International Journal of Thermophysics, Vol. 10, No. 3, 1989

A Data-Base System for the Thermophysical Properties of 400 Pure Fluids and Their Binary Mixtures[1]

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In order to provide the newest and most reliable numerical data of thermophysical properties of fluids to the scientific and technical community as quickly as possible, the present data-base system was designed and constructed. This data base is concerned with 12 kinds of thermophysical properties at 7 defined physical states for about 400 pure fluids and their binary mixtures. The present system is constructed by means of a data-base management system, INQ, on our computer ACOS series System-2020 produced by Nippon Electric Co. Ltd. The data base is usable as (i) the conversational processing by TSS, (ii) the tabulation of property data in batch processing, and (iii) one of the subroutine libraries in the computation of a user's program. For users' convenience, 10 kinds of application programs have been prepared for the multipurpose retrievals, and anyone can use this data base liberally without any special knowledge on the structure or languages of this system. Furthermore, the function of graphic display of property data has been added recently.

KEY WORDS: data-base system; density; dielectric constant; enthalpy; entropy; heat capacity; refractive index; surface tension; thermal conductivity; vapor pressure; viscosity.

1. INTRODUCTION

Nowadays, accurate numerical data on the thermophysical properties of fluids are essential to both scientific research and industrial design. For scientists and engineers, it is extremely important to obtain the best information quickly. With the recent progress of computer technologies, a

[1] Invited paper presented at the Tenth Symposium on Thermophysical Properties, June 20–23, 1988, Gaithersburg, Maryland, U.S.A.

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0195-928X/89/0500-0727$06.00/0

number of data-base systems have been created in order to store and retrieve raw information. Although an enormous amount of literature has been published every year, there often exist unexpected large discrepancies among the experimental data, reported by different authors, of a fluid under the same conditions. Therefore, it is quite risky to use raw data, which one finds out from the massive information, without critical evaluation. Thus, the complete collection, critical evaluation, systematic organization, and quick dissemination of numerical data should be indispensable to improve scientific communication.

The present data-base system has been designed and constructed on 12 kinds of the thermophysical properties of nearly 400 fluids and their binary mixtures, in order to provide reliable selected values to the scientific and technical community as accurately and quickly as possible.

Although the present data base is relatively small in capacity and, for instance, numbers of registered substances and input data are limited, the system has a number of distinguishing features as described elsewhere (1). The present research has been conducted to pursue an ideal form of the data-base system and its functions to be endowed.

2. OUTLINE OF THE PRESENT DATA BASE

In consideration of the present situation of scientific information, a new data-base system on the thermophysical properties of fluids (TPPF) has been designed and created. The present system is constructed by means of a data-base management system, INQ, on our ACOS series System-2020 computer produced by Nippon Electric Co. Ltd.

Our TPPF is concerned with 12 kinds of thermophysical properties of fluids at all the possible physical states, where a substance exists as gas or liquid. The properties and the physical states are listed in Table I, where their codes are defined for the simplification and convenience of processing work and users' retrieval.

The fluids registered were selected on reflection of practical demands in science and technology, including nearly 50 elements and 120 inorganic and 230 organic compounds. According to the availability of selected data, new substances will be added from time to time. As one compound often has several names in practical or commercial use, a thesaurus of the substance names has been provided for the user's convenience. In this system, therefore, one can find out the retrieval key of a fluid from its various names, its chemical formula, or the registry number of the *Chemical Abstracts*. Each fluid is accompanied by the fundamental constants, such as molecular weight, normal melting and boiling points, critical temperature, pressure, volume, and density.

Table I. Codes of Properties and Physical States

Code	Property	Code	Physical state
D	Density	GO	Ideal-gas state
V	Specific volume	GA	Gas at 101.3 kPa
Z	Compressibility factor	GS	Gas at saturation
P[a]	Vapor pressure	GP	Gas at high pressure
C	Isobaric specific heat		
H	Specific enthalpy	LA	Liquid at 101.3 kPa
S	Specific entropy	LS	Liquid at saturation
R	Viscosity	LP	Liquid at high pressure
K	Thermal conductivity		
G[a]	Surface tension		
N	Refractive index		
E	Dielectric constant		

[a] Two-phase property (data are available only at LS).

