New International Formulation for the Thermal Conductivity of H2O

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New International Formulation for the Thermal Conductivity of H$_2$O

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The International Association for the Properties of Water and Steam (IAPWS) encouraged an extensive research effort to update the IAPS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance, leading to the adoption of a Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance. This paper describes the development and evaluation of the 2011 formulation, which provides a correlating equation for the thermal conductivity of water for fluid states from the melting temperature up to 1173 K and 1000 MPa with uncertainties from less than 1% to 6%, depending on the state point. © *2012 by the U.S. Secretary of Commerce on behalf of the United States. All rights reserved.* [http://dx.doi.org/10.1063/1.4738955]

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1. Introduction

An accurate characterization of the thermophysical properties of water and steam (H_2O) is very important for both science and technology. For this purpose, the International Association for the Properties of Water and Steam (IAPWS) tries to develop and standardize state-of-the art formulations for the thermophysical properties of H_2O. The most recent IAPWS formulations for the thermodynamic properties of H_2O are the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use[1,2] (referred to as IAPWS-95) and the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam[3,4] (referred to as IAPWS-IF97). After these formulations for the thermodynamic properties had been adopted, IAPWS coordinated an international research project in collaboration with the International Association for Transport Properties (IATP) to also develop updated formulations for the transport properties of H_2O. These efforts led to the adoption of the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance[5] and of the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance.[6] The new formulation for the viscosity of H_2O was described in a previous paper in this journal.[7] The present paper is concerned with the updated recommendations for calculating the thermal conductivity of H_2O.

A first set of skeleton tables for the thermal conductivity of H_2O, covering pressures up to 50 MPa and temperatures up to 700 °C, together with some interpolating equations excluding the critical region, was issued in 1964 upon the instruction of the 6th International Conference on the Properties of Steam.[8,9] It was not clear at that time how to represent the thermal conductivity of H_2O in the critical region. The presence of a pronounced critical enhancement of the thermal conductivity

in fluids, such as carbon dioxide, had just been discovered.[10,11] However, the research group of Amirkhanov *et al.* had not been able to confirm the presence of a pronounced critical thermal-conductivity enhancement for carbon dioxide[12] or for steam.[13] Hence, the possibility of such an enhancement in steam was discarded, and the thermal conductivity of H_2O in the critical region was estimated from smooth graphical interpolations along isobars from low temperatures to high temperatures.

In the 1970s, it was demonstrated experimentally that the thermal conductivity of H_2O also exhibits a pronounced enhancement in the critical region.[14,15] The 8th International Conference on the Properties of Steam, held in 1974, established a special committee for the purpose of completing new formulations for the transport properties of H_2O. This effort led to the adoption of a Release on the Dynamic Viscosity of Water Substance in 1975, as was discussed in a previous recent publication,[7] and a Release on the Thermal Conductivity of Water Substance in 1977.[16–19] The 1977 Release contained a table of critically evaluated thermal-conductivity data covering pressures up to 100 MPa and temperatures up to 800 °C, a table of critically evaluated thermal-conductivity data of the saturated vapor and liquid as a function of temperature, a recommended interpolating equation for industrial use in which the thermal conductivity remained finite at the critical point, and a recommended interpolating equation for scientific use in which the thermal conductivity diverges at the critical point as predicted by theory. Both interpolating equations yield the thermal conductivity of H_2O as a function of density and temperature. The interpolating equation for scientific use, developed by Sengers *et al.*,[19] was to be used in conjunction with the 1968 IFC Formulation for Scientific and General Use[20,21] for the thermodynamic properties, while the interpolating equation for industrial use, developed by Yata and Minamiyama,[22] was to be used in conjunction with the 1967 IFC Formulation for Industrial Use[23] for the thermodynamic properties. The 1968 IFC Formulation was replaced by a Provisional IAPS Formulation 1982 for the Thermodynamic Properties of Ordinary Water Substance for Scientific and General Use based on an equation of state developed by Haar *et al.*,[24] which was subsequently recast in dimensionless form as the IAPWS 1984 Formulation for the Thermodynamic Properties of Ordinary Water Substance.[25] It was certified by the International Association for the Properties of Steam (IAPS) that the recommended interpolating equation for the thermal conductivity for scientific use could be used in conjunction with the IAPWS 1984 Formulation for the Thermodynamic Properties without any loss of accuracy.[19,26] This formulation was issued as the Release on the IAPS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance.[27]

As mentioned earlier, the current recommended formulations for the thermodynamic properties of H_2O are the IAPWS-95 and IAPWS-IF97 formulations. Moreover, the International Practical Temperature Scale of 1968 was replaced by the International Temperature Scale of 1990 (ITS-90).[28] For these reasons, the IAPS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance

was slightly revised, the last revision having been adopted in 2008 to make the information consistent with both the IAPWS-95 and IAPWS-IF97 formulations for the thermodynamic properties, with ITS-90, and with the recent IAPWS Formulation 2008 for the viscosity.[29] Nevertheless, we should emphasize that these recommended equations for the thermal conductivity are still the same as the equations adopted in 1977, which are based on the experimental thermal-conductivity information available at that time.[30] Moreover, these equations do not cover the higher temperatures and pressures covered by the IAPWS-95 formulation for the thermodynamic properties. Hence, as for the viscosity, development of a new formulation for the thermal conductivity of H_2O had become desirable, culminating in the adoption of the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance.[6]

2. Experimental Data

As part of a joint project between IAPWS and IATP, experimental data on the viscosity and thermal conductivity of water and steam were collected, converted to the ITS-90 temperature scale and a common set of units, and evaluated. Unless the temperature scale was explicitly stated in a publication or additional information was available, the year of publication was used to determine the appropriate temperature scale for the conversion. Thus the assigned temperature associated with each thermal conductivity data point was adjusted. In principle, also the values of the thermal conductivity may be affected by a change in the temperature scale because of its possible influence on the temperature gradient. This issue was investigated by Mares and Kalova,[31] who concluded that the effect of converting from IPTS-68 to ITS-90 for properties like heat capacity and thermal conductivity never exceeds 0.2% and, therefore, can be neglected when analyzing thermal conductivity data for water. The resultant database for the thermal conductivity of water, containing 5107 points covering the range of temperatures from 256 K to 1191 K with pressures to 785 MPa, is described in detail in Ref. 32. This database contains data collected through bibliographic efforts under the auspices of IAPWS and documented in unpublished reports through 1988, as well as including later data through the year 2000.

In the work reported here, we used the database described in Ref. 32 as a starting point. Several works that appeared after the year 2000 were added.[33–36] In addition, we included a table of data provided by Sirota[37] to IAPWS that summarizes the results based on a series of papers written from 1973 to 1981 (Refs. 14,38–44) and that supersedes the original publications. Furthermore, we calculated thermal conductivities from the thermal-diffusivity data of Abramson.[45] The Abramson data are at very high pressures (to 4 GPa) that exceed the range of applicability of the IAPWS-95 formulation[1,2] and were not included in the 2000 database. However, we used these data to guide the high-pressure extrapolation behavior of the correlation. Finally,
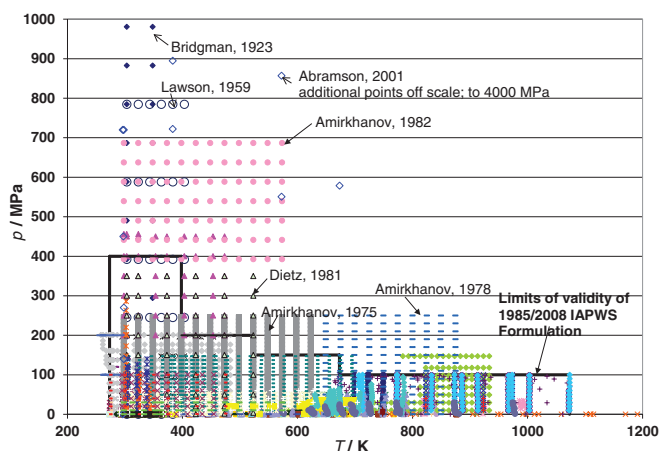
FIG. 1. Distribution of experimental thermal-conductivity data in the temperature-pressure plane.

there are three sets of thermal-diffusivity data[46–48] that are not in the database, but that were used in this work. Two sets in the supercooled liquid region[46,47] were used to examine the extrapolated behavior of the formulation in the supercooled region. Thermal conductivity derived from thermal-diffusivity data in the critical region[48] were also used in the development of the formulation.

The temperature and pressure range of the available data are shown in Fig. 1 along with the range of applicability of the 1985/2008 IAPWS formulation for the thermal conductivity of water.[29] The 2008 formulation is a minor revision of the 1998 release[49] that is itself a minor modification of the formulation adopted in 1985.[19] Table 1 summarizes all data considered in this work, including an estimate of their uncertainty, the temperature and pressure ranges of the data, the experimental method, and the number of individual data points. Densities have been calculated from the IAPWS-95 Formulation for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use.[1,2] The resultant dataset used for regression comprises 7162 data points from 103 sources that cover a temperature range from 255.75 K to 1191.1 K and pressures up to 1176.8 MPa.

3. Development of the Correlation

In order to provide consistency with the conventions adopted by IAPWS in its releases on the transport properties of water, we use the following dimensionless variables for temperature T, density ρ, pressure p, and thermal conductivity λ,

$$\overline{T} = \frac{T}{T^*}, \quad \overline{\rho} = \frac{\rho}{\rho^*}, \quad \overline{p} = \frac{p}{p^*}, \quad \overline{\lambda} = \frac{\lambda}{\lambda^*}, \qquad (1)$$

where the reference constants are $T^* = 647.096$ K, $\rho^* = 322.0$ kg m^{-3}, $p^* = 22.064$ MPa, and $\lambda^* = 1.00$ mW m^{-1} K^{-1}. The reference values for temperature, pressure, and density are in agreement with the presently accepted critical parameters recommended by IAPWS.[139] All temperatures are expressed in terms of the ITS-90 temperature scale.

The formulation for the thermal conductivity of water has the general form[26]

$$\overline{\lambda} = \overline{\lambda}_0(\overline{T}) \times \overline{\lambda}_1(\overline{T}, \overline{\rho}) + \overline{\lambda}_2(\overline{T}, \overline{\rho}). \qquad (2)$$

The first factor $\overline{\lambda}_0$ of the product represents the thermal conductivity in the zero-density limit and is a function of temperature only. The second factor $\overline{\lambda}_1$ represents the contribution to thermal conductivity due to increasing density, while the third factor $\overline{\lambda}_2$ represents an enhancement of the thermal conductivity in the critical region. The determination of each of these contributions will be considered in Secs. 3.1–3.3.

3.1. Thermal conductivity in the limit of zero density

In order to develop an expression for the thermal conductivity in the limit of zero density, all points from the database for densities less than 50 kg m^{-3} were considered. This resulted in a total of 1008 points from 42 sources. These are denoted in Table 1 with italics, along with the experimental method used and an estimate of the uncertainty of the measurement.[32] As indicated in Table 1, the measurements were made by several independent groups with different experimental methodologies. We did not select any of the points published by Sirota *et al.* in journal publications from 1970 to 1981,[14,38–40,42–44,140–142] since they are also incorporated in a report[37] that summarizes all of the experiments of that time period. This report is considered to have the best values incorporating recommended corrections. We also did not consider the 1968 work of Le Neindre *et al.*,[77] since the data reported are dependent upon the IAPS 1964 Skeleton Tables. In addition, we excluded 21 points from Milverton[52] corresponding to pressures below 13.3 kPa (10 cm Hg) that were considered to be subject to severe temperature jumps.[19] Following the procedure used in the development of the formulation for the viscosity of water,[7] the remaining points were then sorted into temperature "bins" of at least three points that covered temperature ranges up to 8 K and included at least one point with a density less than 10 kg m^{-3}; the average bin size was approximately 4 K. This procedure is based on the concept of Key Comparison Reference Values[143] that incorporates statistical analysis of the data reflecting the uncertainties from different data sources. Some points could not be included in the bins and were removed from consideration. The four data points of Miroshnichenko and Makhrov[122] were treated separately as zero-density points and were not included in bins. The nominal temperature of an isotherm was computed as the average temperature of all points in a bin. The thermal conductivity of each point was then corrected to the nominal temperature, T_{nom}, by use of the following equation:

$$\lambda_{\mathrm{corr}}(T_{\mathrm{nom}}, \rho) = \lambda_{\mathrm{exp}}(T_{\mathrm{exp}}, \rho) + [\lambda(T_{\mathrm{nom}}, \rho) - \lambda(T_{\mathrm{exp}}, \rho)]_{\mathrm{calc}}, \qquad (3)$$

where the calculated values were obtained from the 1985/2008 IAPWS thermal-conductivity formulation.[29]

TABLE 1. Summary of experimental data for the thermal conductivity of water.

