International Journal of Thermophysics, Vol. 7, No. 4, 1986

The MIDAS Data-Bank System for the Transport Properties of Fluids[1]

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The development of the MIDAS Data-Bank System from its origin as part of the first DECHEMA properties data project in 1977 is described. The system concentrates the rapidly increasing amount of data for the viscosity and thermal conductivity for pure fluids and fluid mixtures by evaluation of the most reliable data sets. The data sets are represented by density–temperature correlations which are the customary method to correlate transport properties. To allow for a direct calculation of the transport properties from given pressures and temperatures, a new type of equation has been developed. As an example, the simultaneous representation of the viscosity and thermal conductivity of oxygen by one transport equation of state is discussed.

KEY WORDS: correlation; data bank; fluid mixtures; oxygen; pure fluids; transport equation of state; thermal conductivity; viscosity.

1. INTRODUCTION

The need for accurate thermophysical properties information and its impact on technological progress have received increasing recognition, particularly in the decade 1972–1982. A number of memoranda [1–3] pointed out that noncritical use of literature data in engineering calculations may bias considerably equipment design and performance and may even cause dangerous failures. However, the divergence between the scientific experimental "data production" diffused in numerous publications and the

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0195-928X/86/0700-0973$05.00/0

industrial need for data with a known quality became more and more obvious at that time.

To improve the situation and to satisfy the applicational requirements, it was necessary to concentrate the rapidly growing quantity of data in evaluation projects as in the research on the properties of Water and Steam [4] and in the TPRC project, later called CINDAS [5]. In several countries joint industry–university projects on data evaluation were established, of which the German "Entwicklungsgruppe Stoffdatencompiler" (EG-SDG), starting in 1977, was among the first initiatives. Initially sponsored by the government, companies from the chemical industry and university institutes formed a task group under the auspices of DECHEMA to compile the most reliable thermodynamic and transport properties data and to develop improved calculation methods on this basis. The results of this continuing project are implemented in the DETHERM Thermophysical Property Information System [6, 7], which provides on-line access for end-users. Other projects of this kind developed, for instance, in the United Kingdom as the Physical Properties Data Service (PPDS) and in the United States as the Design Institute for Physical Property Data (DIPPR).

2. THE MIDAS DATA-BANK SYSTEM

Being one of the founding members of the EG-SDC, the Institute for Technical Thermodynamics and Thermal Process Design, University of Stuttgart (ITT), was assigned to evaluate the transport properties, viscosity, and thermal conductivity of pure fluids with a special emphasis on their pressure dependence. In the following step, the recommended values should be represented by correlations to reduce the amount of data needed in process design calculations and to complement the DETHERM system. Finally, new methods to represent transport properties directly in terms of pressure and temperature and covering the entire fluid region of a substance should be developed.

The initial contribution of the ITT to the task group consisted of a compilation of viscosity data which was published later in a monograph [8]. As the scope of the new project included both viscosity and thermal conductivity, it was necessary to reorganize the data evaluation by making more extensive use of computer facilities to handle the large amount of literature data. An electronic data bank was established to store not only bibliographic references but also the numerical data published therein. This data bank ensures a quick availability of the relevant experimental results to the evaluation procedure supported by a set of computer programs. The programs were developed to perform routine steps in the generation of recommended values such as the interpolation of different data sets on a

common pressure and temperature grid and the generation of various graphical representations which would be very time-consuming if carried out manually. Derived from its purpose this system was designated by the acronym MIDAS (Multiple ITT Data Analysis System). A connection to the gold-addicted king of this name in the Greek mythology exists only insofar as "gold-plated" numbers play a certain role in the research on thermophysical properties [9].

MIDAS serves as a link between the primary field of thermophysical properties research, namely, the experimental sector and the end-user who asks for reliable data. The latter need is being satisfied since the beginning of the project through its continuing contribution to the EG-SDC and the DECHEMA system DETHERM. However, MIDAS has ever since been equally understood as a science-oriented tool. This role became reinforced in 1983 when MIDAS was incorporated in the IUPAC Subcommittee on Transport Properties. The data bank became available to the members of the subcommittee, who make use of it in their data correlation. In turn, a questionnaire is circulated annually among the members to invite experimentalists to submit papers accepted for publication so that the data can be included in MIDAS in the sense of a central depository.