One of the distinguishing features of the present data base is that only the most probable values, which were critically evaluated in advance, have been included. Each set of property data is accompanied by the source bibliography and the grade of estimated reliability. The uncertainties of the input data were determined by critical evaluation, taking account of the inaccuracy of the original work and judging the possible departures from auxiliary data taken from other sources. The property data of pure substances are compiled as a function of temperature and pressure in the form of either numerical data tables or correlation formulas. The property data are entered in their original units and converted into the international system of units (SI) in this system. Therefore, the output data are given completely in SI units.

Taking the primary object of this data base into consideration, it is clearly not sufficient to store the collected information in the system, and it is rather important to retrieve the desired information effectively and to disseminate it quickly. In order to fulfill this purpose, an original retrieval system was designed and 10 kinds of retrieval routines, which would be helpful in common usage, are provided for both on-line searches through TSS terminals and batch processings with line printers. The retrieval routines are summarized in Table II, and the details were described in earlier papers [1, 2]. Using the codes of the retrieval routines, one can search thermophysical properties of assigned fluids quite easily without any special knowledge of the structure or machine language of this system.

Furthermore, the present data base has installed a function of the graphic representation. It would be convenient for users to understand the inclusive trend in the behavior of a property with temperature or pressure and to compare the data with those obtained from other sources. One could obtain a graph of the property data versus temperature for the one-

Table II. Retrieval Routines Installed

Classification	Code	Function
Retrieval of registered information	REGI	To search a REGIstered Fluid (thesaurus of names of the fluid)
	COMB	To output a COMBination table of property vs physical state, where data are available
	INDI	To search registered information on an INDIvidual property of all fluids
	DATA	To search registered DATA information for a property of a designated fluid
Retrieval of supplementary information	BIBL	To output BIBLiographies from an author's name
	LITE	To output source LITErature information
	ADDI	To output ADDITIONAL information on fundamental physical constants of a designated fluid
Main retrieval of numerical data or substances	PROP	To output a PROPerty value of a fluid at a designated condition, interpolated if necessary
	TABL	To output a property data TABLe of a designated fluid at a given physical state.
	SUBS	To retrieve SUBStances which have the designated property values at a given condition

dimensional data when the assigned physical state is GO, GA, GS, LA, or LS. For two-dimensional data at the physical state of GP or LP, one can draw five isobars in a property versus temperature diagram.

3. CONFIGURATION OF THE DATA-BASE SYSTEM

The present data-base management system (DBMS), INQ, belongs to a relational inverted file type and is able to represent naturally the relations among compiled data in the form of tables, that is, sets of numerical data in one- or two-dimensional arrangements. As the individual INQ files are completely independent of each other, it is easy to add new data or to revise the compiled information by partial revisions of the INQ file concerned. The addition or change of the retrieval routines is also possible by the revision of an INQ section which combines the INQ files.

The database consists of five INQ files as follows:

(A) property data information file for pure substances,

(B) property data information file for mixtures,

(C) substance information file,

(D) bibliography information file, and

(E) formula type information file.

The property data files A and B are linked mutually with files C, D, and E by substance codes, reference codes, and formula codes, respectively.

Table III. FDL Description of Mixture File B[a]

Level No.	Data item	Data attribute	Data type
02	Substance code-1	9(4)	RK
02	Substance code-2	9(4)	RK
02	Property code	X(1)	RK
02	Physical state code	X(2)	RK
02	Reference code	9(5)	RK
02	Grade code	9(1)	DSP
02	Property data table [N]		
03	Pressure	FB	DSP
03	Data set 1 [N]		
04	Temperature	FB	DSP
04	Data set 2 [N]		
05	Composition	FB	DSP
05	Property data	FB	DSP

[a] [N], indefinite repeating set; 9(n), figures of n places; X(n), characters of n places; FB, floating binary; RK, retrieval key; DSP, display item.

The data configuration in each INQ file is described in a "file description language" (FDL), which is similar to the COBOL language in data description. As the FDL description of files A, C, D, and E were reported elsewhere [1, 2], the configuration of file B, which was designed for mixtures and added later [3], is given in Table III. The items marked by RK constitute a retrieval mode since the inverted index was prepared for them. The present retrieval system has seven INQ sections, which supply a suitable user view by combining some INQ files concerned.

Employing the DBMS INQ on the host computer, it is possible to retrieve the assigned property data effectively. In addition to the features of INQ mentioned above, it is an important merit that INQ has FORTRAN as the host language, because numerical data processings are indispensable in the design of various application programs in scientific research. Thus, one can use this data base as one of the subroutine libraries through the computation of users' programs.