First author[a]	Year	Method[b]	Uncertainty (%)	Temperature range (K)	Pressure range (MPa)	Number of data
Bridgman[50]	1923	CC	5	303–348	0.1–1176.8	25
Schmidt[51]	1932	CC	3	282–542	0.1–7.4	24
Milverton[52]	1935	SHW	2	345–368	0.0–0.05	77
Timrot[53]	1935	SHW	3	342–526	0.01–0.01	10
Vargaftik[54]	1935	SHW	3	562–750	0.00–0.01	11
Vargaftik[55]	1937	SHW	3	523–628	0.51–2.84	14
Timrot[56]	1940	SHW	3	529–797	0.10–29.42	33
Vargaftik[57]	1946	SHW	3	325–1057	0.0–0.1	8
Riedel[58]	1951	CS	1	293	0.1	1
Schmidt[59]	1955	CC	0.3	293–357	0.1	8
Challoner[60]	1956	PP	1	273–353	0.1	5
Vargaftik[61]	1956	CC	2	504–715	0.1	4
Lawson[62]	1959	CC	2	303–403	0.1–784.5	35
Vargaftik[63]	1959	SHW	2	623–998	0.5–34.3	61
Vargaftik[64]	1959	SHW	2	294–623	0.1–21.3	35
Vargaftik[65]	1960	SHW	2	593–841	0.5–49.0	41
Vines[66]	1960	CC	2	543–833	0.1	2
Tarzimanov[67]	1962	SHW	2	505–624	0.2–14.7	33
Vargaftik[68]	1962	SHW	1	399–727	0.1–14.9	29
Vukalovich[69]	1963	CC	5	583–933	9.8–147.1	135
Vargaftik[70]	1963	SHW	3	389–767	0.1	10
Keyes[71]	1964	CC	3	412–644	0.1–17.2	46
Vargaftik[72]	1964	SHW	3	611–1191	0.1	21
Venart[73]	1964	CC	1.5	370–528	0.1–29.6	163
Baker[74]	1964	SHW	3	381–526	0.1	4
Venart[75]	1965	CC	2	290–527	0.1–29.6	56
Brain[76]	1967	CC	1.5	416–432	0.1	3
Le Neindre[77]	1968	CC	2	383–603	0.1–12.5	65
Tarzimanov[78]	1968	SHW	1	302–428	2.9–98.3	19
Brain[79]	1969	CC	2	443–877	0.1	33
Bach[80]	1970	OPT	1	294–363	0.1	374
Cherneeva[81]	1970	CC	4.3	373–974	10–100	130
Rastorguev[82]	1970	CC	1.6	294–454	0.1–196	54
Stupak[83]	1970	CC	2	316–352	0.1	4
Cherneeva[84]	1970	CC	4.3	373–974	10–100	88
Gazdiev[85]	1971	CC	1.5	313–433	0.1–0.6	8
Papadopoulos[86]	1971	THB	3	298	0.1	1
Turnbull[87]	1971	THW	1.5	298	0.1	1
Dijkema[88]	1972	CC	0.5	298–333	0.00–0.02	2
Mustafaev[89]	1972	TCC	3	423–677	0.1	14
Potienko[90]	1972	THW	3	292	0.1	1
Le Neindre[15]	1973	CC	2	612–788	0.1–50.7	145
Tarzimanov[91]	1973	CC	3	440–773	0.1–100	87
Vargaftik[92]	1973	SHW	1.5	430–998	0.1	11
Castelli[93]	1974	CC	1	275–305	1–140	62
Shurygin[94]	1974	RD	5	293	0.1	1
Rastorguev[95]	1974	CC	1.5	258–484	0.1–201	443
Amirkhanov[96]	1975	PP	2	298–623	0.1–245.3	351
Bury[97]	1975	CC	2	377–790	0.1–50	111
Takizawa[98]	1975	THW	2	273–373	0.1–48.7	29
Le Neindre[99]	1976	CC	1.5	310–643	0.2–50.7	215
Tsederberg[100]	1976	CC	2	707–1072	9.9–98.2	147
Popov[101]	1977	CC	4	597–1074	0.1–98.3	75
Rastorguev[102]	1977	CC	2	296–393	0.1–0.3	29
Amirkhanov[103]	1978	PP	2	649–875	0.1–250	136
Takizawa[104]	1978	THW	1.5	273–353	0.1	9
Varchenko[105]	1978	HW	3	303	0.1	16
Amirkhanov[106]	1979	PP	3	298–473	200–456	57
Curtiss[107]	1979	SHW	2	358–386	0.01–0.13	54
Filippov[108]	1979	THW	4	293	0.1	1
Popov[109]	1979	PP	4	773–1072	9.9–98.2	240
Tufeu[110]	1979	CC	3	680–748	0.02–12.5	16
Yata[111]	1979	CC	2	304–473	9.8–147.4	180
Yata[112]	1979	CC	2.5	377–693	9.8–147	241
Frohn[113]	1980	CC	3	300–650	0.003	8

TABLE 1. Summary of experimental data for the thermal conductivity of water.—Continued

First author[a]	Year	Method[b]	Uncertainty (%)	Temperature range (K)	Pressure range (MPa)	Number of data
Popov[114]	1980	CC	6	713–1073	10–100	50
Popov[115]	1980	CC	4	707–1072	9.9–98.2	148
Venart[116]	1980	THW	1.5	273–368	0.1	22
Dietz[117]	1981	PHW	1	303–523	0.0–350	54
Nagasaka[118]	1981	THW	1	274–319	0.1	4
Sirota[37]	1981	PP	3	481–704	0.1–35	555
Amirkhanov[119]	1982	PP	4	298–573	392.4–686.5	84
Alloush[120]	1982	THW	3	297–315	0.1	3
Nagasaka[121]	1984	SHW	1	274–354	0.1–40	25
Miroshnichenko[122]	1984	THW	2	303–365	0	4
Tufeu[123]	1986	CC	0.5	256–294	100–200	12
Tufeu[124]	1987	CC	2	623–786	0.93–94.5	209
Guseinov[125]	1987	PP	1.8	293–368	0.1	10
Wakeham[126]	1987	THW	0.5	298	0.1	2
Assael[127]	1988	THW	0.5	304–333	0.1	12
Zalaf[128]	1988	THW	0.5	302–342	0.1–285.7	78
Tarzimanov[129]	1989	THW	1.3	573–978	1–30	104
Venkateshan[130]	1990	TH	4	298	0.1	1
Eldarov[131]	1991	CC	2	298–353	0.1	6
Gross[132]	1992	THS	2	293	0.1	1
Assael[133]	1993	THW	0.5	285–328	0.1	4
Ramires[134]	1993	THW	0.5	299–364	0.1	38
Watanabe[135]	1994	SPH	2	296	0.1	2
Grigorev[136]	1995	CC	2	295–454	0.1–100	54
Mensah-Brown[137]	1996	THW	0.5	304–339	0.1–140.1	38
Ramires[138]	2000	THW	0.5	297–355	0.0–0.05	31
Abdulagatov[33]	2004	CC	2	308–704	0.1–60	39
Abdulagatov[34]	2004	CC	2	291–575	1–40	22
Abdulagatov[36]	2004	CC	1.6	273–473	0.0–100	42
Abdulagatov[35]	2005	CC	2	298–574	0.1–30	31
Benchikh[47]	1985[c]	OPT	5	250–311	0.1	19
Taschin[46]	2006[c]	TG	5	256–353	0.1	13
Desmarest[48]	1989[c]	DLS	10	647–648	22.1–22.3	15
Abramson[45]	2001[c]	OPT	10	295–673	0.1–3700	29

[a]Primary data sources used in the analysis of the zero-density function are indicated by italic font.
[b]CC: concentric cylinders; CS: concentric spheres; DLS: dynamic light scattering; HW: heated wire; OPT: optical; PHW: pulsed heated wire; PP: parallel plates; RD: rotating disk; SHW: steady-state heated wire; SPH: spot heating; TCC: transient concentric cylinders; TG: transient grating; TH: transient heated foil; THB: thermistor bead; THS: transient hot strip; THW: transient hot-wire.
[c]Data derived from thermal-diffusivity measurements not included in database.

Weighted linear least-squares regression was then used to extrapolate the nominal isotherms in order to obtain the value at zero density, λ_0. Points were weighted with a factor equal to the inverse of the square of the estimated relative uncertainty. Both linear and quadratic density regressions were performed and the best fit was selected for λ_0. Confidence intervals[144] constructed from the regression statistics were 95%. Some isotherms that had unusually large uncertainty bands due to inconsistencies in the underlying data were rejected from further consideration. In addition, for the isotherms of Miroshnichenko and Makhrov,[122] the experimental uncertainty was used directly since regression was not performed on these isotherms. Also, it was not possible to perform a regression on the highest temperature isotherm, 1111.58 K, since all points were at the same pressure. In this case an average value was taken and estimated to be equivalent to the value at zero density, with an uncertainty equivalent to the experimental uncertainty.

In order to supplement the experimental dataset at very low and at high temperatures where data are unavailable or sparse, we incorporated selected theoretical data points from the recent work of Hellmann *et al.*[145] We first adjusted the theoretical values by increasing their magnitude by 1% (as recommended by the authors),[146] and ascribed to the theoretical values an uncertainty compatible with that of the experimental data, namely, 2% (at a 2σ confidence level) for points below 800 K and 3% for points at higher temperatures. Six theoretical points covering 250–300 K and six high-temperature theoretical data points covering 800–1100 K were added to the λ_0 dataset. In addition, in agreement with a decision made at the IAPWS meeting in 2009, the uncertainties of the experimental values were increased so that the theoretical values were within the uncertainty band.

We selected a form of equation similar to that used previously[49] for the dimensionless thermal conductivity in the
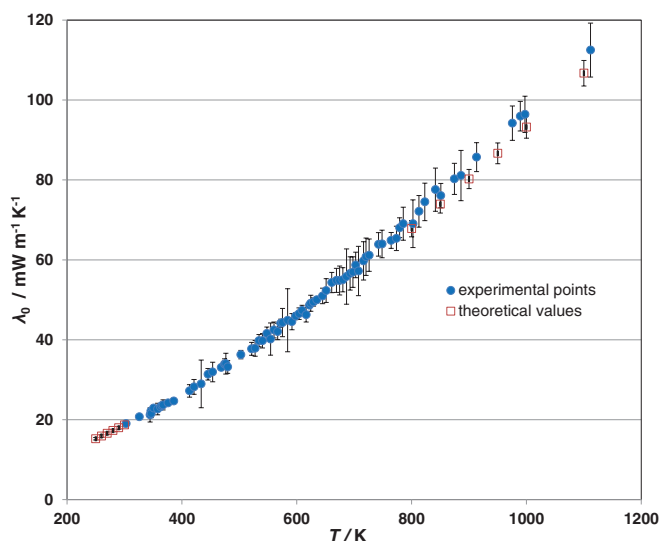
FIG. 2. Dataset for λ_0 used in the regression.

limit of zero density,

$$\overline{\lambda}_0(\overline{T}) = \frac{\sqrt{\overline{T}}}{\sum_{k=0}^{4} \frac{L_k}{\overline{T}^k}}.\qquad(4)$$

We explored weighted least squares and weighted orthogonal distance regression[147] for 3, 4, and 5-term expressions of the form of Eq. (4) with integer and half-integer exponents, k. Preliminary regressions identified statistical outliers,[148] which were then excluded from the final regression. The final set of λ_0 values contained 86 data points from 250 K to 1100 K and is shown in Fig. 2. The coefficients obtained from the regression are given in Table 2. The weights were equal to the inverse of the square of the estimated uncertainty. Figure 3 displays the percent deviation $(100(\lambda_{0,\text{exp}}-\lambda_{0,\text{calc}})/\lambda_{0,\text{calc}})$ between the λ_0 data and both the 1985/2008 IAPWS Formulation[29] and the new proposed correlation. Due to the lack of available experimental data at low and high temperatures, the 1985/2008 IAPWS Formulation shows deviations up to almost 5% at 250 K and about 6% at 2000 K from the theoretical values of Hellmann et al.[145] The present formulation attempts to address this deficiency by incorporating theoretical values to guide the extrapolation behavior of the correlation in regions where experimental data are unavailable or sparse. Figure 4 shows the present equation, the experimental λ_0 data, the 1985/2008 IAPWS Formulation,[29] and also the recent theoretical λ_0 values from the work of Hellmann et al.[145] that have been adjusted upward by 1%, as mentioned earlier. The theoretically calculated values were obtained in the rigid-rotor approximation with the CC-pol intermolecular potential-energy

FIG. 3. Comparisons of λ_0 correlations with the theoretical and experimental data.

surface by Bukowski et al.[149–151] and the classical trajectory method. The proposed correlation represents both the experimental and theoretical values within the experimental uncertainty of 3% in its range of validity of temperatures up to 1173 K. Although there are data up to 1191 K, we limit the upper temperature on the range of validity to be consistent with the viscosity formulation[5] used in the calculation of the enhancement of thermal conductivity discussed in Sec. 3.3.