3. PRESENT STATUS

An outline of the MIDAS Data-Bank System in its present configuration is given in Fig. 1. Besides the originating institute, ITT at Stuttgart, two other institutes now contribute to the evaluation of transport properties and to the development of new correlation concepts:

the Institute for Thermo- and Fluid Dynamics (ITF), Ruhr-University, Bochum; and

the Institute for Fluid and Thermodynamics (IFT), University-GH, Siegen.

The tasks of the project are shared among the participating institutions according to their respective research interests and experiences, which complement each other smoothly. Such parts which require an extensive amount of computer time can be performed effectively at the ITT using the powerful computer equipment at the University of Stuttgart. Therefore, the ITT is assigned to the maintenance of the MIDAS data bank, the continuous input of new data, and its evaluation. The generated recommended values are subsequently used to establish correlations for the transport properties. These include customary formulations in terms of density and temperature as well as the newly developed concept of transport equations of state in terms of pressure and temperature so that the user can employ

the form most convenient in his/her application. The correlations are added as subprograms to a library package.

The ITF at Bochum contributes to the project by its expertness in optimization strategies for equations of state which originated in the work of Wagner [10, 11]. For complex problems as the structural optimization of equations of state, Ewers and Wagner [12] developed a superior random strategy which incorporates principles of biological evolution and

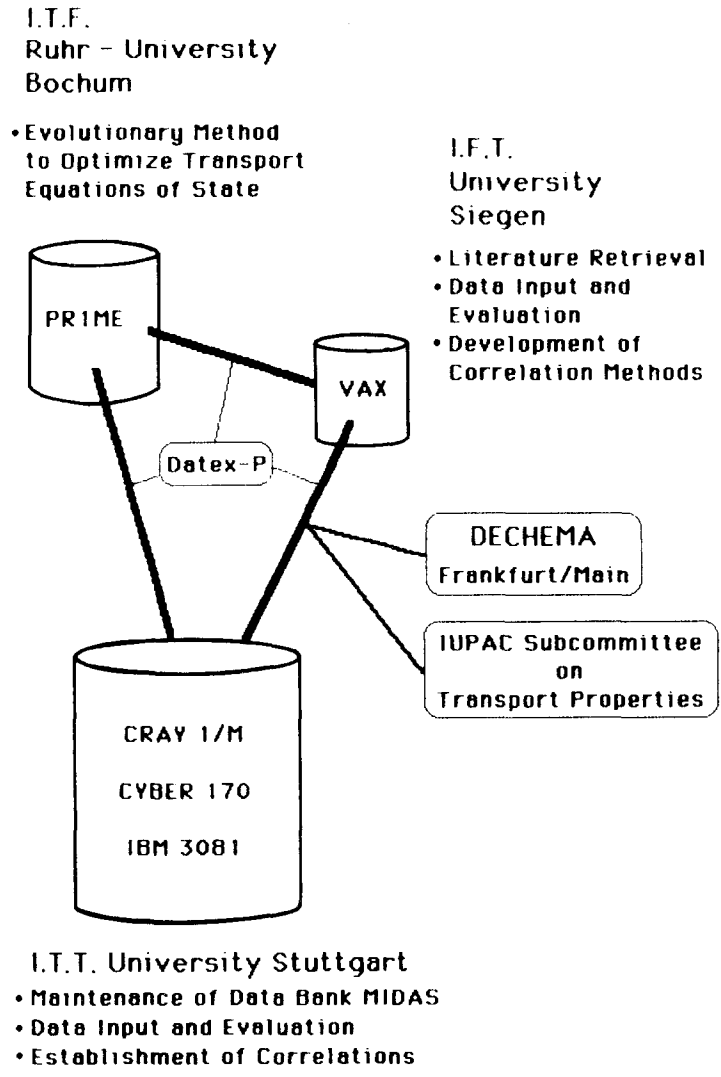

Fig. 1. Organization of the MIDAS Data-Bank System.

consequently is called the evolutionary optimization method (EOM). This method has been successfully employed by Schmidt and Wagner [13] to establish a more effective fundamental equation of state for oxygen, with an improved accuracy over an extended range of the fluid region of that substance. Because of their similarity to thermal equations of state, the EOM is now also being employed to find optimal functional forms for transport equations of state.