4. EXPANSION TO THE MIXTURES

Knowledge of the thermophysical properties of fluid mixtures is of practical importance in the field of science and technology, especially of theoretical interest in connection with the intermolecular force between different molecules. However, studies of fluid mixtures are relatively limited, and little is known about the application of various mixture rules. From this point of view, the present data base has been expanded to binary fluid mixtures [3], whose software configuration is shown in Table III.

The input data of mixtures have been selected after critical evaluation using several sets of experimental data from the open literature, as in the

Table IV. Mixing Rule Formulas of Binary Systems

Group A	Values of pure components Q_1 and Q_2 and mole fractions x_1 and x_2
10	$Q_m = x_1 Q_1 + x_2 Q_2$
11	$1/Q_m = x_1/Q_1 + x_2/Q_2$
12	$\log Q_m = x_1 \log Q_1 + x_2 \log Q_2$
13	$Q_m^{1/2} = x_1 Q_1^{1/2} + x_2 Q_2^{1/2}$
14	$Q_m^{1/3} = x_1 Q_1^{1/3} + x_2 Q_2^{1/3}$
15	$Q_m^{1/4} = x_1 Q_1^{1/4} + x_2 Q_2^{1/4}$
16	$Q_m = x_1 Q_1 + x_1 x_2 (Q_1 - Q_2) + x_2 Q_2$
17	$Q_m = x_1 Q_1 - x_1 x_2 (Q_1 - Q_2) + x_2 Q_2$
18	$Q_m = x_1 Q_1 + x_1 x_2 (Q_1 - Q_2)^2 + x_2 Q_2$
19	$Q_m = x_1 Q_1 - x_1 x_2 (Q_1 - Q_2)^2 + x_2 Q_2$

Table IV. *(Continued)*

Group B	Including other properties of pure components: M, molecular weight; ρ, density; T_c, critical temperature
20	$Q_m = \dfrac{x_1\rho_1 + x_2\rho_2}{x_1(\rho_1/Q_1) + x_2(\rho_2/Q_2)}$
21	$Q_m = \dfrac{x_1 Q_1 M_1^{1/3} + x_2 Q_2 M_2^{1/3}}{x_1 M_1^{1/3} + x_2 M_2^{1/3}}$
22	$Q_m = \dfrac{x_1 Q_1 (M_1 Tc_1)^{1/2} + x_2 Q_2 (M_2 Tc_2)^{1/2}}{x_1 (M_1 Tc_1)^{1/2} + x_2 (M_2 Tc_2)^{1/2}}$
23	$Q_m = \dfrac{Q_1}{1 + A_1(x_2/x_1)} + \dfrac{Q_2}{1 + A_2(x_1/x_2)}$
24	Wilke's approximation for gas viscosity $A_1 = \left[1 + \left(\dfrac{Q_1}{Q_2}\right)^{1/2}\left(\dfrac{M_2}{M_1}\right)^{1/4}\right]^2 \Big/ 2\sqrt{2}\left[1 + \dfrac{M_1}{M_2}\right]^{1/2}$ $A_2 = (Q_2/Q_1)(M_1/M_2)\,A_1$
25	Brokaw's approximation for gas viscosity $A_1 = K_1(Q_1/Q_2)^{1/2}$ $A_2 = K_2(Q_2/Q_1)^{1/2}$ $K_1 = L\left(\dfrac{M_2}{M_1}\right)^{1/2}\left(1 + \dfrac{(M_1/M_2) - (M_1/M_2)^{0.45}}{2\left(1 + \dfrac{M_1}{M_2}\right) + \dfrac{1 + (M_1/M_2)^{0.45}}{1 + L}L}\right)$ $K_2 = L\left(\dfrac{M_1}{M_2}\right)^{1/2}\left(1 + \dfrac{(M_2/M_1) - (M_2/M_1)^{0.45}}{2\left(1 + \dfrac{M_2}{M_1}\right) + \dfrac{1 + (M_2/M_1)^{0.45}}{1 + L}L}\right)$ $L = (4M_1M_2/(M_1 + M_2)^2)^{1/4}$
26	Mason–Saxena's approximation for gas thermal conductivity $A_1 = \dfrac{1.065}{2\sqrt{2}}\dfrac{[1 + (Q_1/Q_2)^{1/2}(M_1/M_2)^{1/4}]^2}{[1 + (M_1/M_2)]^{1/2}}$ $A_2 = \dfrac{1.065}{2\sqrt{2}}\dfrac{[1 + (Q_2/Q_1)^{1/2}(M_2/M_1)^{1/4}]^2}{[1 + (M_2/M_1)]^{1/2}}$

