Thermal Conductivity of Ordinary Water Substance in the Ideal-Gas Limit

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Values of the thermal conductivity coefficient in the ideal-gas limit have been determined from experimental data. A data bank developed in the frame of the joint project of the IAPWS and the Subcommittee on Transport Properties Commission of the IUPAC was utilised. Low density values on selected isotherms were correlated and extrapolated to zero density. A virial type equation of thermal conductivity for low density was applied in this procedure. Extrapolated values of thermal conductivity coefficient were correlated. Three equations with different number of coefficients are discussed.

1. Introduction

In this paper we analysed the data of the H_2O Thermal Conductivity Data Bank [1] and propose new forms of the equation for the thermal conductivity in the ideal-gas limit $\lambda_0(T)$.

2. Source Data

The database [1] contains 5107 experimental values for thermal conductivity with ranges of temperature 256 K to 1191 K and pressure 0.00314 MPa to 785 MPa. Temperatures of old experiments have been converted to the ITS-90. Values of thermal conductivity coefficients have not been converted because of low influence from the change of temperature scales. The change would not exceed 0.2 % in conversion from IPTS-68 and 0.42 % in conversion from IPTS-48 [2].

3. Elaboration of Experimental Data

3.1. Extrapolation Equation The values of the coefficient of thermal conductivity in the ideal-gas limit were derived by extrapolation of selected experimental data to zero density. For extrapolation a virial type equation of thermal conductivity [3], [4], [5] was applied

$$\lambda(\rho,T)=\lambda_{tr}(\rho,T)+\lambda_{int}(\rho,T) \qquad (1)$$
$$=\lambda_{0tr}(T)\left[1+B_{\lambda,tr}(T)\rho\right]+\lambda_{0\,int}(T)\left[1+B_{\lambda,int}(T)\rho\right]$$

On each isotherm the virial conductivity coefficients have constant values. Equation (1) for $T = const.$ was simplified to the form

$$\lambda(\rho) = \lambda_0 + K \cdot \rho \qquad (2)$$
$$(T = const.)$$

3.2. Data Selection Extrapolation using equation (2) requires data of low density. For that reason only the data with density lower than 50 $kg.m^{-3}$ were accepted in calculations like in [6].

Density values from the database [1] were compared with density calculated from formulation IAPWS 1995 [7]. It was found that 15 experimental points were significantly different. Those points were removed. The differences are given in Table 1.

3.3. Experimental isotherms The data were divided into 62 sets. Points within a set had equal temperature and formed an experimental isotherm. Those, which contained at least three points and which had at least one point with density lower than 1 $kg.m^{-3}$, were accepted for extrapolation.

This restriction diminished the number of acceptable data to 231 on 36 experimental isotherms in temperature range from 345.45 K to 748.08 K. These experimental points are displayed in Fig. 1.

3.4. Conversion of Thermal Conductivity Values to Nominal Isotherms To increase the number of isotherms, the remaining values of thermal conductivity were converted to nominal isotherms. In a nominal isotherm data within the temperature range of 10 K were grouped together. The conductivity value was converted from its original value to a nominal value at T_{nom} defined according to (3). The conversion was done via equation (4).

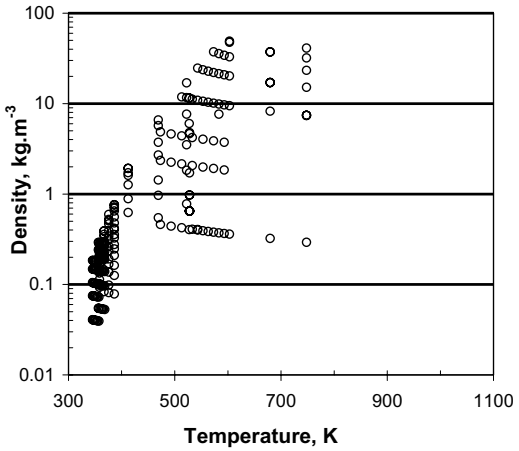


Fig. 1. Points on the experimental isotherms.

$$T_{nom} = (T_{max} + T_{min})/2 \qquad (3)$$

where T_{max} and T_{min} were the maximum and minimum temperature within a nominal isotherm. Points on those isotherms are displayed in Fig. 2. The number of nominal isotherms was 46 and the total number of points on all of them was 829 in temperature range from 350.325 K to 1066.5 K.

A typical diagram with points along straight line is displayed in Fig. 3.

3.5. Conversion Equation Temperature conversion

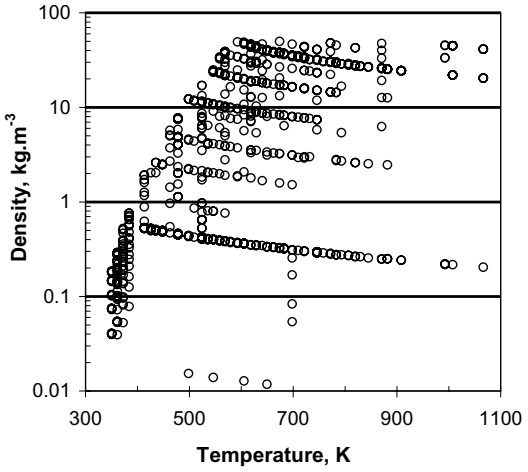


Fig. 2. Points on the nominal isotherms.

