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DIPPR® Project 801 evaluated process design data

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Abstract

Since 1980, the Design Institute for Physical Property Data® has sponsored Project 801 to develop, organize and make available to project sponsors a complete, critically evaluated compilation of thermophysical properties of industrial important chemicals. The database currently contains the properties of over 1700 chemicals and is arguably the best process design database in the world. Project 801 will continue to serve the needs of engineers and scientists in the future as new compounds and data are incorporated into the database and as new capabilities and technologies are implemented.

Keywords: Data compilation; Thermophysical data

1. Introduction

DIPPR® Project 801, Data Compilation, originated in the late 1970s as the flagship project of the Design Institute for Physical Property Data®. T.E. Daubert and R.P. Danner of The Pennsylvania State University (PSU) were selected as the principal investigators of the project, and the project has remained at PSU since the project's inception. With Dr. Daubert's approaching retirement, the steering committee of DIPPR® Project 801 began a search in 1996 for a new contractor for the project and, at the November 1996 AIChE meeting in Chicago, awarded the contract to Brigham Young University (BYU) with R.L. Rowley, W.V. Wilding and J.L. Oscarson as principal investigators. The project officially transfers January 1, 1998.

This paper reviews the history of Project 801 and looks to the future of the project.

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2. History

In the early to mid-1970s, the need for accurate data for process design and simulation led to efforts to develop cooperative projects to develop thermophysical property databases. In other countries, there were at the time government-sponsored database projects such as DECHEMA in Germany, but these projects did not satisfy the needs of industry in the US due to difficulties of distance, lack of access to source data, and lack of industry involvement. Although some companies were pooling their efforts in small cooperative consortia, there was not an industry-wide, comprehensive undertaking in the US [1,2].

As part of his work in the mid-1970s to revise his book on physical property predictions, Professor Robert Reid invited a few companies to submit to him their physical property databases to potentially be combined into a single database in the book. Although there was reluctance on the part of these companies to share their databases, several agreed on conditions of confidentiality and anonymity. Reid met with representatives of these companies at the November 1975 AIChE meeting and through the use of anonymous graphs of some of the data illustrated that, although they all had excellent databases, each database had major errors. Significantly, the errors differed from company to company [3].

In 1976, the National Bureau of Standards, with encouragement from Union Carbide, invited industry representatives to Gaithersburg where Project Evergreen, a data compilation project similar to that being worked on by Reid, was proposed. There was lively discussion at this meeting about issues of funding, principal investigators and the need for experimental measurements to be included in the effort. Although there was no clear consensus reached on the project structure or operations, there was agreement that cooperative data compilation was a good idea and the sooner such an effort was begun the better.

In January of 1977, the first International Conference on Properties and Phase Equilibria for Product and Process Design was held at Asilomar, CA. This meeting provided the opportunity for relaxed discussion of data compilation ideas between industry representatives and a variety of university faculty. These discussions led to formalized meetings to develop a cooperative data compilation effort. The first of these meetings was hosted by Allied Chemical Research in Morristown, NJ with D.W.H. Roth presiding. Allied suggested that one of the first items of business should be the selection of an appropriate umbrella organization within which to operate the project and proposed the Manufacturing Chemists Association (MCA), which is now the Chemical Manufacturers Association (CMA).

During 1977, three meetings were held at MCA headquarters in Washington DC, at which the participants debated the form and scope of the project. Some representatives desired the project to produce data books, similar to the API data book, while other representatives preferred computer products. There were also debates about the types of experimental measurements that should be undertaken and who should do them. Despite disagreements on these issues, there was agreement on the balloting procedure for project sponsors and on weighting factors based on company size [3].

Insurmountable difficulties surfaced at the second of the MCA meetings, and it became obvious that a different umbrella organization was needed. D.A. Palmer of Amoco Chemicals approached F.J. Van Antwerpen and J.C. Forman (outgoing and incoming Executive Secretaries of AIChE) about the possibility of AIChE assuming this role.

The response from AIChE was positive, and at the third of the meetings held at MCA a proposal to

join with AIChE was accepted by the group. In 1978, Roth made a formal presentation to the AIChE Council and A.H. Larsen of Monsanto prepared by-laws both of which were accepted by the council. J.W. Prados was appointed as the Council liaison to help with the organization of what would be called the Design Institute for Physical Property Data®. Prados had the requisite skills to bring the different factions with their different points of view together and at the November 1978 AIChE meeting DIPPR® was launched. Roth was elected Chairman of the Administrative Committee, Prados was elected Chairman of the Technical Committee and Palmer was elected Vice-Chairman. The steering committee for the data compilation project and other project chairmen were also elected.