case of pure fluids. However, we often encounter difficulty in evaluating property data of binary mixtures. For instance, only one set of data was available in the literature for a property of the specified mixture. The majority of the existing data would cover the limited ranges of temperature or pressure. Even if there exist several sets of experimental data, the behaviors of the property with respect to composition were not always similar at different temperatures, and the data of pure components in a mixture often did not agree with the most probable values of the corresponding pure fluids. In some works, furthermore, the data of pure components were not given, or only the effect of temperature was measured at a few constant compositions. In these cases, it becomes difficult to determine the most probable values of the mixture as a function of composition, and therefore, the uncertainty accompanied by the selected data should be greater than that of pure fluids.

Taking into account the present mixture information, retrieval modes of mixture properties have been designed by a different version from those of pure fluids. In the retrieval procedure, when one designates two substance codes of the components, property code and physical state code, in turn, the computer displays the grade of data, source reference, and available range of temperature and pressure. Then while the searcher designates a temperature range where he needs data at a constant pressure, results can be displayed on the terminal screen as a data table, in which the property data are given as a function of composition at each temperature. If one needs the graphic representation, isotherms in a property versus composition diagram are also displayed.

In order to supply the insufficiency of experimental data of mixtures, it will be more convenient for users to estimate the property values by means of appropriate mixture rules. Therefore, various mixture rules [4] were examined and the proper formulas were selected for the present purpose. Some examples of registered formulas are given in Table IV.

A function to fit the input data to the mixture rule formulas has been added to the present retrieval routine. Results of the comparison of the input data with all the formulas can be displayed in the order of their average deviations. If necessary, the comparison also can be displayed in a graphic form, examples of which are shown in Figs. 1 and 2. Thus, the best formula of mixture rules can be selected in each temperature range. If one designates a composition at a temperature, an estimated property value can be output by means of the best correlation formula.

Using the present retrieval routine, we determined the best correlation formulas for the viscosity of 65 binary gaseous mixtures and for the thermal conductivity of 75 systems at various temperatures [5].

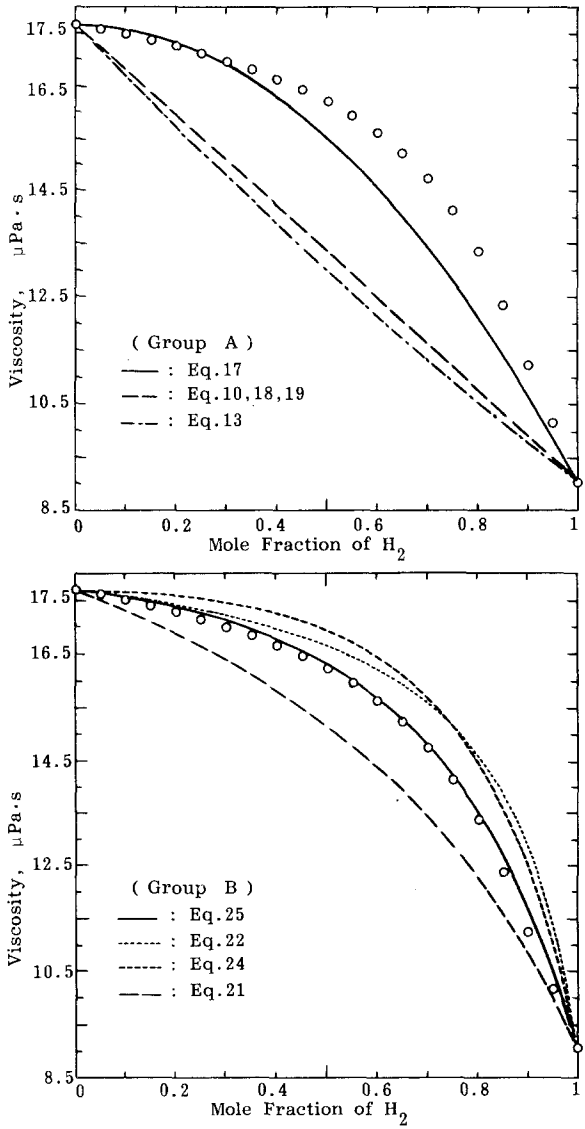

Fig. 1. Viscosity of $(N_2 + H_2)$ mixture at 307.2 K (data-base output). (○) Stored data. Equations are given in Table IV.