The IFT at Siegen shares in the time-consuming activity of observing and retrieving publications related to the transport properties of fluids and, especially, of acquiring new experimental data from the actual literature. It is also responsible for circulating anually a questionnaire among the members of the IUPAC Subcommittee on Transport Properties. The data received are entered to the local computer at Siegen and transmitted to the MIDAS data bank either via magnetic storage media or via the Datex-P network which links remote computer systems. In turn, this communication is used to access MIDAS interactively within the process of data evaluation which is also carried out at Siegen. Furthermore, theoretical studies are under way to apply transport equations of state to viscosities and thermal conductivities of various pure substances and to improve the capabilities of the equations.

4. DATA EVALUATION METHOD

In general, our knowledge on transport properties is estimated to be much lower than on equilibrium properties, which is due to the historical development of thermodynamics [14]. Scheffler et al. [15] have analyzed the time dependence of the increase in experimental data for the viscosity of water substance. It turned out that in the decade 1964–1974 more measurements were carried out than since the beginning of viscometry in 1840. This example is certainly not typical for other substances because water is a very well-investigated fluid with respect to its transport properties. For most of the other fluids the situation may be even worse.

One reason for the avalanche-like increase in data for transport properties is the progress in the measurement techniques. Experiments on transport properties involve a fluid being exposed to a nonequilibrium condition and its response to that being detected. Electronic data recording devices have facilitated such measurements more than in any other field and even made possible the introduction of new methods. For example, the transient hot-wire method became, within a very short time, the standard thermal conductivity experiment. Also, the scope of the measurements was extended and includes now substances relevant for chemical processes [16].

The major steps in the evaluation of viscosity and thermal conductivity data are illustrated in Fig. 2. The procedure follows closely the IUPAC principles for the preparation of thermodynamic tables and correlations of the fluid state which were laid down recently in the guide of Angus [17]. After the retrieval of all available data sources for the transport property of a substance, the most relevant data sets are preselected. Normally, some sources must be omitted because they contain too few data points or present their data in a form not suitable for further evaluation. On the average, 50% of all collected references can be used. The bibliographic section of the MIDAS data bank contains currently about 3000 selected references.

In a second step, the data sets are entered to the computer and converted to SI units if necessary. Before getting loaded into the numerical section of the MIDAS data bank, all data sets are checked for typing errors and misprints. Of great advantage for this purpose are three-dimensional representations [18, 19], which give a good impression of the internal consistency of the data and allow for a first rough assessment of their quality. This is demonstrated in Fig. 3, which gives a depiction of the experimental thermal conductivity data for liquid *n*-undecane by Mustafaev [20]. The peak was revealed as a misprint and was corrected before the data set was loaded to MIDAS. Likewise, corrected versions of experimental results have been produced in many other cases. At present, the data bank contains 211 viscosity sets with a total of 22,552 data triples for 84 fluids and 960 thermal conductivity sets with a total of 98,461 data triples for 119 fluids.

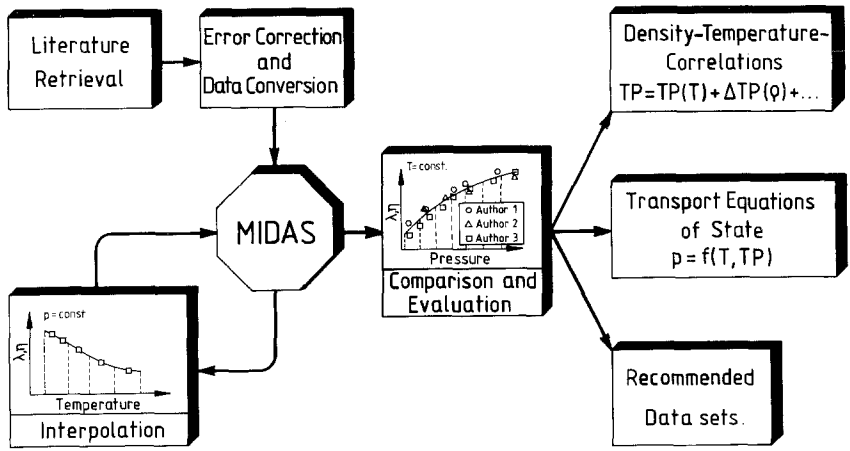

Fig. 2. Data evaluation method.