The data compilation project was central to all of DIPPR®'s purposes and so a special meeting was held in September 1979 at NBS in Gaithersburg to select the contractor for this project. The contract was awarded to Professors T.E. Daubert and R.P. Danner of the Pennsylvania State University. Later that year, contractors for other projects were selected. Funded work began in 1980 on the data compilation project and three other DIPPR® projects.

3. Project 801 today

DIPPR® 801 has been the largest DIPPR® project both in terms of financial support and number of sponsoring companies. The early years of the project focused on adding compounds to the database, but as the number of compounds included in the database has increased, more emphasis has been placed on systematic review of the data in the database. Presently, there are over 1700 chemicals included in the sponsor version of the database with 29 property constants and 15 temperature-dependent property correlations. Figs. 1 and 2 show a typical data sheet (for water) from the database.

The objective of the DIPPR® data compilation project is to develop, organize, and make available to the project sponsors a complete, critically evaluated compilation of thermophysical properties of industrial important chemicals. Four operational concepts have been critical to the success of Project 801 [4].

3.1. Industrial sponsor control

The steering committee is made up of thermophysical property experts from the sponsoring companies who are very active in the operations of the project. These individuals understand best the data needs of their companies. All procedural matters, such as correlation forms, property units, or properties to be included are discussed and voted on by the steering committee before they are implemented. The committee also determines the annual project budget and the project contractor.

The committee is divided into review panels that evaluate proposed information (data, correlations, estimations) to be included in the database. Only after mutual agreement between the review panels and the project staff is the change incorporated into the database.

3.2. Critical evaluation

There are many compilations of property data, but the 801 database is unique in its emphasis on the 'best value' available. The database gives single values for property constants and single correlations for temperature dependent properties. The original sources are available in the database, but the listed

PROPERTY CONSTANTS

Chemical Abstracts Name: WATER H2O
IUPAC NAME: WATER WATER
Synonyms: DIHYDROGEN OXIDE ICE
REFRIGERANT 718 STEAM
Chemical Abstracts Number: 7732-18-5 Structural Formula: HOH

PROPERTY	UNITS	VALUE	NOTE	QUALITY CODE	ACCEPTED REFERENCE(S)			REJECTED REFERENCE(S)		
Molecular Weight	kg/kmol	18.015			1					
Critical Temperature	K	647.13		XE1	2909	2729	1886			
Critical Pressure	Pa	2.2055×10^{7}		XE1	2909	2984	2729			
Critical Volume	m^3/kmol	0.05595		XE1	2909	1886	2984	424	5	3
Crit Compress Factor		0.229		D	PS					
Melting Point	K	273.15		XE1	424	2729	3			
Triple Pt Temperature	K	273.16		XE1	424	48	2909			
Triple Pt Pressure	Pa	6.1173×10^{2}		XE1	2909	424	1319			
Normal Boiling Point	K	373.15		XE1	2909	424	2729			
Liq Molar Volume	m^3/kmol	0.018069		XE1	2909	424	3			
IG Heat of Formation	J/kmol	-2.4181×10^{8}		XE1Z	1314	1124	47			
IG Gibbs of Formation	J/kmol	-2.2859×10^{8}	1	D 1	PS	1124	48			
IG Absolute Entropy	J/kmol·K	1.8872×10^{5}		XE1Z	1314	1124				
Heat Fusion at Melt Pt	J/kmol	6.0017×10^{6}		XE1Z	424	48				
Stand Net Heat of Comb	J/kmol	0.0	2		PS					
Acentric Factor		0.3449		D	PS	43	11	22		
Radius of Gyration	m	6.1500×10^{-11}		D 3	11	12				
Solubility Parameter	$(J/m^3)^{0.5}$	4.7813×10^{4}		D 3	PS					
Dipole Moment	C·m	6.1700×10^{-30}		XE2Z	25	1518				
van der Waals Volume	m^3/kmol	0.01237	3	D 3	72	389				
van der Waals Area	m^2/kmol	2.2600×10^{8}	4	D 4	1092					
Refractive Index		1.3325		XE1	43	8				
Flash Point	K		5							
Flammibility Limits	vol %		5							
Autoignition Temp	K		5							

Issue Data: JULY 1981 Revision Date: AUG. 1988

NOTES:
1. Calculated from the enthalpy of formation and the absolute entropy.
2. Product of combustion.
3. Do not use this value to calculate r for the UNIQUAC equation.
4. Estimated by method of Vera et al. Do not use to calculate q for the UNIQUAC equation.
5. Property inappropriate for this substance.