TABLE 2. Coefficients in Eq. (4) for $\overline{\lambda}_0(\overline{T})$.

k	L_k
0	$2.443\,221 \times 10^{-3}$
1	$1.323\,095 \times 10^{-2}$
2	$6.770\,357 \times 10^{-3}$
3	$-3.454\,586 \times 10^{-3}$
4	$4.096\,266 \times 10^{-4}$
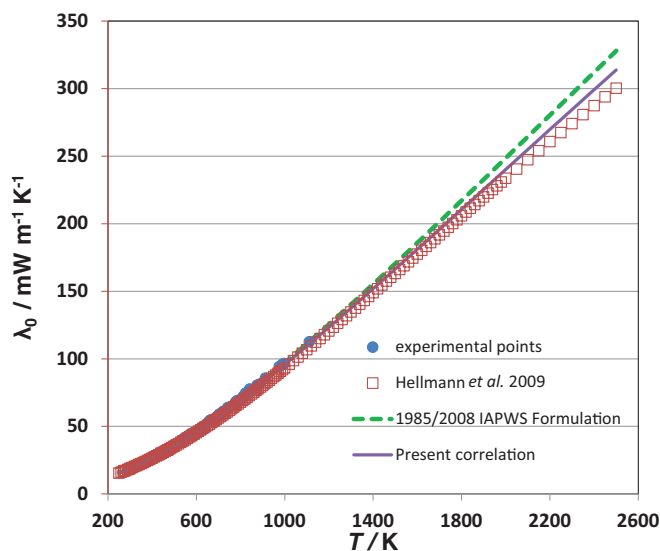
FIG. 4. λ_0 as a function of temperature.

The extrapolation to higher temperatures (2000 K) agrees with the theoretically predicted behavior to within about 3%.

3.2. Residual contribution

The second factor $\overline{\lambda}_1$ of the product in Eq. (2) is the residual thermal conductivity and represents the contribution to thermal conductivity due to increasing density. This term is sometimes referred to in the literature as the excess thermal conductivity, but here we follow the alternative nomenclature of residual thermal conductivity. The critical region is not considered here; it will be treated separately in Sec. 3.3. We adopt the same general form for $\overline{\lambda}_1$ as in an earlier work,[19]

$$\overline{\lambda}_1(\overline{T}, \overline{\rho}) = \exp\left[\overline{\rho} \sum_{i=0}^{4} \left(\frac{1}{\overline{T}} - 1\right)^i \sum_{j=0}^{5} L_{ij}(\overline{\rho} - 1)^j\right], \quad (5)$$

with coefficients L_{ij} to be determined by regression of experimental data and the dimensionless density as defined in Eq. (1).

All points were initially assigned weights $1/u^2$, where u is the estimated relative experimental uncertainty. The uncertainties are given in Table 1; they are those given by Assael *et al.*,[32] or the original author's recommendation when available. All densities were computed with IAPWS-95. Also, any points that exhibited differences of more than three standard deviations from preliminary regressions were considered outliers and were not used in further regression analysis. In order to extend the behavior of the correlation to higher pressures, we derived thermal conductivities from the thermal-diffusivity data of Abramson[45] and included these data in our regressions even though the data are not included in the experimental database. The thermal conductivity is related to the thermal diffusivity D with the relationship $\lambda = D\rho c_p$, where the density and heat capacity are obtained from the equation of state. The Abramson data are listed in Table 3, and contain points at pressures as high as 3.7 GPa, which is outside of the range of applicability of the equation of state;[2] however, we include these data to guide the extrapolation behavior of the correlation at extreme pressures. The 1985/2008 IAPWS Formulation[29] has very unrealistic behavior in this region (for example, at 800 K and 2 GPa the thermal conductivity from the 1985/2008 IAPWS Formulation[29] is too large by more than 2 orders of magnitude) and it was desired to improve upon this behavior.

Equation (5) contains a maximum of 30 empirical terms; there is no theoretical motivation for the form or the total number of terms necessary, or which terms will best represent the experimental data. We used the orthogonal distance regression package ODRPACK (Ref. 147) and eliminated statistically insignificant terms as indicated by ODRPACK. Some datasets received additional weight in order to represent them to near, or within, their experimental uncertainty. We also required the correlation to reproduce the value (0.6065 W m^{-1} K^{-1}) at 298.15 K and 0.1 MPa recommended by Ramires *et al.*[152] The critical region was represented by a

TABLE 3. Very-high-pressure thermal-conductivity data derived from the work of Abramson *et al.*[45]

T(K)	p(MPa)	λ (mW m^{-1} K^{-1})
295.15	1278	866.05
296.15	0.1	609.12
296.15	0.1	600.78
296.15	720	829.45
296.15	1098.9	861.09
297.15	450	764.1
298.15	140	673.85
298.15	270	722.07
298.15	720	821.83
383.15	722.23	932.64
383.15	894.91	989.59
383.15	1724.1	1167.4
384.15	1113.5	1047.5
384.15	2046	1221.5
469.15	1080	1038
469.15	1390	1142
469.15	1450	1152.4
469.15	2220	1318.5
469.15	2250	1363.1
470.15	3699.8	1594.5
521.15	3546.8	1603.4
571.15	3548.4	1628.1
572.15	550.77	921.26
572.15	856.94	1058.6
673.15	578.51	882.06
673.15	1113.9	1110.7
673.15	2015.7	1331.5
673.15	2829.8	1519.9
673.15	3413.5	1641.2

theoretical formulation[153] that contains a single parameter $\overline{q}_D^{-1}$, as is discussed in Sec. 3.3. A residual-term formulation with a total of 28 terms provided the best representation of the data with the fewest number of terms. The final values of the coefficients for the residual function are given in Table 4. A detailed comparison of the correlation with experimental data will be presented in Sec. 4.

3.3. Critical region

To represent the critical region term $\overline{\lambda}_2$ in Eq. (2), we use a simplified crossover model developed by Olchowy and Sengers,[153] which has yielded a good practical representation of the thermal conductivity of many fluids in the critical region[154–162]

$$\overline{\lambda}_2(T, \rho) = \frac{\rho c_p R_D k_B T}{6\pi \mu \xi \lambda^*}\left\{\overline{\Omega}(\overline{q}_D \xi) - \overline{\Omega}_0(\overline{q}_D \xi)\right\}, \quad (6)$$

where the specific heat capacity at constant pressure, $c_p(T, \rho)$, is obtained from the equation of state,[1,2] and the viscosity, $\mu(T, \rho)$, from the IAPWS standard[5,7] that includes a critical enhancement term. The crossover functions $\overline{\Omega}$ and $\overline{\Omega}_0$ are given by

$$\overline{\Omega}(y) = \frac{2}{\pi}\left[\left(1 - \kappa^{-1}\right)\arctan(y) + \kappa^{-1}y\right] \quad (7)$$

TABLE 4. Coefficients L_{ij} in Eq. (5) for $\overline{\lambda}_1(\overline{T}, \overline{\rho})$.

j	0	1	2	3	4	5
i						
0	1.603 973 57	−0.646 013 523	0.111 443 906	0.102 997 357	−0.050 412 363 4	0.006 098 592 58
1	2.337 718 42	−2.788 437 78	1.536 161 67	−0.463 045 512	0.083 282 701 9	−0.007 192 012 45
2	2.196 505 29	−4.545 807 85	3.557 772 44	−1.409 449 78	0.275 418 278	−0.020 593 881 6
3	−1.210 513 78	1.608 129 89	−0.621 178 141	0.071 637 322 4	0	0
4	−2.720 337 0	4.575 863 31	−3.183 692 45	1.116 834 8	−0.192 683 05	0.012 913 842

and

$$\overline{\Omega}_0(y) = \frac{2}{\pi}\left[1 - \exp\left(\frac{-1}{y^{-1} + y^2/3\overline{\rho}^2}\right)\right], \qquad (8)$$

where $\kappa = c_p/c_V$ is the ratio of the isobaric and isochoric heat capacities, and where

$$y = \overline{q}_{\mathrm{D}}\xi(\overline{T}, \overline{\rho}). \qquad (9)$$

In these equations, $R_D = 1.01$ is a universal dynamic amplitude ratio, k_{B} is the Boltzmann constant, $\overline{q}_{\mathrm{D}}$ is a cutoff wave number, and $\xi(\overline{T}, \overline{\rho})$ is a correlation length to be specified below, so that y is a dimensionless variable. We note that the cutoff wave number $\overline{q}_{\mathrm{D}}$ appearing in the crossover function for the critical thermal-conductivity enhancement is physically similar to, but numerically different from, the cutoff wave number q_{D} appearing in the crossover function for the critical viscosity enhancement.[7,153,163]

We find it convenient to introduce a dimensionless function Z defined by

$$Z(y) = \frac{2}{\pi y}\left\{\left[(1 - \kappa^{-1})\arctan(y) + \kappa^{-1}y\right]\right.$$
$$\left. - \left[1 - \exp\left(\frac{-1}{y^{-1} + y^2/3\overline{\rho}^2}\right)\right]\right\}. \qquad (10)$$

Equation (6) for $\overline{\lambda}_2$ can then be rewritten as

$$\overline{\lambda}_2(T, \rho) = \frac{\rho c_p R_D k_{\mathrm{B}} T \overline{q}_{\mathrm{D}}}{6\pi\mu\lambda^*} Z(y). \qquad (11)$$

To express Eq. (10) in terms of dimensionless quantities, we introduce a dimensionless isobaric specific heat capacity $\overline{c}_p$ and a dimensionless viscosity $\overline{\mu}$,

$$\overline{c}_p = \frac{c_p}{R}, \quad \overline{\mu} = \frac{\mu}{\mu^*}, \qquad (12)$$

where $R = 0.461\,518\,05\ \mathrm{kJ\,kg^{-1}\,K^{-1}}$ is the specific gas constant as defined by the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use[1] and where $\mu^* = 1 \times 10^{-6}\ \mathrm{Pa\,s}$ as defined by the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance.[5] From Eq. (10), it then follows that the dimensionless critical thermal-conductivity enhancement is given by

$$\overline{\lambda}_2(\overline{T}, \overline{\rho}) = \Lambda \frac{\overline{\rho}\,\overline{c}_p\overline{T}}{\overline{\mu}} Z(y), \qquad (13)$$

where

$$\Lambda = \frac{\rho^* T^* R R_D k_{\mathrm{B}} \overline{q}_{\mathrm{D}}}{6\pi\mu^*\lambda^*} \qquad (14)$$

is a numerical constant. To avoid numerical truncation issues in Eq. (10) for small values of y, the function $Z(y)$ is subject to the condition

$$Z(y) = 0 \quad \text{for} \quad y < 1.2 \times 10^{-7}. \qquad (15)$$

We note that the calculation of $Z(\overline{q}_{\mathrm{D}}\xi)$ from Eq. (10) may be sensitive to the order of addition/subtraction of terms, so that parentheses have been put around the terms representing the separate contributions from $\overline{\Omega}$ and $\overline{\Omega}_0$ to the function Z.

A procedure has already been developed for calculating the correlation length ξ for use in the formulation for the viscosity of H₂O.[5,7] The same procedure can be used in the present formulation for the thermal conductivity of H₂O,

$$\xi = \xi_0\left(\frac{\Delta\overline{\chi}}{\Gamma_0}\right)^{\nu/\gamma} \qquad (16)$$

in terms of $\Delta\overline{\chi}(\geq 0)$ defined by

$$\Delta\overline{\chi}(\overline{T}, \overline{\rho}) = \overline{\rho}\left[\left(\frac{\partial\overline{\rho}(\overline{T}, \overline{\rho})}{\partial\overline{p}}\right)_{\overline{T}} - \left(\frac{\partial\overline{\rho}(\overline{T}_{\mathrm{R}}, \overline{\rho})}{\partial\overline{p}}\right)_{\overline{T}}\frac{\overline{T}_{\mathrm{R}}}{\overline{T}}\right] \qquad (17)$$

or

$$\Delta\overline{\chi}(\overline{T}, \overline{\rho}) = \overline{\rho}\left[\varsigma(\overline{T}, \overline{\rho}) - \varsigma(\overline{T}_{\mathrm{R}}, \overline{\rho})\frac{\overline{T}_{\mathrm{R}}}{\overline{T}}\right], \qquad (18)$$

with

$$\varsigma = \left(\frac{\partial\overline{\rho}}{\partial\overline{p}}\right)_{\overline{T}}. \qquad (19)$$

In these equations, $\nu = 0.630$ and $\gamma = 1.239$ are critical exponents, $\xi_0 = 0.13$ nm and $\Gamma_0 = 0.06$ are critical amplitudes, and $\overline{T}_{\mathrm{R}} = 1.5$ is a reduced reference temperature. When $\Delta\overline{\chi}$ calculated from Eq. (17) is less than zero, it must be set to zero for calculations to proceed.

For general and scientific use, the specific heat capacity $\overline{c}_p$ in Eq. (13), the ratio κ of the specific heat capacities in Eq. (9) for the function Z, and the derivatives $(\partial\overline{\rho}/\partial\overline{p})_{\overline{T}}$ in Eq. (17) are to be calculated from the IAPWS-95 formulation for the thermo-dynamic properties[1] and the viscosity $\overline{\mu}$ in Eq. (13) from the

IAPWS Formulation 2008 for the viscosity.[5] For industrial use, the specific heat capacity $\overline{c}_p$ in Eq. (13), the ratio κ of the specific heat capacities in Eq. (10) for the function Z, and the derivatives $(\partial\overline{\rho}/\partial\overline{p})_{\overline{T}}$ in Eq. (17) may be calculated from IAPWS-IF97 (Ref. 3) and the viscosity $\overline{\mu}$ in Eq. (13) may be approximated by the background viscosity $\overline{\mu}_b$ without the critical viscosity enhancement.[5] Here, we only consider the results when Eq. (13) for $\overline{\lambda}_2(\overline{T},\overline{\rho})$ is calculated in conjunction with IAPWS-95.[1] Further discussion of the formulation for industrial use is provided in Sec. 5.