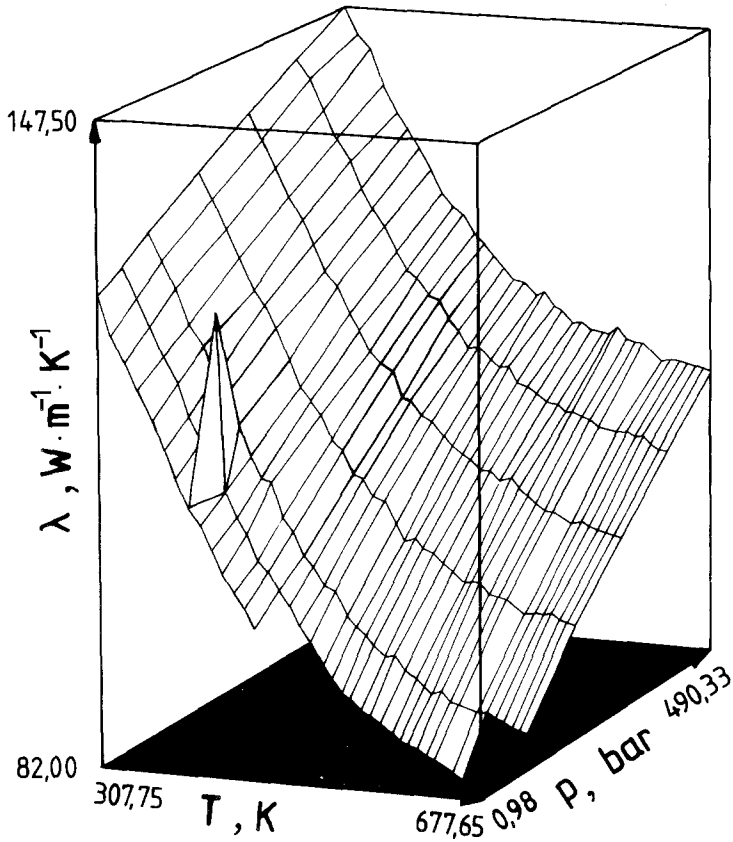

Fig. 3. Representation of a literature data set with experimental scatter and a misprint. Thermal conductivity measurements of *n*-undecane by Mustafaev [20].

Unfortunately, experiments from different laboratories are not carried out at the same thermodynamic states, which prevents an immediate comparison. It is therefore necessary to interpolate the original data sets on a common temperature grid, the spacing of which has to be adjusted to the temperature dependence of the property under consideration. The interpolated data sets are also loaded to MIDAS.

Next, original and interpolated values are plotted along isotherms. Weight factors are assigned to every data set to fit auxiliary correlations which describe the pressure as a function of the transport property along each isotherm. From these correlations the recommended values are calculated at a fixed pressure grid and their uncertainty can be estimated. The evaluation cannot be done only on the basis of objective criteria such

as the accuracy and scatter of the original data, adopted experimental method, purity of the sample, etc. Also, more subjective criteria are of same importance and cannot be excluded.

So far, the viscosity of 51 pure fluids and the thermal conductivity of 44 pure fluids have been evaluated in wide ranges of pressures and temperatures. These data are stored in MIDAS and can be provided as skeleton tables when quick values are needed. They are the basis to establish the aforementioned types of correlations, which are discussed in the next paragraph.

5. CORRELATIONS

Transport properties of fluids are usually represented as functions of density and temperature (Fig. 4). This choice of independent variables has evolved from the Enskog solution of the Boltzmann equation for moderately dense gases, which has been modified to describe also dense fluid states [14, 21]. As demonstrated for the viscosity of methane (Fig. 5), the surfaces of the transport properties yield a rather simple and smooth shape in view of this formulation. Hence, they can be represented by simple functions with only a limited number of adjustable parameters. Such a correlation [22] was used to generate the surface in Fig. 5; numerous other