Fig. 1. Property constants for water.

value is the single best value as determined by the project staff and steering committee. The listed value may be derived from many experimental determinations or, when no reliable experimental data are available, estimated from tested correlations and prediction methods. The evaluation procedure is at the heart of the project, and the procedures and practices are rigorous and thorough to ensure that the best value is indeed selected based on available information.

3.3. Consistency

Not all of the properties in the database are independent. For those that are interdependent, such as the properties associated with vaporization (heat of vaporization, vapor pressure, boiling point and

EQUATION CONSTANTS

Chemical Abstracts Name: WATER								H2O WATER
				COEFFICIENTS				
Property	Note	Equation	Quality	A	B	C	D	E
Solid Density Min(233.15, 51.202) Max(273.15, 50.888)		100	2	53.030	-7.8409×10^{-3}			
Liquid Density Min(273.16, 55.583) Max(333.15,54.703)	1	105	1	5.4590	0.30542	647.13	0.081000	
Vapor Pressure Min(273.16, 610.056) Max(647.13, 2.1940×10^{7})	2	101	1	73.3649	-7258.2	-7.3037	4.1653×10^{-6}	2.000
Heat of Vaporization Min(273.16, 4.4733×10^{7}) Max(647.13, 0.00)		106	2	5.2053×10^{7}	0.31990	-0.21200	0.25795	
Solid Heat Capacity Min(3.15, 180.15) Max(273.15, 38121)		100	3	-262.49	140.52			
Liquid Heat Capacity Min(273.16, 76150) Max(533.15, 89394)		100	2	2.7637×10^{5}	-2090.1	8.1250	-0.014116	9.3701×10^{-6}
Ideal Gas Heat Capacity Min(100.00, 33363) Max(2273.15, 52760)		107	2	33363	26790	2610.5	8896.0	1169.0
Second Virial Coefficient Min(273.15, -1.7827) Max(2273.10, 9.1885×10^{-3}		104	4	0.022220	-26.380	-1.6750×10^{7}	-3.8940×10^{19}	3.1330×10^{21}
Liquid Viscosity Min(273.16, 1.7016×10^{-3}) Max(646.15, 5.0277×10^{-5})		101	3	-52.843	3703.6	5.8660	-5.8790×10^{-29}	10.0
Vapor Viscosity Min(273.16, 8.9078×10^{-6}) Max(1073.15, 4.0603×10^{-5})		102	2	6.1839×10^{-7}	0.67779	847.23	-73930	
Liquid Thermal Conductivity Min(273.16, 0.56716) Max(633.15, 0.42715)		100	2	-0.4320	5.7255×10^{-3}	-8.0780×10^{-6}	1.861×10^{-9}	
Vapor Thermal Conductivity Min(273.16, 0.017019) Max(1073.15, 0.10748)		102	2	2.1606×10^{-3}	0.76839	3940.5	-4.4534×10^{5}	
Surface Tension Min(273.16, 0.077919) Max(647.13, 0.00)		106	2	0.18548	2.7170	-3.5540	2.0470	

Issue Date: JULY 1981 Revision Date: JAN. 1993

Notes: 1. For the temperature range 333.15 to 403.15 K use the coefficients: A = 4.9669, B = 0.2788, C = 647.13, D = 0.18740. For the temperature range 403.15 to 647.13 K use A = 4.391, B = 0.2487, C = 647.13, D = 0.2534.

2. For sublimation pressures in the temperature range of 149.3 K to 273.16 K use the coefficients: A = 35.169, B = -6149.4, C = -1.3785, D = 5.4788×10^{-3}, E = 1.000.

	Accepted References								
Property	Used in Regression			Not Used in Regression					Rejected References
Solid Density	424			48					
Liquid Density	2909			47	174	424			
Vapor Pressure	509	2909	424	47	175				
Heat of Vaporization	2909			175	1348				1932
Solid Heat Capacity	174								
Liquid Heat Capacity	2909			174					
Ideal Gas Heat Capaccity	2909			424	47	432	1611		
Second Virial Coefficient	2909			3	890	891	4143		3
Liquid Viscosity	3830			175	47	546	2416	2909	
Vapor Viscosity	2909	3830		174	2416	2909			
Liquid Thermal Conductivity	3830			175	23	174	1976	2659	
				2909	3830				
Vapor Thermal Conductivity	2909	3830		174	2659	2909			
Surface Tension	2909			6	1961				33

Fig. 2. Temperature-dependent correlation coefficients for water.

acentric factor) it has been a deliberate objective of the project to ensure that the values for these properties are consistent.