Equation (13) completely specifies the critical enhancement term $\overline{\lambda}_2(\overline{T},\overline{\rho})$ except for the selection of a suitable value for the universal dynamic amplitude ratio R_D and the system-dependent cutoff wave number $\overline{q}_D$. The most reliable predictions for R_D obtained from the dynamic renormalization group theory seem to be the values $R_D = 1.038$ found by Paladin and Peliti[164,165] and $R_D = 1.063$ found by Folk and Mozer.[166] The mode-coupling theory yields in first approximation $R_D = 1.00$,[167] but when memory and non-local effects are included, one obtains an improved estimate of $R_D = 1.03$.[168] Hence, Luettmer-Strathmann *et al.*[169,170] adopted as a probable theoretical estimate $R_D = 1.05 \pm 0.03$. Experimental values for R_D have been reviewed by Privman *et al.*[171] and by Sengers *et al.*[170,172] The experimental values appear to be consistent with a value of R_D slightly larger but close to unity. In a previous publication, Sengers *et al.*[170] have reported an attempt to determine an optimum value for R_D from measurements of the decay rate of the critical fluctuations obtained by Desmarest and co-workers for H_2O.[48,173–175] For this purpose, an estimate was needed for the value of the background thermal conductivity λ_b at the critical density $\rho = \rho_c$ which was obtained from the 1985/2008 IAPWS Formulation for the Thermal Conductivity of H_2O (Ref. 29) available at that time. It was then concluded that the dynamic light-scattering data were consistent with $R_D = 1.05 \pm 0.05$. However, a new analysis of the experimental thermal-conductivity data has yielded an estimate for λ_b substantially larger than the one implied by the 1985/2008 IAPWS Formulation[29] for the Thermal Conductivity. Hence, we have repeated the analysis with the new background λ_b,

$$\lambda_b = \lambda^* \times \overline{\lambda}_0(\overline{T},\overline{\rho}) \times \overline{\lambda}_1(\overline{T},\overline{\rho}). \quad (20)$$

This re-analysis[170] of the light-scattering data yielded $R_D = 1.01 \pm 0.05$, which turns out to be close to the experimental value $R_D = 1.00 \pm 0.04$ obtained by Wilkinson *et al.* for xenon.[176] Hence, in the present formulation for the thermal conductivity of H_2O we have adopted $R_D = 1.01$ to determine Λ in Eq. (14). We note that the initial conclusions in Ref. 170 were based on use of the 1985/2008 IAPWS Formulation for the Thermal Conductivity for λ_b and not on a background thermal conductivity proposed by Le Neindre *et al.*,[15] as was erroneously stated in Ref. 170.

The cutoff wave number was determined by an iterative process. Starting with an estimate for $\overline{q}_D$, the critical enhancement $\overline{\lambda}_2(\overline{T},\overline{\rho})$ was calculated and subtracted from experimental thermal-conductivity data in the critical region to get an

TABLE 5. Critical-region constants.

Constant	Value
Λ	177.8514
$\overline{q}_D^{-1}$	0.40 nm
ν	0.630
γ	1.239
ξ_0	0.13 nm
Γ_0	0.06
$\overline{T}_R$	1.5

improved estimate of the background contribution. This process was repeated until a consistent representation of the thermal-conductivity data in the critical region was obtained with $\overline{q}_D^{-1} = 0.4$ nm. This value for $\overline{q}_D^{-1}$ is similar to those found for some other simple fluids.[153] The values of the constants needed to compute the critical enhancement $\overline{\lambda}_2(\overline{T},\overline{\rho})$ from Eq. (13) for H_2O are summarized in Table 5. Note that the value of Λ in Table 5 should be used in the formulation, rather than computing Λ from Eq. (14).

There are three sources of detailed experimental information for H_2O in the critical region: thermal-conductivity data obtained by Sirota *et al.*[14,37–44] with a parallel-plate apparatus,[177] thermal-conductivity data obtained by Le Neindre and co-workers[15,124] with a coaxial-cylinder apparatus,[177] and dynamic light-scattering measurements for the decay rate of the critical fluctuations obtained by Desmarest and co-workers.[48,173–175]

Dynamic light scattering yields values for the thermal diffusivity $D(q)$ at a finite wave number q. A procedure for converting the experimental measurements for $D(q)$ into values for the thermal diffusivity D in the hydrodynamic limit $q = 0$ has been presented in a previous publication.[170] In implementing the procedure, an estimate for the background thermal conductivity λ_b deduced from the 1985/2008 IAPWS Formulation[29] was adopted, as mentioned earlier. For the present project, the procedure was repeated but with the background thermal conductivity λ_b calculated from Eq. (20). The values thus deduced from the light-scattering data reported by Desmarest *et al.*[48] for the thermal diffusivity D as a function of $\Delta T = T - T_c$ are presented in Table 6 (which is identical to Table 1 in the Erratum of Ref. 170), together with the corresponding thermal-conductivity values $\lambda = \rho c_p D$ with c_p calculated from IAPWS-95.[1] On comparing this information with the values listed in Table 1 of Ref. 170, one sees that the values deduced for D and, hence, for λ, from the light-scattering measurements are insensitive to the estimates adopted for the background thermal conductivity. Thus we adopt the thermal-conductivity values in Table 6 as primary experimental data for the thermal conductivity of H_2O close to the critical temperature.

A plot of these thermal-conductivity data as a function of $\Delta T = T - T_c$ is presented in Fig. 5. The curve in this figure represents the values calculated from the present formulation, Eq. (2). The present formulation reproduces these experimental conductivities with a standard deviation of 3%, which is within the experimental accuracy of 3%–5% in D and ± 5 mK in ΔT.[48,175]

TABLE 6. Thermal diffusivity $D(q)$ at $\rho = \rho_c$ measured at $q = 1.549 \times 10^7 \, \mathrm{m}^{-1}$ by Desmarest et al.[48] and the corresponding values for $D = D(0)$ and λ as a function of $\Delta T = T - T_c$.

ΔT (K)	$D(q)$ $(m^2 \, s^{-1})$	D $(m^2 \, s^{-1})$	$\lambda = \rho c_p D$ (W m^{-1}K^{-1})	μ/μ_b
0.020	2.79×10^{-10}	1.84×10^{-10}	4.320	1.18
0.036	3.28×10^{-10}	2.52×10^{-10}	3.266	1.16
0.077	4.36×10^{-10}	3.80×10^{-10}	2.278	1.13
0.106	4.79×10^{-10}	4.33×10^{-10}	1.868	1.12
0.118	5.28×10^{-10}	4.82×10^{-10}	1.863	1.12
0.159	6.26×10^{-10}	5.84×10^{-10}	1.661	1.11
0.245	8.29×10^{-10}	7.92×10^{-10}	1.437	1.09
0.286	9.39×10^{-10}	9.04×10^{-10}	1.392	1.09
0.351	10.61×10^{-10}	10.28×10^{-10}	1.275	1.08
0.438	11.73×10^{-10}	11.44×10^{-10}	1.120	1.07
0.522	13.10×10^{-10}	12.83×10^{-10}	1.039	1.07
0.550	13.52×10^{-10}	13.26×10^{-10}	1.014	1.07
0.668	15.61×10^{-10}	15.36×10^{-10}	0.950	1.06
0.740	16.58×10^{-10}	16.34×10^{-10}	0.903	1.06
0.877	18.62×10^{-10}	18.40×10^{-10}	0.841	1.05

Since the critical enhancement of the viscosity μ is only significant in a very small range of temperatures and densities around the critical point,[7,163] one often approximates the viscosity μ in Eq. (11) for the critical thermal-conductivity enhancement by the background viscosity μ_b.[153] However, the light-scattering data provide information sufficiently close to the critical temperature where this approximation is no longer justified, as demonstrated by the values listed for μ/μ_b in Table 6. Thus, for an accurate representation of the thermal conductivity very close to the critical point, the full viscosity $\overline{\mu}$ is to be kept in Eq. (13).

Experimental data for the thermal conductivity in the critical region were reported by Sirota in a series of eight papers during the period from 1973 to 1981.[14,38–44] The thermal-conductivity data were obtained with a parallel-plate apparatus.[177] Articles in the series discuss various corrections applied to the original measurements. Our analysis is based on a summary table of the final data provided by Sirota for use by
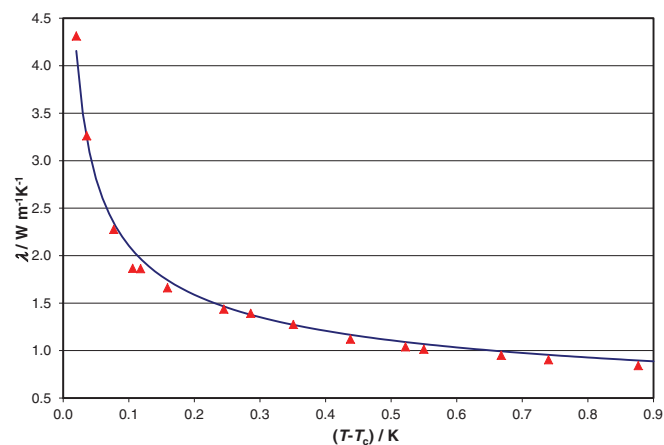

FIG. 5. Thermal conductivity λ as a function $\Delta T = T - T_c$ at $\rho = \rho_c$ very close to the critical temperature. The symbols represent the thermal-conductivity data deduced from the dynamic light-scattering measurements as listed in Table 6. The curve represents the values calculated from the present formulation.

IAPWS.[37] The experimental data are along isobars as a function of temperature on IPTS-48. The temperatures have been converted to ITS-90 and the densities have been recalculated according to IAPWS-95.[1]

Le Neindre et al.[15,124] published two sets of experimental thermal-conductivity data obtained with a coaxial-cylinder apparatus.[177] While the data of Sirota et al.[37] were obtained along isobars as a function of temperature, the data of Le Neindre et al. were obtained along isotherms as a function of pressure. The temperatures reported by Le Neindre et al. in 1973 (Ref. 15) are based on IPTS-48, while the data reported in 1987 (Ref. 124) are based on IPTS-68. Again all temperatures were converted to ITS-90 (Ref. 32) and the densities were recalculated according to the IAPWS Formulation 1995 for the thermodynamic properties.[1]

The work of Tufeu and Le Neindre[124] represents an extensive effort to improve upon the experimental information earlier obtained by Le Neindre et al.[15] in the same laboratory. The authors state that the two datasets agree within their respective 2% claimed accuracy. They also appear to be consistent with the dynamic light-scattering data for the thermal diffusivity.[175] The thermal-conductivity data of Sirota et al. deviate from the data obtained by Le Neindre and co-workers by as much as 10% in the density range from 200 to 400 kg m^{-3} at supercritical temperatures up to 673 K.[124] On the 22.6 MPa isobar, there are deviations amounting to 25%.[175] Moreover, as we shall see below, the data of Sirota et al. exhibit some unphysical behavior regarding the location of the thermal-conductivity maxima in the critical region. Hence, we have adopted the experimental data of Tufeu and Le Neindre,[124] together with the dynamic light-scattering data of Desmarest et al.,[48] as the primary experimental information to validate the present thermal-conductivity formulation for describing the thermal conductivity of H$_2$O in the critical region.

The thermal conductivity of H$_2$O at supercritical temperatures is shown as function of the density in Fig. 6. The symbols indicate the experimental data reported by Tufeu and Le Neindre.[124] The curves represent the values calculated from the present formulation. There are some deviations at $T = 652$ K, which is only 5 K above T_c, where it becomes difficult to measure the thermal conductivity with the coaxial-cylinder measurement technique very accurately. Moreover, close to the critical temperature the effects of increased uncertainty in the density on the thermal conductivity become appreciable. However, we know from Fig. 5 that the thermal-conductivity formulation does reproduce the correct limiting behavior near the critical temperature. This is further demonstrated in Fig. 7, which includes the thermal conductivity as a function of density at temperatures very close to T_c. Hence, we conclude that the formulation does yield a satisfactory description of the critical enhancement consistent with the available experimental accuracy.

The experimental thermal conductivity data reported by Sirota et al.[37] are shown in Fig. 8. A comparison of the data of Sirota et al.[37] in Fig. 8 with those of Tufeu and Le Neindre[124] in Fig. 6 reveals some considerable inconsistencies between the two datasets. While the two datasets show similar magnitudes
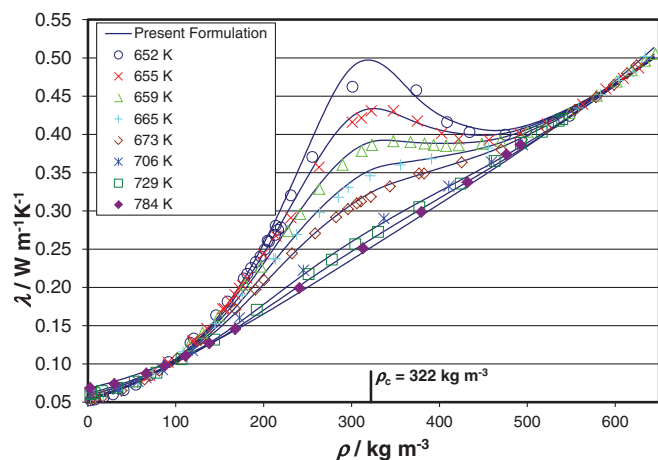
FIG. 6. Thermal conductivity λ as a function of the density ρ at supercritical temperatures. The symbols indicate the experimental data reported by Tufeu and Le Neindre.[124] The curves represent values calculated from the present formulation.