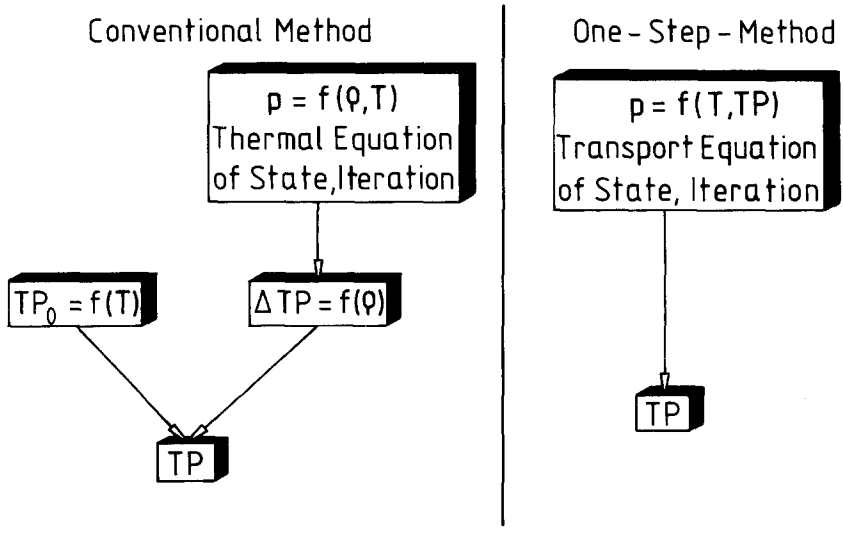

Fig. 4. Possible formulations to correlate transport properties of fluids.

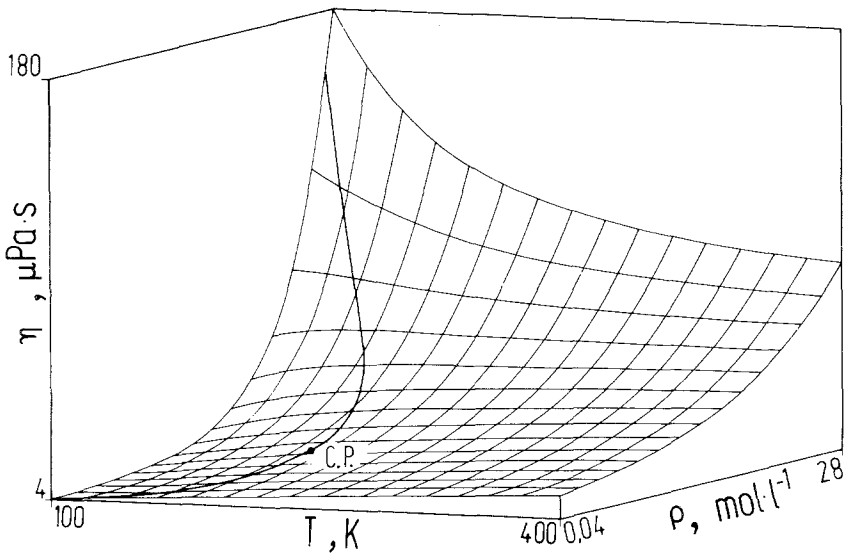

Fig. 5. The viscosity of methane over density and temperature.

examples can be found in the book of Vargaftik et al. [16], and we adopted it in our work on the thermal conductivity of fluid air [23].

One of the major drawbacks of this common approach is that from a given pair of pressure and temperature, the density must first be obtained from a thermal equation of state before any transport property can be calculated. This two-step procedure (Fig. 4) is unsatisfactory not only in its practical applicability but also from a more principal point of view. Transport processes result from the same molecular phenomena as the macroscopic equilibrium properties of a substance [24]. The complete information about the molecular interaction of a fluid is given by its fundamental equation of state. Therefore, it should be possible to represent also transport properties directly in terms of pressure and temperature as indicated in Fig. 4.

To develop such a formulation, the pressure–temperature dependence of the transport properties was studied in a phenomenological analysis of the evaluated data sets. Figure 6 shows as a typical example the thermal conductivity of oxygen over the pT plane. To represent these surfaces it turned out that a pressure-explicit formulation,

$$p = f(T, \mathrm{TP}) \tag{1}$$

where T is the temperature and TP is a transport property, i.e., either viscosity or thermal conductivity, is superior to the two other possible combinations of these variables [25]. Self-evidently, this formulation