3.4. Completeness

To satisfy the needs for property data in process design and development, it is important to have complete sets of data. The project strives to provide values for all properties for all chemicals included in the database. Critically evaluated estimation methods are relied upon when experimental data are lacking. The only gaps in the compilation are for compounds for which estimation methods are inconsistent or for inapplicable properties such as vapor properties for inorganic salts.

The efforts over the past seventeen years by the PSU staff and the project steering committee to apply these four principles in accomplishing the objectives of Project 801 has produced what is arguably the best process design database in the world.

4. The future

At the start of 1998, DIPPR® 801 moves from PSU to BYU. The goal of the new project staff is to continue to improve the database to meet the needs of its industrial sponsors. There are several key objectives to ensure the continued success of Project 801.

4.1. Efficient database transfer

The project staffs from BYU and PSU met in May (1997) to begin the transfer of the project to BYU. At that meeting the methods used by PSU to collect and evaluate data, to enter data into the database, and to disseminate the results to the sponsors and to the publishers of public versions of the database were discussed. The software that is used by PSU to accomplish the various tasks of the project was also examined. Toward the end of 1997 the hard files which contain all of the information on the compounds and the evaluations that have been accumulated over the past 17 years will be moved to BYU. An up-to-date electronic version of the database will also be sent as soon as Penn State finishes their revisions for 1997.

Space for the project, already committed by the university, will be available by September 1, 1997. Once this space is acquired, it will be prepared to accommodate the project operations. A file server for the database has already been acquired and a second has been ordered. Other computers will be obtained later in the year. Two graduate students are currently working on computer projects to enhance the database. The Project Coordinator, a key individual in the success of the project, has been hired. The goal of the BYU staff is that there will be no interruption in service to the project sponsors and the work of maintaining and improving the database will continue smoothly.

4.2. Improve existing database

Using Microsoft ACCESS®, the database will be made fully relational. A relational database permits sophisticated user-defined searches on properties, conditions, compounds, etc. For example, a search for all compounds with boiling points within a certain range could easily be performed. This search

could also include additional conditions such as the requirement of a certain functional group. One of the graduate students mentioned above is working on this aspect of the project and a prototype of the relational database is already functioning.

Many project sponsors will want to continue to receive the database in its current format since they have software set up to interface with this format. The relational database is able to output the database in its current format. The database will maintain this backwards compatibility as long as the project sponsors desire it. It is expected, however, that as new capabilities are added to the database which can not be accommodated in its current, restricted format that format changes will be more desirable to the sponsors.

4.3. Extend accessibility and flexibility

A website will be established for access to the database by project sponsors. This will facilitate quick, flexible, and complete access to the database, raw data, staff evaluations of data, and recommendations. There will be immediate access to modifications and additions to the database. The flexibility of database access will be enhanced through the use of the website which will include graphical and computational capabilities. The combination of the website with the relational database will permit on-line searches of the database. Communications between the project staff and the steering committee will also be facilitated through the use of the Internet. There are also possibilities of individual sponsors establishing intranet access to the database for all users in their company.

The BYU staff developed a prototype website as part of the proposal process for Project 801. Although rudimentary in its capabilities, this website demonstrated some of the exciting possibilities of Internet access to the database. The second graduate student mentioned above is currently working on the design of the website. At this point communication between the website and the relational database has been established. The development of the website will continue for the next several months.

4.4. Augment the database

One of the main objectives of Project 801 has always been the addition of new compounds to the database. This work will continue with new compounds being added to the database at a rate of about 50 chemicals per year. The project sponsors develop the priority list of chemicals to be added each year. New properties will be added from time to time as approved by the steering committee. Some possibilities include molecular structure, safety, or environmental properties.

4.5. Maintain the database

Procedures for the efficient, accurate maintenance of the database will be implemented. Statistical process control concepts will be used to systematically eliminate errors in the database. Systematic reviews of the database will be performed in which the quality of the data will be evaluated, consistency tests will be performed, and new data will be incorporated into the database.

The correlations used to represent temperature dependent properties and the estimation methods used in the absence of reliable data will also be updated as better methods are developed. The project staff will be actively involved in development and evaluation of these methods.

5. Conclusion

The DIPPR® 801 Project has been an extremely valuable undertaking for the industrial sponsors of the project and for all engineers and scientists who rely on the database. The operational philosophies that have made the project successful will continue to guide the project, and new capabilities and technologies will be added to ensure that the DIPPR® Project 801 evaluated process design database continues to meet the needs of industry.

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