FIG. 8. Thermal conductivity λ as a function of the density ρ at constant pressures. The symbols indicate experimental data reported by Sirota *et al.*[37] The curves represent values calculated from the present formulation.

for the thermal conductivity, the density dependence of the thermal-conductivity data of Sirota *et al.*[37] appears to be unphysical, displaying a maximum at some isobars well above the critical density $\rho = \rho_c$. This problem was already noticed in the development of the previous IAPWS formulation for the thermal conductivity of H_2O, when the densities were calculated from the reported pressures and temperatures by using other equations of state.[19] In the critical region, the density becomes very sensitive to small errors in either the pressure or the temperature. While Sirota *et al.*[37] put great efforts in determining the thermal conductivity, we conclude that either the reported pressures or temperatures are not sufficiently accurate to deduce reliable values for the corresponding densities.
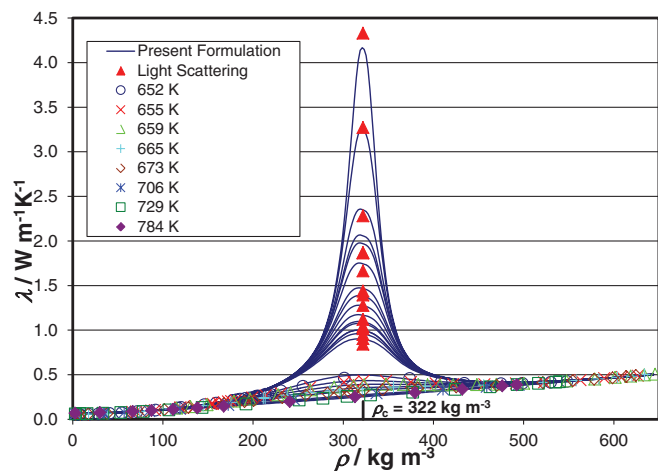
3.4. Computer-program verification

Tables 7 and 8 are provided to assist the user in computer-program verification. The thermal-conductivity values are calculated as a function of the tabulated temperatures and densities. Regarding Table 7, we note that some derivatives from IAPWS-95 (Ref. 1) diverge at $\rho = 0$; for those points in Table 7 $\bar{\lambda}_2$ must be set to zero. For the liquid points at 298.15 K, $\Delta\bar{\chi}$ calculated from Eq. (17) is less than zero, so (as stated in Sec. 3.3) it must be set to zero for calculations to proceed and $\bar{\lambda}_2 = 0$.

3.5. Liquid H_2O at 0.1 MPa

It is useful to have simplified correlating equations for the properties of liquid water at atmospheric pressure with uncertainties no greater than those of the more complex formulations that cover wide ranges of temperature and pressure. For this purpose, IAPWS has recommended formulations for the properties, including thermal conductivity, of liquid water as a function of absolute temperature T at a standard pressure of 0.1 MPa.[178] Details on these correlations are presented in Ref. 178; we present only the thermal-conductivity correlation here. An older recommended correlation for the thermal conductivity of liquid water at 0.1 MPa is provided in Ref. 179; Eq. (21) below replaces that correlation.

The dimensionless thermal conductivity $\bar{\lambda}$ of liquid water at a pressure of 0.1 MPa is described by the following

FIG. 7. Thermal conductivity λ as a function of the density ρ at temperatures very close to T_c. The solid triangles indicate the thermal-conductivity data deduced from the dynamic light-scattering measurements of Desmarest *et al.*[48] Additional symbols show the experimental data reported by Tufeu and Le Neindre.[124] The curves represent values calculated from the present formulation.
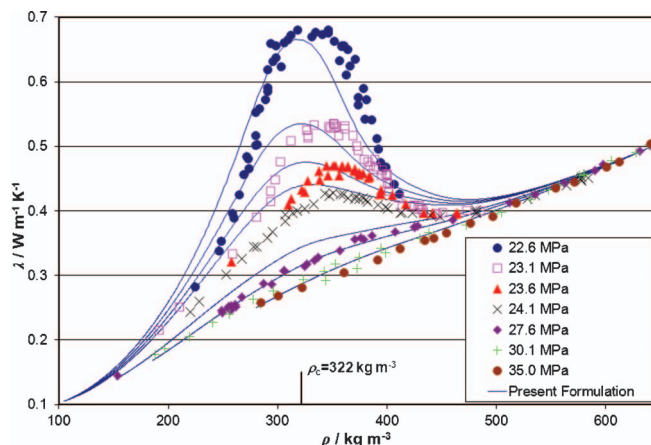
TABLE 7. Sample points for computer-program verification of the correlating equation, Eq. (2). At these points, $\bar{\lambda}_2 = 0$.

T (K)	ρ (kg m^{-3})	λ (mW m^{-1} K^{-1})
298.15	0	18.434 188 3
298.15	998	607.712 868
298.15	1200	799.038 144
873.15	0	79.103 465 9

TABLE 8. Sample points for computer-program verification of the correlating equation, Eq. (2), including the critical-enhancement contribution $\bar{\lambda}_2$. For all points, $\bar{\lambda}_0(647.35\,\text{K}) = 51.576\,479\,7$.

T (K)	ρ (kg m^{-3})	$\bar{\lambda}_1$	$\bar{\lambda}_2$	λ (mW m^{-1} K^{-1})
647.35	1	1.006 849 7	0.000 130 0	51.929 892 4
647.35	122	2.144 517 3	20.316 232 0	130.922 885
647.35	222	3.484 073 6	188.091 206	367.787 459
647.35	272	4.223 370 8	540.133 176	757.959 776
647.35	322	4.968 195 3	1187.513 54	1443.755 56
647.35	372	5.696 125 0	356.533 33	650.319 402
647.35	422	6.397 342 9	118.931 062	448.883 487
647.35	750	11.587 053 2	3.341 930 3	600.961 346

TABLE 9. Coefficients c_i and d_i in Eq. (21) for the thermal conductivity of liquid water at 0.1 MPa.

i	c_i	d_i
1	1.663 0	−1.15
2	−1.778 1	−3.4
3	1.156 7	−6.0
	−0.432 115	−7.6

equation:

$$\bar{\lambda} = \sum_{i=1}^{4} c_i (\tilde{T})^{d_i}, \tag{21}$$

where $\tilde{T} = T/(300\,\text{K})$ and c_i and d_i are coefficients and exponents given in Table 9. Equation (21) is recommended for use in the following temperature range:

$$273.15\,\text{K} \le T \le 383.15\,\text{K} \tag{22}$$

and extrapolates in a physically reasonable manner down to 253.15 K, as shown in Fig. 9. At some temperatures within this range, the equilibrium phase at 0.1 MPa is a vapor (above approximately 372.26 K), or is a solid (below approximately 273.15 K), and at these conditions Eq. (21) describes the thermal conductivity of a metastable phase. Equation (21) is fitted to values from Eq. (2) in this work, and the uncertainty is the same as that of Eq. (2) that will be discussed in Sec. 4.2.

4. Evaluation

In summary, the recommended formulation for the thermal conductivity is given by Eq. (2),

$$\bar{\lambda} = \bar{\lambda}_0(\overline{T}) \times \bar{\lambda}_1(\overline{T}, \overline{\rho}) + \bar{\lambda}_2(\overline{T}, \overline{\rho}).$$

The function $\bar{\lambda}_0(\overline{T})$ is given by Eq. (4) with coefficients in Table 2. The function $\bar{\lambda}_1(\overline{T}, \overline{\rho})$ is given by Eq. (6) with coefficients in Table 4. The function $\bar{\lambda}_2(\overline{T}, \overline{\rho})$ is given by Eq. (13) with the parameters presented in Table 5, thermodynamic properties from the IAPWS-95 release[1] and the viscosity $\overline{\mu}$ from the IAPWS Formulation 2008 for the Viscosity.[5]

4.1. Comparisons with experimental data and previous IAPWS formulation for thermal conductivity

In order to evaluate performance, we have compared the results of the new formulation, Eq. (2), as well as the previous IAPWS formulation for the thermal conductivity,[29] with the experimental database. Comparisons with all sources in the experimental database are presented in Table 10, which gives the number of data points, estimated uncertainty of the data, average percent deviation, average absolute percent deviation, and the standard deviation of each data source. Some points are extrapolations of the previous IAPWS correlation,[29] because they are outside of the recommended range of temperatures and densities. We define the percent deviation as $P = 100*$ $(\lambda_{\text{exp}} - \lambda_{\text{calc}})/\lambda_{\text{exp}}$, where λ_{exp} is the experimental value of the thermal conductivity, and λ_{calc} is the value calculated from the present correlation, Eq. (2). The average absolute percent deviation (AAD) is found with the expression AAD $= (\Sigma |P|)/n$, where the summation is over all n points; the average percent deviation (bias) is AVG $= (\Sigma P)/n$, and the standard deviation is STDEV $= ([n\Sigma P^2 - (\Sigma P)^2]/n^2)^{1/2}$. As indicated in Table 10, the results of the new formulation and the previous IAPWS formulation for the thermal conductivity[29] are in most cases comparable, with significant differences observed in only a few cases, especially at very high pressures, as discussed below.

Selected graphical comparisons of the new correlation and the 1985/2008 IAPWS Formulation[29] are shown in Figs. 10–14. Figures 10a and 10b show the percent deviation of selected high-pressure experimental data from the model proposed here, as well as from the 1985/2008 IAPWS Formulation. In the very-high-pressure region, above 500 MPa,
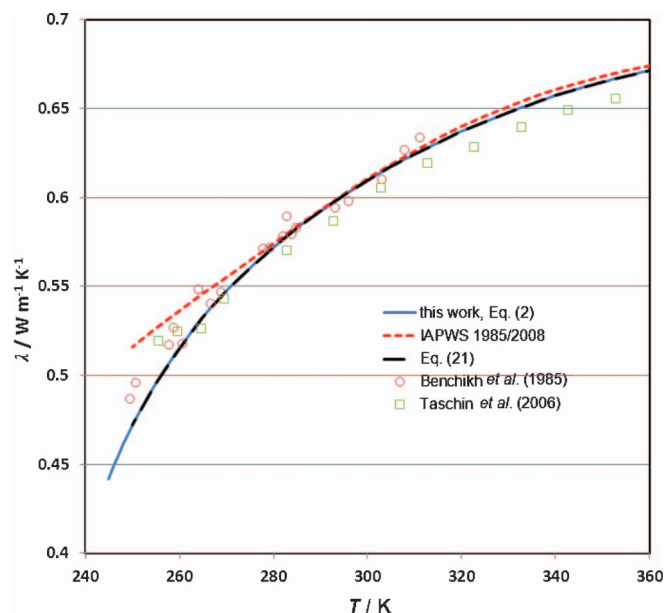

FIG. 9. Thermal conductivity of liquid water at 0.1 MPa, showing supercooled region. Experimental data have been converted from thermal-diffusivity data.

TABLE 10. Summary of comparisons of Eq. (2) with experimental data and of the previous IAPWS formulation for the thermal conductivity with experimental data.