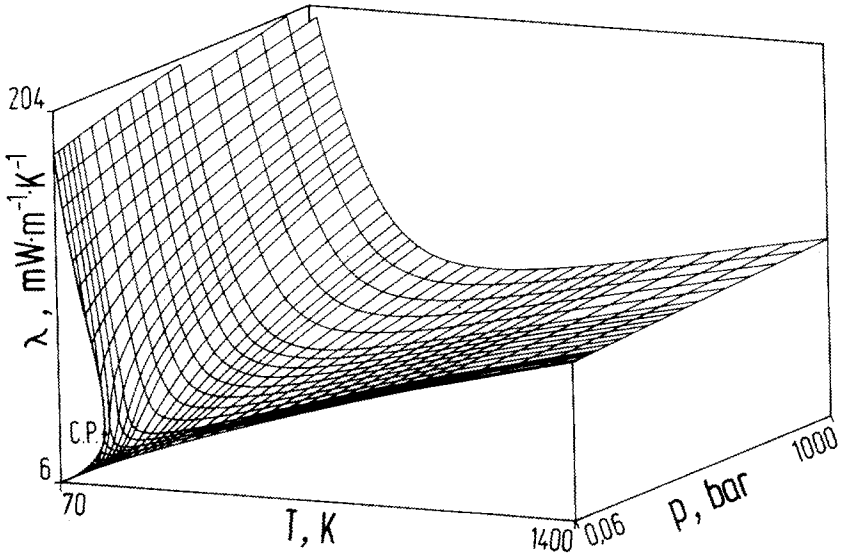

Fig. 6. The thermal conductivity of oxygen over pressure and temperature.

agrees with the basic structure of thermal equations of state and was consequently called the transport equation of state.

The concept of transport equations of state was first applied to the viscosity of water, which could be represented with a comparable accuracy as by the conventional method [25]. Meanwhile, equations of this type have been established for the viscosities and thermal conductivities of most of the simple fluids. For example, the equation for the transport properties of oxygen reads

$$p_R = A \cdot \mathrm{TP}_R + B \cdot \mathrm{TP}_R{}^2 + C \cdot \mathrm{TP}_R{}^3 + D \cdot \mathrm{TP}_R{}^4 + E \cdot \mathrm{TP}_R{}^5 + F \cdot \mathrm{TP}_R{}^6 + (G \cdot \mathrm{TP}_R{}^3 + H \cdot \mathrm{TP}_R{}^5) \cdot \exp(-I \cdot \mathrm{TP}_R{}^2) \tag{2}$$

with the temperature functions

$$\begin{aligned} A &= a_1 T_R{}^{-0.5} + a_2 T_R{}^{0.5} + a_3 T_R + a_4 T_R{}^{1.5} + a_5 T_R{}^2 \\ B &= a_6 + a_7 T_R + a_8 T_R{}^{1.5} + a_9 T_R{}^2 \\ C &= a_{10} T_R{}^{0.5} + a_{11} T_R + a_{12} T_R{}^2 \\ D &= a_{13} T_R + a_{14} T_R{}^2 \\ E &= a_{15} T_R{}^2 \\ F &= a_{16} T_R{}^2 \\ G &= a_{17} + a_{18} T_R + a_{19} T_R{}^2 \\ H &= a_{20} T_R{}^{0.5} + a_{21} T_R{}^{2.5} \end{aligned} \tag{3}$$

Pressure and temperature were reduced as usual by their respective critical values $p_R = p/p_C$ and $T_R = T/T_C$, which is not reasonable for the transport properties. Hence, a new reduction mode was adopted according to

$$TP_R = \ln(TP/TP^* + 1) \tag{4}$$

where the transport properties appear not only as reduced quantities but additionally by their natural logarithm, which was introduced to account for the strong temperature dependence in the liquid region. The reduction constant for the viscosity is given by

$$TP^* = (M^{1/2} \cdot {p_C}^{2/3})/({T_C}^{1/6} \cdot R^{1/6} \cdot {N_A}^{1/3}) \tag{5}$$

and for the thermal conductivity similarly by

$$TP^* = (R^{5/6} \cdot {p_C}^{2/3})/({T_C}^{1/6} \cdot M^{1/2} \cdot {N_A}^{1/3}) \tag{6}$$

These modules have already been derived by Kamerlingh Onnes [26] and contain the universal gas constant R, the molar mass M, and Avogadro's number N_A. A unit constant was added arbitrarily in Eq. (4) to avoid singularities of the logarithm in the gas region.