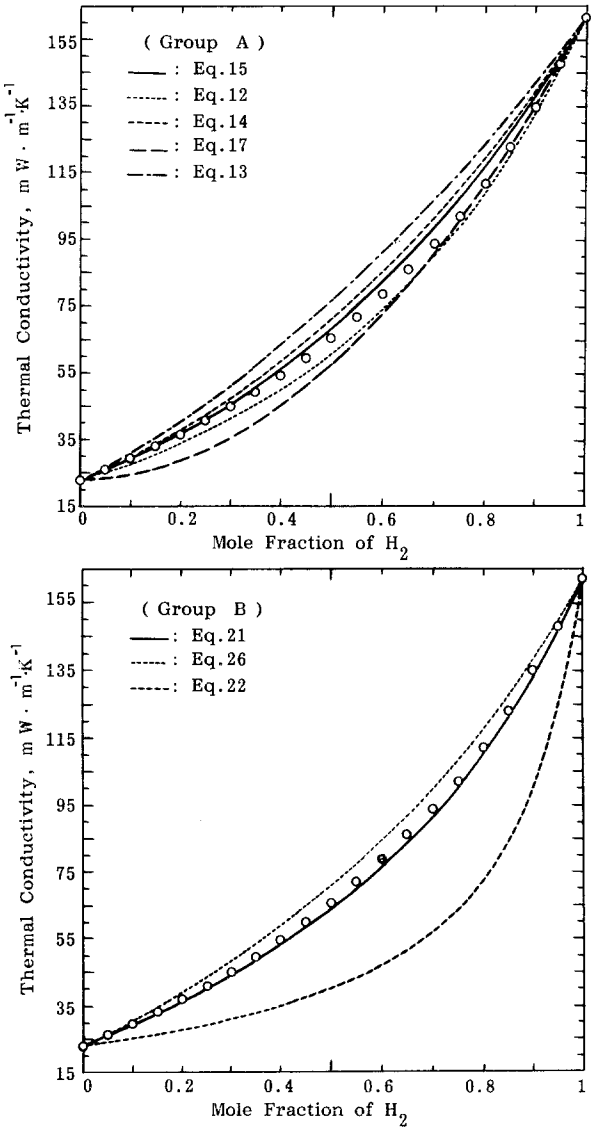

Fig. 2. Thermal conductivity of $(N_2 + H_2)$ mixture at 258.3 K (data-base output). (○) Stored data. Equations are given in Table IV.

5. MAINTENANCE OF THE DATA-BASE SYSTEM

The present data-base system, through which one can retrieve the updated most probable values on thermophysical properties of fluids quickly, has been open to academic researchers since 1981, in order to examine the system, retrieval routines, and input data. At present, as the software functions of the system are considered to have attained the desired end, our efforts are concentrated upon the maintenance of stored data.

Of course, it is most important to keep the compiled data accurate and up-to-date. However, mistakes in data processing or questionable values in the outputs are sometimes pointed out by users. Therefore, the correction of mistakes, recheck of data evaluation processes, renewal of input data, and addition of new data have been continued on a daily basis. The supplemental working programs on an off-line microcomputer are also designed for convenience in such maintenance works.

In the present data-base system, as individual INQ files are independent of each other, it is easy to revise the stored data or to add new data by the partial revisions of the INQ file concerned. This should be a distinguishing merit of the data-base system on a large host computer, in comparison with the small data base recorded on sets of floppy disks which are often sold commercially.

The present data base will be connected with the interuniversity network in the near-future.

ACKNOWLEDGMENTS

This investigation has been supported partly by a Scientific Research Grant of the Ministry of Education (1979, 1980, 1983–1988), Research and Development Funds of Hyogo Foundation for Promotion of Science and Technology (1982), and funds of the Information Processing Center, Kobe University (1978–1988). The author wishes to express his appreciation to our co-workers at Kobe University: Professor T. Takamori and Dr. Y. Takaoka for the design of the system, Professor Y. Tanaka for the data evaluation, Mr. S. Kominami for the graphic design, and Mr. H. Sugitani for the mixture base. He also thanks Mr. M. Tanaka and Miss K. Hamaoka for their extensive work in data processing. The author should like to acknowledge Professors H. Iwasaki, S. Saito (Tohoku University), K. Watanabe (Keio University), and J. Osugi and Y. Takesaki (Kyoto University) for their valuable advice on the early design of this system.

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