First author	No. Points	Unc. (%)	Present work			1985/2008 IAPWS formulation[29]		
			AAD (%)	AVG	STDEV	AAD (%)	AVG	STDEV
Bridgman[50]	25	5	3.0	2.4	2.2	5.3	5.3	4.9
Schmidt[51]	24	3	0.5	−0.3	0.5	0.4	0.0	0.4
Milverton[52]	77	2	1.2	−1.2	1.0	1.2	−1.2	0.6
Timrot[53]	10	3	0.9	0.8	0.7	0.7	0.2	0.8
Vargaftik[54]	11	3	1.0	0.0	1.4	1.0	0.1	1.3
Vargaftik[55]	14	3	1.5	0.8	1.9	1.5	0.4	2.0
Timrot[56]	33	3	4.5	−3.0	5.4	4.3	−2.9	5.1
Vargaftik[57]	8	3	1.9	0.6	2.2	1.8	1.3	2.2
Riedel[58]	1	1	0.5	0.5	0.0	0.6	0.6	0.0
Schmidt[59]	8	0.3	0.4	0.0	0.5	0.5	0.4	0.4
Challoner[60]	5	1	0.9	−0.9	0.2	0.4	−0.4	0.3
Vargaftik[61]	4	2	1.6	−1.5	1.4	1.8	−1.5	1.4
Lawson[62]	35	2	1.1	0.3	1.4	1.2	0.8	1.7
Vargaftik[63]	61	2	2.9	−2.0	2.7	2.5	−1.8	2.3
Vargaftik[64]	35	2	1.9	1.8	3.4	1.8	1.7	2.7
Vargaftik[65]	41	2	2.3	−1.3	2.2	2.1	−1.3	2.0
Vines[66]	2	2	1.8	1.8	1.8	2.3	2.0	2.3
Tarzimanov[67]	33	2	2.9	−0.4	3.3	3.3	−1.3	3.7
Vargaftik[68]	29	1	1.2	0.0	1.5	1.0	−0.4	1.1
Vukalovich[69]	135	5	13.6	12.6	13.7	9.6	8.7	9.2
Vargaftik[70]	10	3	1.7	1.7	0.7	1.8	1.8	0.8
Keyes[71]	46	3	3.0	0.5	3.4	2.4	0.7	2.7
Vargaftik[72]	21	3	1.4	−0.9	1.5	1.2	0.2	1.4
Venart[73]	163	1.5	2.0	0.5	2.6	2.2	1.0	2.8
Baker[74]	4	3	1.7	1.7	1.0	1.8	1.8	0.9
Venart[75]	56	2	1.5	0.3	1.9	1.5	0.8	2.0
Brain[76]	3	1.5	1.0	0.6	0.9	1.0	0.7	0.9
Le Neindre[77]	65	2	1.5	1.1	1.7	1.7	1.1	2.0
Tarzimanov[78]	19	1	0.8	0.3	0.9	0.7	0.1	0.8
Brain[79]	33	2	2.3	0.8	2.4	1.9	0.7	2.0
Bach[80]	374	1	0.6	−0.4	0.7	0.6	0.0	0.7
Cherneeva[81]	130	4.3	4.4	2.6	6.6	3.6	2.4	5.0
Rastorguev[82]	54	1.6	3.1	−3.1	1.7	2.9	−2.9	1.6
Stupak[83]	4	2	0.7	−0.7	0.3	0.2	−0.2	0.3
Cherneeva[84]	88	4.3	1.8	−0.8	3.5	1.5	−0.3	3.2
Gazdiev[85]	8	1.5	0.2	0.1	0.2	0.4	0.4	0.2
Papadopoulos[86]	1	3	3.1	3.1	0.0	3.3	3.3	0.0
Turnbull[87]	1	1.5	1.0	−1.0	0.0	0.9	−0.9	0.0
Dijkema[88]	2	0.5	1.7	−1.7	1.2	1.2	−1.0	1.2
Mustafaev[89]	14	3	1.6	−1.2	1.3	1.7	−1.3	1.3
Potienko[90]	1	3	0.9	0.9	0.0	1.0	1.0	0.0
Le Neindre[15]	145	2	6.5	−0.3	10.2	6.6	−2.2	10.8
Tarzimanov[91]	87	3	2.4	0.2	3.0	2.5	−0.3	3.1
Vargaftik[92]	11	1.5	1.0	−0.5	1.0	1.0	−0.2	1.1
Castelli[93]	62	1	1.5	1.5	0.6	1.0	1.0	0.4
Shurygin[94]	1	5	6.8	6.8	0.0	6.9	6.9	0.0
Rastorguev[95]	443	1.5	0.6	−0.4	0.7	0.6	−0.1	0.7
Amirkhanov[96]	351	2	2.0	−1.6	1.8	1.1	−0.7	1.2
Bury[97]	111	2	2.6	2.0	2.6	2.6	2.1	2.3
Takizawa[98]	29	2	1.6	−1.5	0.7	1.3	−1.2	0.7
Le Neindre[99]	215	1.5	0.5	0.0	0.7	0.7	0.2	0.8
Tsedeberg[100]	147	2	2.2	0.4	2.9	2.2	−0.3	2.8
Popov[101]	75	4	1.8	−1.0	2.7	3.3	−2.6	3.3
Rastorguev[102]	29	2	0.3	−0.2	0.3	0.4	0.1	0.4
Amirkhanov[103]	136	2	2.2	1.1	2.4	2.9	−2.4	3.1
Takizawa[104]	9	1.5	1.9	−1.9	0.4	1.5	−1.5	0.5
Varchenko[105]	16	3	0.9	−0.9	0.2	0.8	−0.8	0.2
Amirkhanov[106]	57	3	1.1	−0.8	1.3	0.9	0.2	1.2
Curtiss[107]	54	2	0.8	0.7	0.7	1.2	1.2	0.2
Filippov[108]	1	4	2.0	−2.0	0.0	1.9	−1.9	0.0
Popov[109]	240	4	2.4	1.5	2.5	2.9	0.6	3.4
Tufeu[110]	16	3	3.6	3.6	2.0	3.5	3.5	1.7

TABLE 10. Summary of comparisons of Eq. (2) with experimental data and of the previous IAPWS formulation for the thermal conductivity with experimental data.—Continued

First author	No. Points	Unc. (%)	Present work			1985/2008 IAPWS formulation[29]		
			AAD (%)	AVG	STDEV	AAD (%)	AVG	STDEV
Yata[111]	180	2	0.5	−0.4	0.5	0.6	0.0	0.8
Yata[112]	241	2.5	0.6	−0.6	0.5	0.7	0.3	0.8
Frohn[113]	8	3	1.4	−1.4	0.9	1.9	−1.8	1.4
Popov[114]	50	6	2.4	−0.6	3.1	2.2	−1.4	2.7
Popov[115]	148	4	1.9	1.4	2.0	2.1	0.9	2.5
Venart[116]	22	1.5	0.5	0.0	0.6	0.5	0.3	0.5
Dietz[117]	54	1	1.1	0.3	1.7	1.8	1.3	2.7
Nagasaka[118]	4	1	0.4	−0.4	0.3	0.1	0.0	0.1
Sirota[37]	555	3	5.1	3.1	6.0	3.7	0.6	5.3
Amirkhanov[119]	84	4	1.8	−1.5	1.6	8.8	8.1	11.0
Alloush[120]	3	3	1.0	0.6	1.0	1.2	0.9	1.1
Nagasaka[121]	25	1	0.4	0.0	0.5	0.3	0.2	0.4
Miroshnichenko[122]	4	2	1.0	−1.0	0.5	1.6	−1.6	0.3
Tufeu[123]	12	0.5	1.0	0.5	1.0	0.8	0.2	1.2
Tufeu[124]	209	2	2.0	0.1	2.6	2.1	−1.1	2.5
Guseinov[125]	10	1.8	0.2	0.0	0.2	0.5	0.4	0.3
Wakeham[126]	2	0.5	0.3	0.3	0.1	0.4	0.4	0.1
Assael[127]	12	0.5	0.4	−0.4	0.3	0.2	0.0	0.2
Zalaf[128]	78	0.5	0.5	0.2	0.6	0.3	0.3	0.3
Tarzimanov[129]	104	1.3	3.8	3.7	2.5	3.6	3.5	2.3
Venkateshan[130]	1	4	2.3	2.3	0.0	2.4	2.4	0.0
Eldarov[131]	6	2	0.1	0.0	0.1	0.4	0.4	0.0
Gross[132]	1	2	0.8	−0.8	0.0	0.7	−0.7	0.0
Assael[133]	4	0.5	0.2	−0.2	0.0	0.2	0.0	0.2
Ramires[134]	38	0.5	0.3	0.0	0.3	0.4	0.3	0.3
Watanabe[135]	2	2	0.9	0.9	0.4	1.0	1.0	0.4
Grigorev[136]	54	2	0.8	0.7	0.5	1.1	0.9	0.8
Mensah-Brown[137]	38	0.5	0.4	0.2	0.4	0.5	0.4	0.4
Ramires[138]	31	0.5	0.3	−0.2	0.3	0.3	0.2	0.3
Abdulagatov[33]	39	2	0.6	−0.5	0.8	0.5	0.0	0.6
Abdulagatov[34]	22	2	0.4	0.0	0.6	0.5	0.3	0.5
Abdulagatov[36]	42	1.6	0.7	−0.4	0.7	0.4	−0.2	0.4
Abdulagatov[35]	31	2	0.4	−0.2	0.5	0.3	0.1	0.3

there are only four sets of data available: Amirkhanov et al.,[119] Lawson et al.,[62] the very old data of Bridgman[50] and the more recent work of Abramson et al.[45] The 1985/2008 IAPWS Formulation[29] was not designed to be used in this region, and deviations are quite large as is evident from Fig. 10b. Since the equation of state is valid up to 1 GPa, we included the high-pressure data in our regression in order to improve the behavior of the thermal-conductivity formulation at high pressures. Comparisons with the data show that the deviations are within 5% up to 1 GPa, and within 15% to 4 GPa. Figures 11a and 11b emphasize the region between 100 MPa and 500 MPa. In this region, we felt that the most reliable data are those of Dietz et al.[117] covering the temperature range of 303 K–523 K at pressures up to 350 MPa with an estimated uncertainty of 1%. The data of Lawson et al.[62] and the 1979 data of Amirkhanov et al.[106] are consistent with those of Dietz. It had been noted earlier by Sengers et al.[19] that some of the other data from the Amirkhanov group appear to be inconsistent with the data of other investigators, and this is evident in the deviation plots. Finally, we present Fig. 12 to illustrate how the high-pressure behavior of the

proposed equation extrapolates well to high pressures and corrects deficiencies in this region of the 1985/2008 IAPWS Formulation.[29]

Figures 13a and 13b show deviations for liquid water at atmospheric pressure. Deviations from the recommended data of Ramires et al.[152] are also displayed. The recommended data have an uncertainty of 0.7%. Both the proposed correlation and the 1985/2008 IAPWS Formulation[29] represent the recommended data to within their estimated uncertainty, with the exception of one point at 370 K where the deviation from the 1985/2008 IAPWS Formulation[29] slightly exceeds 0.7%. Figures 14a and 14b display deviations for water vapor at low pressures. The behavior of both formulations is similar in this region, although there are some differences for specific datasets. The 1985/2008 IAPWS Formulation[29] represents the dataset of Keyes and Vines[71] better, while the present formulation yields a better representation of the dataset of Tarzimanov et al.[67] Figures 15a and 15b show deviations for supercritical water for both the present model and the 1985/2008 IAPWS Formulation.[29] Again, the performance is
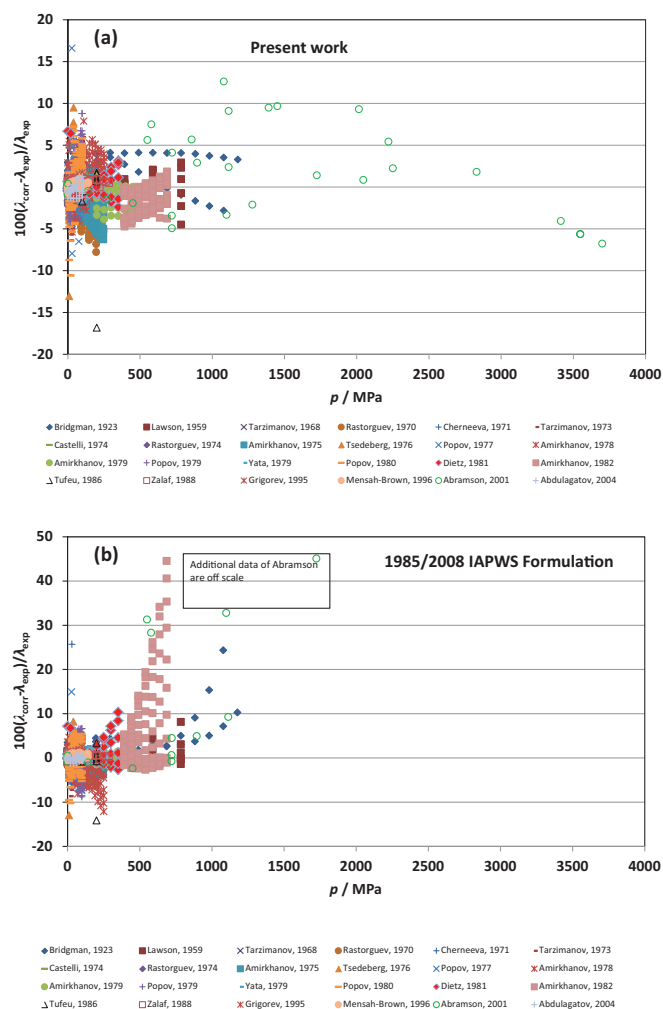
FIG. 10. (a) Percent deviation as a function of pressure for selected high-pressure data, present correlation. (b) Percent deviation as a function of pressure for selected high-pressure data, 1985/2008 IAPWS Formulation.[29]
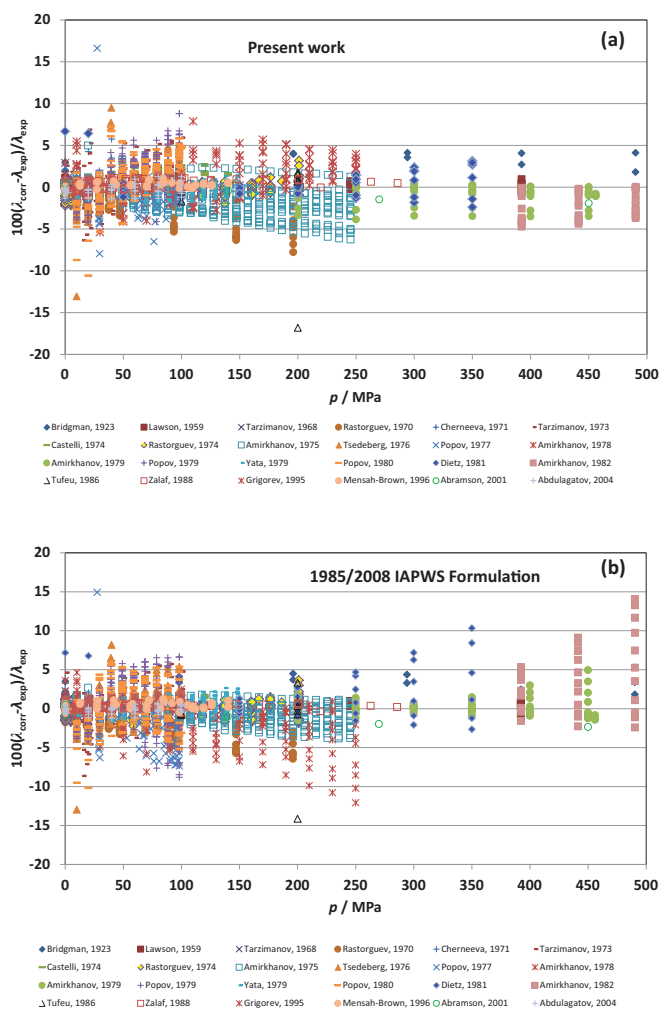
FIG. 11. (a) Percent deviation as a function of pressure for selected high-pressure data, present correlation. (b) Percent deviation as a function of pressure for selected high-pressure data, 1985/2008 IAPWS Formulation.[29]

comparable. The present formulation has a small negative bias in the very-high-temperature region compared to the dataset of Vargaftik *et al.*[72] This is due to the formulation of the zero-density limit having been made compatible with the theoretical values of Hellmann *et al.*,[145] as was described in Sec. 3.1.