Fitting the equation to the recommended viscosity data set of oxygen yielded the following numerical values of the parameters

$a_1 = -7.966\,490\,38$, $a_2 = 6.216\,083\,94$, $a_3 = 3.925\,188\,98 \times 10$
$a_4 = -1.323\,497\,64 \times 10$, $a_5 = -2.656\,190\,45 \times 10$, $a_6 = -5.766\,574\,76$
$a_7 = -5.160\,346\,27 \times 10$, $a_8 = 1.852\,708\,58 \times 10$, $a_9 = 5.827\,971\,22 \times 10$
$a_{10} = 7.694\,654\,90$, $a_{11} = 1.538\,463\,20 \times 10$, $a_{12} = -5.629\,572\,35 \times 10$
$a_{13} = -3.643\,377\,52$, $a_{14} = 2.595\,708\,52 \times 10$, $a_{15} = -5.806\,757\,48$
$a_{16} = 5.187\,468\,82 \times 10^{-1}$, $a_{17} = 6.213\,978\,63 \times 10^2$, $a_{18} = -1.667\,944\,20 \times 10^3$
$a_{19} = 5.292\,049\,66 \times 10^2$, $a_{20} = 3.432\,378\,63 \times 10^3$, $a_{21} = -2.051\,413\,96 \times 10^3$
$I = 15$

The nonlinear parameter I was varied independently until an optimal value was obtained.

Because of the striking similarity between the viscosity and the thermal conductivity surfaces, it was attempted to apply Eq. (2) with the temperature functions (3) to represent also the thermal conductivity of oxygen. Without structural modifications and replacing only the reduction constant TP* according to Eq. (6), the fit to the recommended data set proved even more accurate and yielded the following optimal parameter values:

$a_1 = 6.474\,078\,47 \times 10^{-1}$, $a_2 = -8.376\,886\,69 \times 10$, $a_3 = 2.152\,222\,93 \times 10^2$
$a_4 = -3.211\,170\,60 \times 10$, $a_5 = -1.989\,354\,97 \times 10^2$, $a_6 = 2.837\,561\,38 \times 10$
$a_7 = -1.824\,506\,66 \times 10^2$, $a_8 = 2.109\,530\,58 \times 10$, $a_9 = 3.612\,152\,89 \times 10^2$
$a_{10} = 3.530\,291\,61 \times 10$, $a_{11} = 5.561\,252\,05 \times 10$, $a_{12} = -1.207\,744\,15 \times 10^3$

$a_{13} = -5.510\,231\,86$, $a_{14} = 8.168\,966\,80 \times 10$, $a_{15} = 4.466\,749\,97 \times 10$
$a_{16} = -5.301\,968\,47$, $a_{17} = -1.980\,131\,21 \times 10$, $a_{18} = -1.167\,026\,87 \times 10$
$a_{19} = 9.478\,243\,70 \times 10^{2}$, $a_{20} = -3.470\,179\,52$, $a_{21} = 2.370\,261\,39 \times 10^{-2}$
$I = 0.05$

The accuracy of the transport equation of state for oxygen is summarized in Figs. 7 and 8 in the form of departure surfaces. Percentage deviations between calculated and recommended values are plotted over the range of the recommended data sets as a function of pressure and temperature. The viscosity is represented with maximum deviations of 2.85 and -4.56%, which is within the uncertainty ascribed to the evaluated data set. The mean percentage deviation is -0.14%, with a standard deviation of $\pm 1.14\%$. The shape of the departure surface in Fig. 7 suggests that the equation should not be extrapolated to low temperatures at very high pressures.

In the case of the thermal conductivity (Fig. 8) the maximum deviations are 3.23 and -2.12%. The mean percentage deviation is reduced significantly to 0.01%, as well as the standard deviation to $\pm 0.65\%$. However, the plot indicates a "break-out" of the equation when employed at temperatures below 70 K and above 1400 K.

Nevertheless, the capability of the equation is surprisingly good considering that it represents both the viscosity and the thermal conductivity