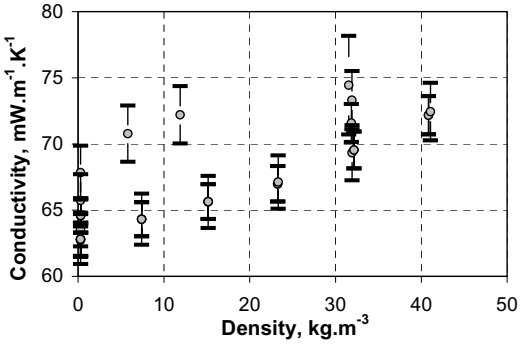


Fig. 3. Points on the isotherm 386.37 K.

of experimental values of the conductivity to the nominal temperature, T_{nom}, was made according to equation (4):

$$\lambda_{conv}(T_{nom}, \rho) = \lambda_{exp}(T_{exp}, \rho) + \Delta\lambda_{calc} \qquad (4)$$

where

$$\Delta\lambda_{calc} = [\lambda(T_{nom}, \rho) - \lambda(T_{exp}, \rho)]_{calc}$$

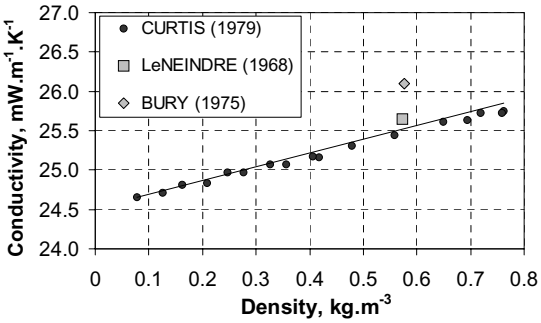
The increment $\Delta\lambda_{calc}$ was calculated from IAPWS equation [8].

3.6. Discrepancies Examples of discrepancies on some isotherms are shown in Fig. 3 to Fig. 6.

Table 1. Difference between database density and IAPWS-95 [7] density calculation. (for density less than 50 kg.m^{-3})

Author	Temp. K	Pressure MPa	Density kg.m^{-3}	Density IAPWS kg.m^{-3}
Tim	342.12	0.029852	0.19005	978.3183
Tim	346.82	0.036513	0.22954	975.6042
Tim	372.52	0.0992	0.58565	958.8003
Dij	297.99	0.00314	0.022833	997.0442
Var	429.89	0.1	0.5148	0.508
Var	455.43	0.1	0.485	0.4787
Var	465.26	0.1	0.4745	0.4683
Var	576.15	0.1	0.382	0.377
Var	646.09	0.1	0.3403	0.3359
Var	685.74	0.1	0.3206	0.3164
Var	810.56	0.1	0.271	0.2675
Var	877.09	0.1	0.2504	0.2472
Var	909.77	0.1	0.24142	0.2383
Var	997.68	0.1	0.22012	0.2172
Fro	299.99	0.003536	0.02554	996.5158

Tim: Timrot 1935, Dij: Dijkema 1972,
Var: Vargaftik 1973, Fro: Frohn 1980



Data from Curtis in Fig. 4 can be linearly approximated but the points by LeNeindre and Bury do not agree with the data of Curtis.

Fig. 5 represents measurements by 6 different authors. Uncertainties are added to each point. It is apparent that in some cases the ranges of uncertainties of corresponding points do no overlap.

A similar comment is possible to make to Fig. 6, where a systematic deviation between two groups of points is apparent.

3.7. Extrapolation of Data on Isotherms to Zero Density Each isotherm was extrapolated to zero density to calculate λ_0. Weighted regression procedure was used in this step.

Together with value λ_0 corresponding uncertainty was calculated for each isotherm. In that way a data set for development of equation $\lambda_0(T)$ was obtained.

That data set of 82 points is displayed in Fig. 7.

4. Equation for Thermal Conductivity in the Ideal-Gas Limit

We utilised the form of the IAPWS equation for $\lambda_0(T)$ [8] in the regression analysis:

$$\lambda_0(\bar{T}) = \frac{\sqrt{\bar{T}}}{\sum_i \frac{E_i}{\bar{T}^{N_i}}} \lambda^*, \qquad (5)$$

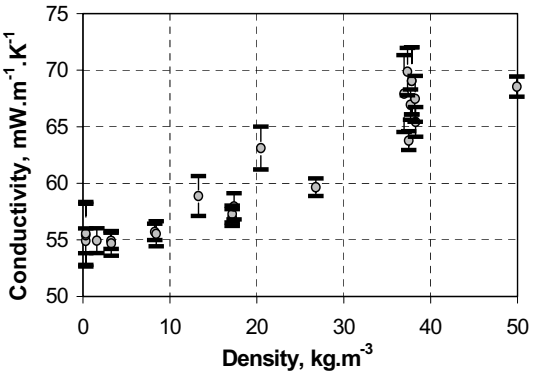


Fig. 5. Uncertainty of experimental values on the isotherm 673.86 K.