4.2. Range and uncertainty estimates for the correlation

The range of validity of Eq. (2) for the thermal conductivity is

$$
\begin{aligned}
&0 < p < p_t \text{ and } 273.16 \leq T \leq 1173.15 \text{ K}, \\
&p_t \leq p \leq 100 \text{ MPa and } T_m(p) \leq T \leq 1173.15 \text{ K}, \\
&100 \text{ MPa} < p \leq 250 \text{ MPa for } T_m(p) \leq T \leq 874 \text{ K}, \\
&250 \text{ MPa} < p \leq 687 \text{ MPa for } T_m(p) \leq T \leq 573 \text{ K}, \quad (23) \\
&687 \text{ MPa} < p \leq 785 \text{ MPa for } T_m(p) \leq T \leq 403 \text{ K}, \\
&785 \text{ MPa} < p \leq 1000 \text{ MPa for } T_m(p) \leq T \leq 348 \text{ K},
\end{aligned}
$$
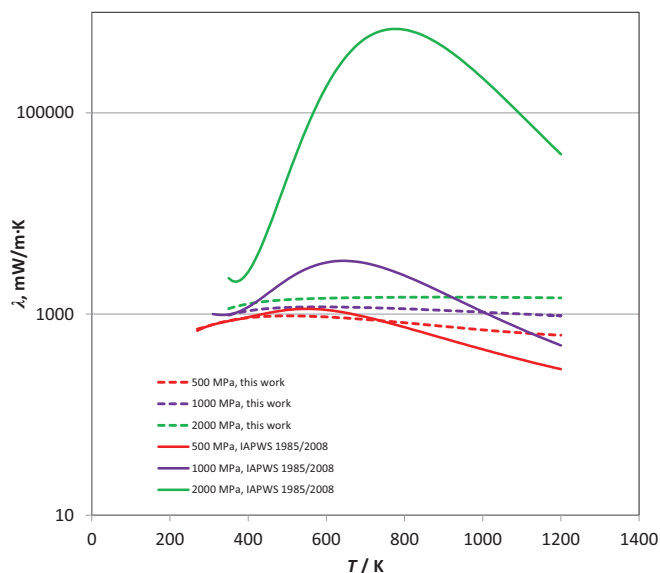
FIG. 12. Selected high-pressure isotherms of the proposed correlation and the 1985/2008 IAPWS Formulation.[29]
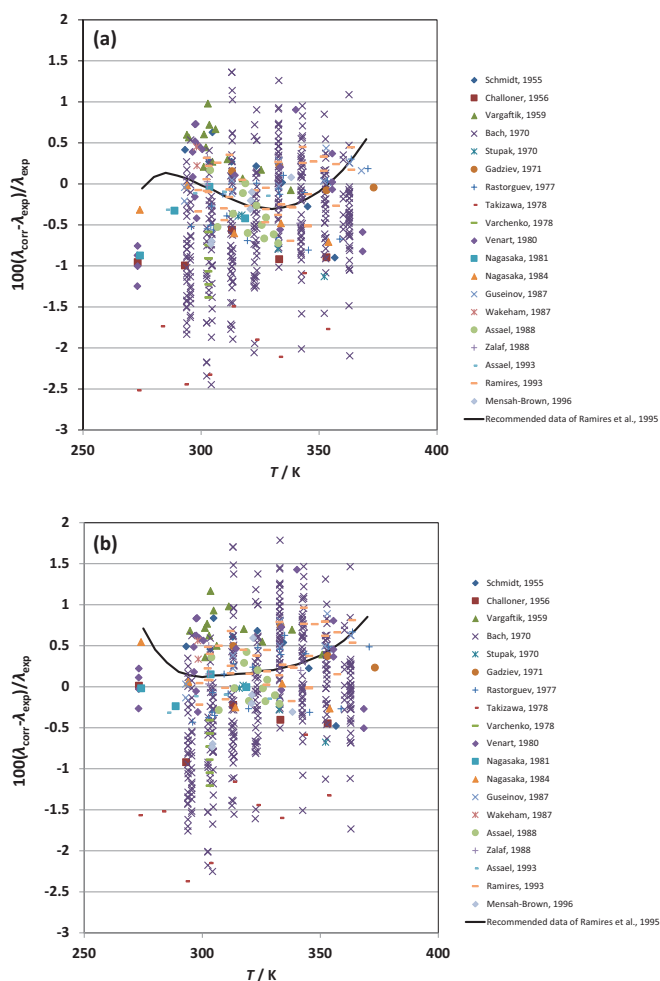
FIG. 13. (a) Comparisons for liquid water at atmospheric pressure, present correlation. (b) Comparisons for liquid water at atmospheric pressure, 1985/2008 IAPWS Formulation.[29]
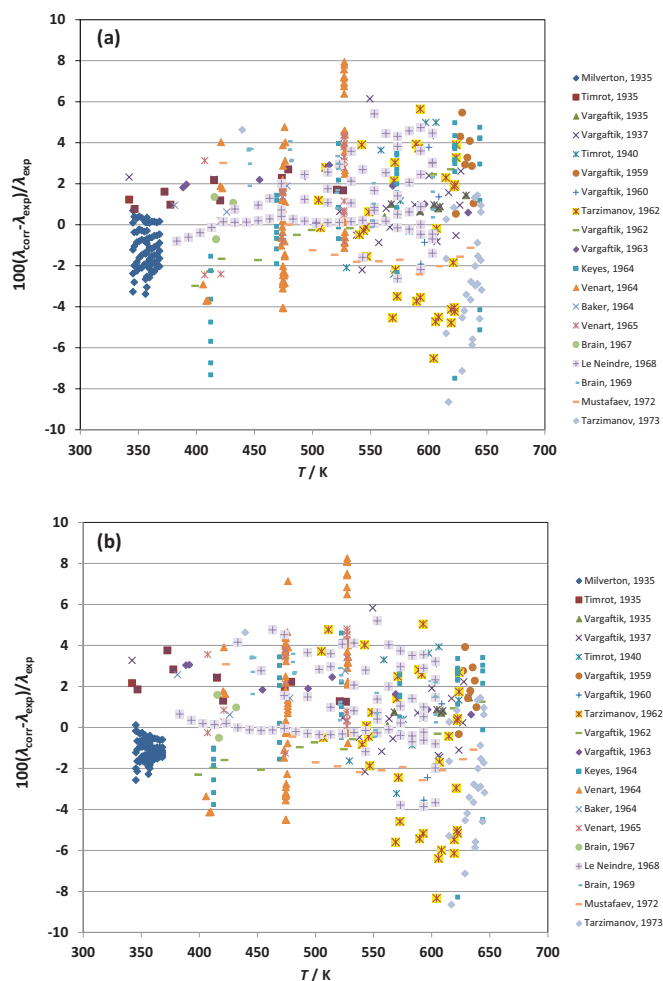
FIG. 14. (a) Comparisons for water vapor at low pressures, present work. (b) Comparisons for water vapor at low pressures, 1985/2008 IAPWS Formulation.[29]

where T_m is the pressure-dependent melting temperature and p_t is the triple-point pressure; both are given in Refs. 180 and 181. In addition, based on comparisons with the data of Abramson *et al.*,[45] Eq. (2) provides reasonable extrapolation behavior for pressures to 4 GPa for temperatures up to 673 K. This is outside the range of applicability of the equation of state[2] (that only extends to 1 GPa), but both the densities and the thermal conductivities show physically realistic behavior. The 1985/2008 IAPWS Formulation[29] is not valid in this region at all as it displays physically unrealistic behavior. In addition, at high temperatures and low densities, Eq. (2) extrapolates in a physically reasonable manner above 1173.15 K, as noted in Sec. 2.1. However, the extrapolation will become increasingly unrealistic above approximately 1400 K, where a contribution to the thermal conductivity due to the dissociation of H$_2$O becomes significant. Kessel'man and Blank[182] show that the thermal conductivity of water with the dissociation effect included at 1400 K and 0.1 MPa is approximately 20% greater than that of non-dissociated water, and recommendations are provided for the thermal conductivity of water with the dissociation effect included at temperatures up to 6000 K.[183] For vapor states at temperatures below the triple-point temperature of 273.16 K and pressures less than

or equal to the sublimation pressure, the calculation of the thermal conductivity is dominated by the dilute-gas term, and this behaves in a physically reasonable manner down to at least 250 K. For the metastable subcooled liquid at atmospheric pressure, Eq. (2) behaves in a physically reasonable manner down to 250 K, as discussed further in Sec. 4.3. Finally, for stable fluid states outside the range of validity of Eq. (2), but within the range of validity of IAPWS-95,[1] the extrapolation behavior of Eq. (2) is physically reasonable.

The critical thermal-conductivity enhancement is significant in a large range of temperatures and densities. This is illustrated in Fig. 16, which shows contours in the temperature-density plane encompassing regions around the critical point where the contribution from the critical enhancement term $\bar{\lambda}_2(\overline{T}, \overline{\rho})$ to the total thermal conductivity $\bar{\lambda}(\overline{T}, \overline{\rho})$ exceeds 5%, 1%, 0.5%, and 0.1%. The information in this figure can be used as a guide to decide at which temperatures and densities the critical-enhancement term needs to be included to calculate the thermal conductivity with a given accuracy. We note that the range of the critical thermal-conductivity enhancement for H$_2$O is comparable to that observed for other fluids such as carbon dioxide.[184]
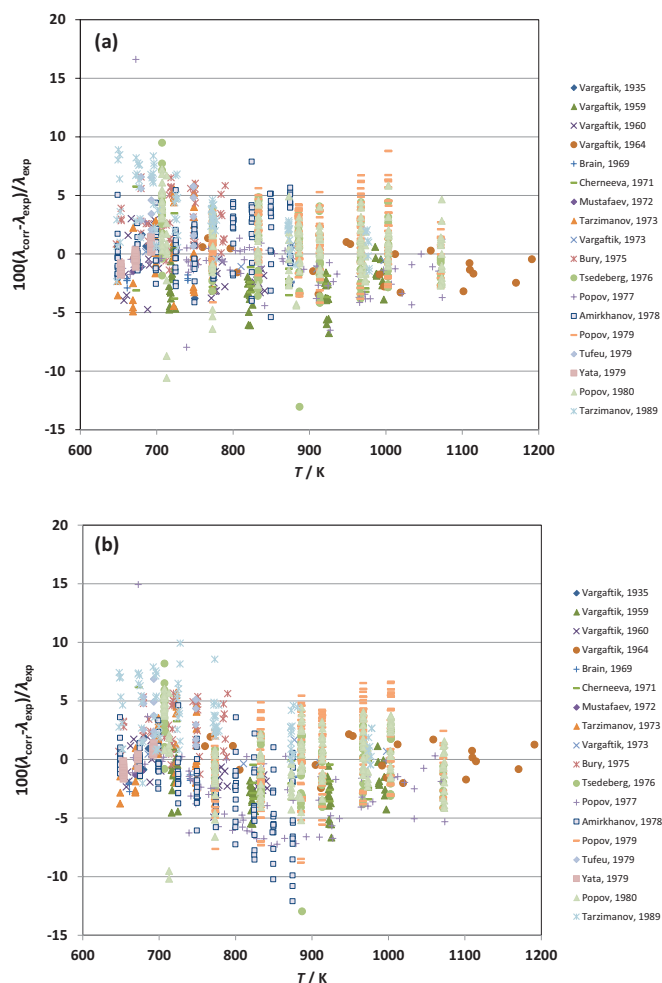
FIG. 17. Estimated uncertainties for Eq. (2).

FIG. 15. (a) Comparisons for supercritical water, present work. (b) Comparisons for supercritical water, 1985/2008 IAPWS Formulation.[29]

marized in Fig. 17 and can be considered as estimates of a combined expanded uncertainty with a coverage factor $k = 2$. Finally, the present formulation reproduces the recommended value[152] of the thermal conductivity at 298.15 K and 0.1 MPa, 0.6065 W m^{-1} K^{-1}, to within the number of significant figures provided, and also represents all recommended values in Ref. 152 from 275 K to 370 K at 0.1 MPa to within the stated uncertainty of 0.7%.