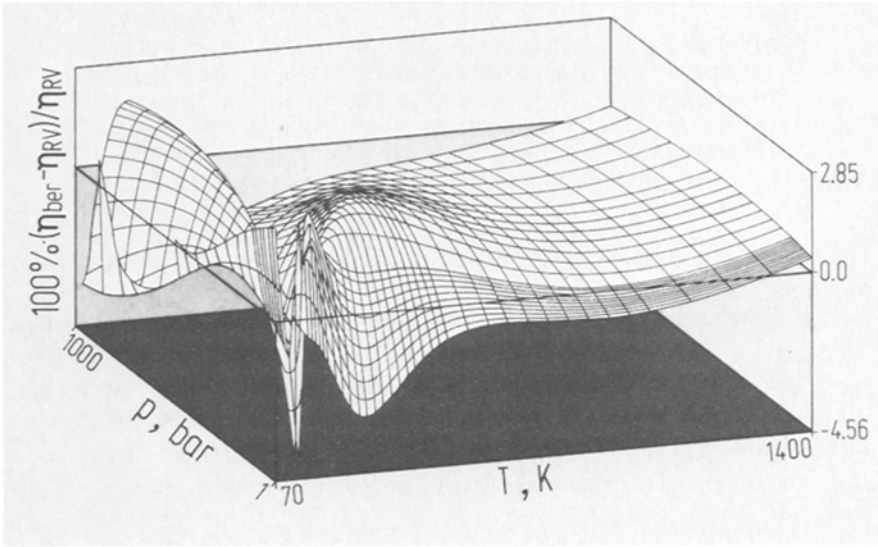

Fig. 7. Departures of the transport equation of state from evaluated data for the viscosity of oxygen over pressure and temperature.

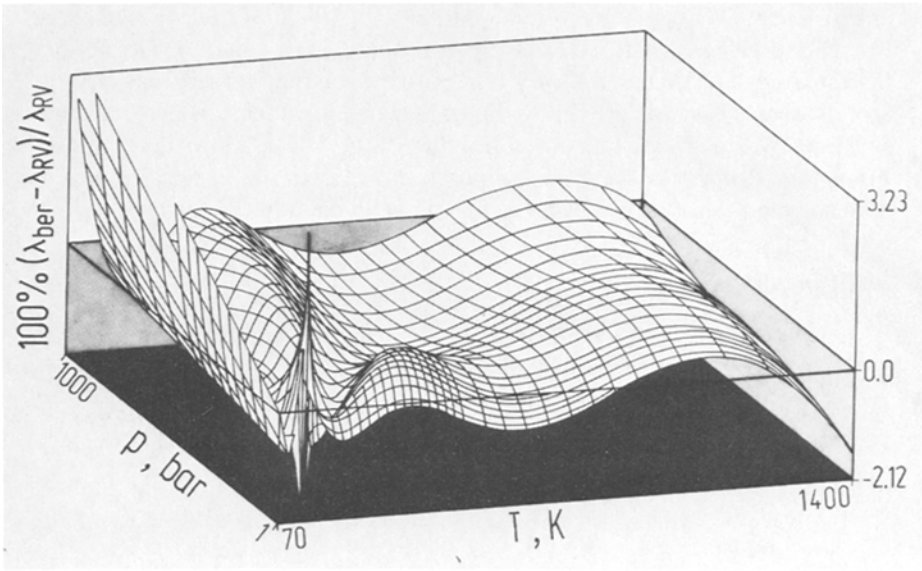

Fig. 8. Departures of the transport equation of state from evaluated data for the thermal conductivity of oxygen over pressure and temperature.

of one substance with the same functional form in a wide range of fluid states. This means a considerable simplification in the practical calculation of transport properties. Transport equations of state have, meanwhile, been applied to other fluids, too.

6. CONCLUSION

The MIDAS Data-Bank System is a cooperative effort to improve the knowledge on the viscosity and the thermal conductivity of fluids. It is felt that a great potential for such improvements still exists because the transport properties have been in the background of the general research on thermophysical properties, which concentrated on equilibrium properties for a long time. Through the evaluation of reliable data and the development of new correlation methods, the system contributes to the industrial as well as the scientific field and can be an opportunity to close the gap between the demand and the availability of transport property information.

ACKNOWLEDGMENTS

We owe sincere thanks for successive financial support to Bundesministerium für Forschung und Technologie (BMFT), Arbeitsgemeinschaft

industrieller Forschungsvereinigungen (AiF), and Deutsche Forschungsgemeinschaft (DFG). Special thanks are due to Dr. Rainer Eckermann of DECHEMA and our partners of the Entwicklungsgruppe Stoffdatencompiler for providing the framework in which this project could develop. We are grateful to our colleagues of the IUPAC Subcommittee on Transport Properties for their cooperation. Thanks are especially due to the chairman, Professor J. Kestin, for his valuable advice.

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