limit in air
Heat of combustion
Sensory, health, and toxicity impacts
A number of acute aquatic toxicity parameters

Table VII. Properties in the Polymer Solution Diffusivities and Thermal Properties Database (Project 922)

Diffusivity of solvent into polymer
Diffusivity of polymer into solvent
Thermal conductivity
Specific heat
Density
Enthalpy of polymerization
Coefficient of thermal expansion

4. CONCLUSIONS

DIPPR has supplied carefully measured and evaluated values of physical, thermodynamic, environmental, safety, and health properties to its supporters and, through its public dissemination, to science and industry in general, for 15 years. Its longevity is due to its creation of useful projects, its responsiveness to its supporters, and the involvement of those supporters in its activities.