Fig. 6. Uncertainty of experimental values on the isotherm 745.77 K.

where λ^* = 0.4945 W.K^{-1}.m^{-1} in the IAPWS equation [8] and λ^* = 1.0000 W.K^{-1}.m^{-1} in equations A, B, C; the dimensionless temperature is $\bar{T} = \frac{T}{T^*}$ and T^* = 647.226 K.

Equation (5) was rearranged to be suitable for linear regression

$$\frac{\lambda^* \sqrt{\bar{T}}}{\lambda_0(\bar{T})} = \sum_i E_i \left(\frac{1}{\bar{T}}\right)^{N_i} \qquad (6)$$

Experimental points in corresponding co-ordinates are displayed in Fig. 8.

5. Results

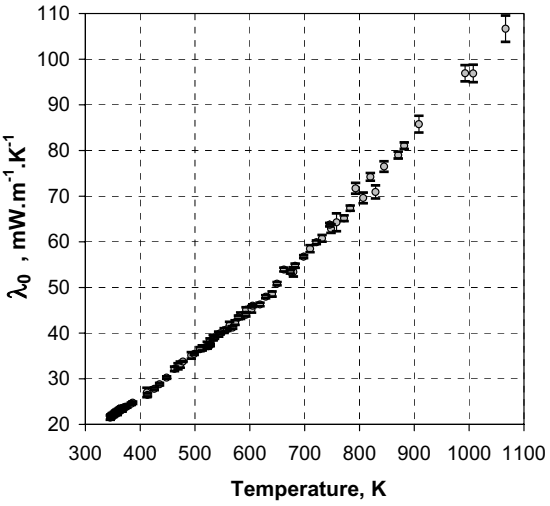
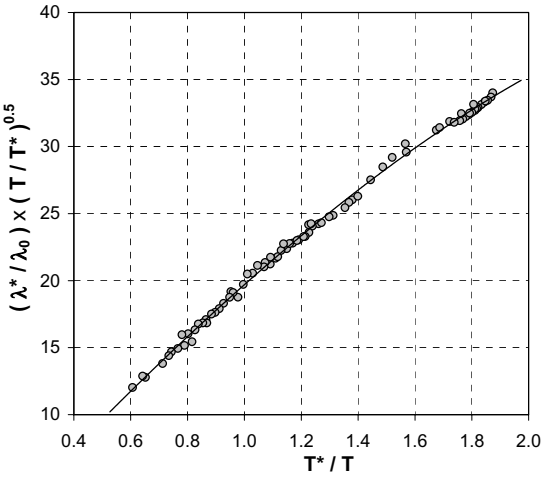


Fig. 7. Predicted values of thermal conductivity coefficient in the ideal-gas limit.

Fig. 8 . Points for correlation.



The results of correlation are summarised in Table 2. The first line in Table 2 brings exponents, coefficients and weighted RMS deviation of the IAPWS equation [8] from predicted values λ_0.

In the second line a new equation with the same number of terms and the same exponents as in [8] is presented. In the following lines new equations with limited number of coefficients are given. It was also accepted to use terms with exponent 0.5, because the root of temperature is necessary to calculate for the numerator on the right side of equation (5). The weighted percentage RMS deviations are given in the last column in Table 2.

6. Conclusions

The final correlation resulted in three equations with different number of terms of the form (5). It is obvious that the number of terms in the equation (5) is possible to diminish in comparison with the current IAPWS equation [8]. Even with equations B and C we reached lower weighted RMS deviations than the IAPWS [8] equation has. Moreover, both equation B and C have a non-oscillating course. Equation B is more precise at high temperatures than equation C. Therefore equation B is the most recommended.

Acknowledgements
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References and Notes

[1] *H_2O Thermal Conductivity Data Bank*. Joint IAPWS and STP/IUPAC Project, February 2000.

Table 2. Numerical values of the coefficients and exponents of the equations.

Equation	i	N_i	E_i	RMS, %
IAPWS [8]	1 2 3 4	0 1 2 3	1.000000 6.978267 2.599096 - 0.998254	1.67
A	1 2 3 4	0 1 2 3	- 4.498188 30.876295 - 7.879375 1.228376	1.29
B	1 2 3	0 0.5 1	-15.905462 33.834773 1.801134	1.29
C	1 2	0 0.5	-17.922937 37.675632	1.30

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