For estimates of uncertainty outside the critical region, we relied upon comparisons with the 1985/2008 IAPWS Formulation[29] in regions where it is applicable, and also with a subset of the experimental data. The uncertainty estimates are sum-
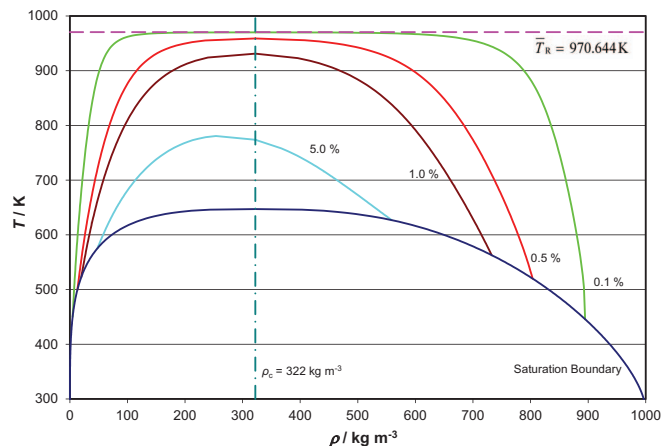
4.3. Supercooled region

The thermal diffusivity of supercooled water has been measured by Benchikh *et al.*[47] and by Taschin *et al.*[46] These data were converted to thermal conductivity with the density and heat capacity calculated from the recommended equations in Ref. 178 for supercooled water. Figure 9 shows the agreement between the correlating Eq. (2) and these two datasets, demonstrating that the extrapolation behavior of Eq. (2) into the supercooled liquid region is reasonable. For comparison purposes, the extrapolation behaviors of the 1985/2008 IAPWS formulation for the thermal conductivity[29] and of the compact equation for 0.1 MPa, Eq. (21), are also shown. Equations (2) and (21) are indistinguishable on the plot.

The isobaric heat capacity c_p of supercooled water exhibits an anomalous increase at temperatures below 270 K as measured by Angell *et al.*[185] and Archer and Carter.[186] The IAPWS-95 formulation in the region of supercooled water was fitted to the c_p measurements of Angell *et al.* The subsequent c_p measurements of Archer and Carter are believed to have a slightly higher accuracy.[187] Conversion of the thermal-diffusivity data to thermal-conductivity data with the aid of an equation that reproduces the c_p measurements of Archer and Carter yields slightly lower values of thermal conductivity, but differ by no more than 1% from the values obtained using c_p from IAPWS-95, which is within the experimental accuracy of the data.[188]

FIG. 16. Contours in the temperature-density plane where the contribution from the critical-enhancement λ_2 to the total thermal conductivity λ equals 5%, 1%, 0.5%, and 0.1%, respectively.
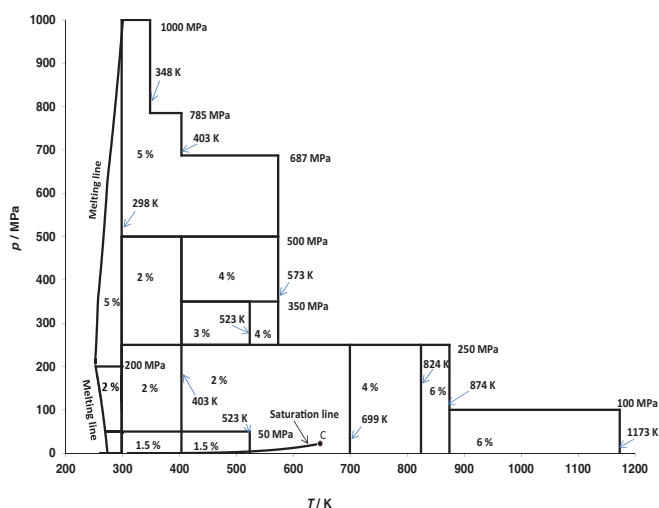
TABLE 11. Coefficients A_{ij} in Eq. (26) for $\zeta_I(\overline{T}_R, \overline{\rho})$.

	$j = 0$	$j = 1$	$j = 2$
$i = 0$	6.537 868 071 995 16	6.527 177 592 817 99	5.355 005 298 961 24
$i = 1$	−5.611 499 549 233 48	−6.308 169 833 875 75	−3.964 156 899 254 46
$i = 2$	3.396 241 673 613 25	8.083 792 854 925 95	8.919 902 089 187 95
$i = 3$	−2.274 926 297 308 78	−9.822 405 101 976 03	−12.033 872 950 579 0
$i = 4$	10.263 185 466 270 9	12.135 841 379 139 5	9.194 948 651 943 02
$i = 5$	1.978 150 503 315 19	−5.543 496 645 712 95	−2.168 662 744 797 12
	$j = 3$	$j = 4$	
$i = 0$	1.552 259 599 066 81	1.119 992 641 999 4	
$i = 1$	0.464 621 290 821 181	0.595 748 562 571 649	
$i = 2$	8.932 373 748 614 79	9.889 525 650 789 20	
$i = 3$	−11.032 196 006 112 6	−10.325 505 114 704 0	
$i = 4$	6.167 809 999 333 60	4.668 612 944 574 14	
$i = 5$	−0.965 458 722 086 812	−0.503 243 546 373 828	

5. Recommendations for Industrial Applications

5.1. Industrial application of the correlating equation

The recommended formulation for calculating the thermal conductivity in conjunction with IAPWS-IF97 (Ref. 3) has a form similar to Eq. (2),

$$\overline{\lambda}_I(\overline{T}, \overline{\rho}) = \overline{\lambda}_0(\overline{T}) \times \overline{\lambda}_1(\overline{T}, \overline{\rho}) + \overline{\lambda}_{2I}(\overline{T}, \overline{\rho}), \qquad (24)$$

where the functions $\overline{\lambda}_0(\overline{T})$ and $\overline{\lambda}_1(\overline{T}, \overline{\rho})$ are identical to those specified in Eqs. (4) and (5), but where for the industrial application we use

$$\overline{\lambda}_{2I}(\overline{T}, \overline{\rho}) = \Lambda \frac{\overline{\rho}\,\overline{c}_p \overline{T}}{\overline{\mu}} Z(\overline{q}_D \xi). \qquad (25)$$

In Eq. (25), the isobaric specific heat capacity $\overline{c}_p$, as well as the density derivatives in Eq. (17) for specifying the correlation length ξ in Eqs. (13) and (16) for the function Z, are to be calculated from IAPWS-IF97.[3] The function $\zeta(\overline{T}_R, \overline{\rho})$ in Eq. (19) is for industrial applications to be calculated from

$$\zeta_I(\overline{T}_R, \overline{\rho}) = \frac{1}{\sum_{i=0}^{5} A_{ij}\overline{\rho}^i} \qquad (26)$$

with coefficients A_{ij} given in Table 11. The dimensionless viscosity, $\overline{\mu}$, in Eq. (25) should be calculated from the recommended viscosity correlation for industrial application as described in the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance.[5] If one needs the thermal conductivity for an industrial application as a function of pressure, rather than as a function of density, the pressures should be converted to densities to be entered into Eqs. (24) and (25) by using the IAPWS Industrial Formulation 1997 for the thermodynamic properties.[3]

The subscript j denotes ranges defined as

$$
\begin{aligned}
&j = 0: \ \overline{\rho} \leq 0.310\ 559\ 006, \\
&j = 1: \ 0.310\ 559\ 006 < \overline{\rho} \leq 0.776\ 397\ 516, \\
&j = 2: \ 0.776\ 397\ 516 < \overline{\rho} \leq 1.242\ 236\ 025, \qquad (27) \\
&j = 3: \ 1.242\ 236\ 025 < \overline{\rho} \leq 1.863\ 354\ 037, \\
&j = 4: \ 1.863\ 354\ 037 < \overline{\rho}.
\end{aligned}
$$

5.2. Range of validity of the industrial equation

The range of validity for the industrial application of the thermal conductivity correlation, Eq. (24), is

$$
\begin{aligned}
&p \leq 100 \text{ MPa for } 273.15 \text{ K} \leq T \leq 1073.15 \text{ K}, \\
&p \leq 50 \text{ MPa for } 1073.15 \text{ K} \leq T \leq 1173.15 \text{ K}.
\end{aligned} \qquad (28)
$$

TABLE 12. Program-verification table for $\lambda(p,T)$ in Region 1 for the industrial application of the correlating equation.

p (MPa)	20	50
T (K)	620	620
λ (mW m^{-1} K^{-1})	0.481 485 195 × 10^3	0.545 038 940 × 10^3
$\overline{\lambda}_0$	0.484 911 627 × 10^2	0.484 911 627 × 10^2
$\overline{\lambda}_1$	0.966 869 008 × 10	0.111 212 177 × 10^2
$\overline{\lambda}_2$	0.126 391 714 × 10^2	0.575 816 285 × 10
ρ (kg m^{-3})	0.613 227 777 × 10^3	0.699 226 043 × 10^3
$(\partial\rho/\partial p)_T$ at ρ, T (kg m^3 MPa^1)	0.520 937 820 × 10	0.184 869 007 × 10
$(\partial\rho/\partial p)_T$ at ρ, T$_R$ (kg m^3 MPa^1)	0.935 037 951	0.639 306 277
ξ (nm)	0.377 694 973	0.189 692 422
c_p (kJ kg^{-1} K^{-1})	0.763 433 705 × 10	0.532 047 725 × 10
c_V (kJ kg^{-1} K^{-1})	0.303 793 441 × 10	0.291 692 653 × 10
$Z(y)$	0.166 942 638	0.113 592 223
μ (μPa s)	0.709 051 068 × 10^2	0.841 527 945 × 10^2

TABLE 13. Program-verification table for $\lambda(p,T)$ in Region 2 for the industrial application of the correlating equation.

p (MPa)	0.3	50
T (K)	650	800
λ (mW m^{-1} K^{-1})	$0.522\,311\,024 \times 10^2$	$0.177\,709\,914 \times 10^3$
$\bar{\lambda}_0$	$0.518\,787\,461 \times 10^2$	$0.698\,329\,394 \times 10^2$
$\bar{\lambda}_1$	$0.100\,678\,943 \times 10$	$0.244\,965\,343 \times 10$
$\bar{\lambda}_2$	$0.129\,246\,457 \times 10^{-3}$	$0.664\,341\,394 \times 10$
ρ (kg m^{-3})	$0.100\,452\,141 \times 10$	$0.218\,030\,012 \times 10^3$
$(\partial\rho/\partial p)_T$ at ρ, T (kg m^3 MPa^1)	$0.336\,351\,419 \times 10$	$0.661\,484\,493 \times 10$
$(\partial\rho/\partial p)_T$ at ρ, T$_R$ (kg m^3 MPa^1)	$0.223\,819\,386 \times 10$	$0.312\,182\,530 \times 10$
ξ (nm)	$0.104\,305\,448 \times 10^{-2}$	$0.193\,491\,903$
c_p (kJ kg^{-1} K^{-1})	$0.207\,010\,035 \times 10$	$0.590\,718\,707 \times 10$
c_V (kJ kg^{-1} K^{-1})	$0.159\,675\,313 \times 10$	$0.252\,343\,426 \times 10$
$Z(y)$	$0.121\,437\,275 \times 10^{-2}$	$0.137\,263\,826$
μ (μPa s)	$0.234\,877\,453 \times 10^2$	$0.393\,727\,534 \times 10^2$

5.3. Estimated uncertainty of the industrial equation

The uncertainty of the industrial equatio
n results from two contributions: (1) the uncertainty of the recommended correlating equation for general and scientific use, illustrated in Fig. 17, and (2) the deviation caused by using the industrial formulation for the thermodynamic properties, industrial equation for the viscosity, and the approximation for the compressibility at the reference temperature T_R. Since the latter is much smaller than the former, the uncertainties shown in Fig. 17 are applicable to the industrial equation except for a small region near the critical point, where deviations of the industrial equation become larger.

5.4. Computer-program verification of the industrial equation

Tables 12–14 are provided to assist the user in computer-program verification for industrial use. The IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam[3] exhibits unphysical behavior for ζ and $\bar{c}_p$ very close

TABLE 14. Program-verification table for $\lambda(\rho,T)$ in Region 3 for the industrial application of the correlating equation.

T (K)	647.35	647.35
ρ (kg m^{-3})	222	322
λ (mW m^{-1} K^{-1})	$0.366\,879\,411 \times 10^3$	$0.124\,182\,415 \times 10^4$
$\bar{\lambda}_0$	$0.515\,764\,797 \times 10^2$	$0.515\,764\,797 \times 10^2$
$\bar{\lambda}_1$	$0.348\,407\,362 \times 10$	$0.496\,819\,532 \times 10$
$\bar{\lambda}_2$	$0.187\,183\,159 \times 10^3$	$0.985\,582\,122 \times 10^3$
$(\partial\rho/\partial p)_T$ at ρ, T (kg m^3 MPa^1)	$0.177\,778\,595 \times 10^3$	$0.692\,651\,138 \times 10^4$
$(\partial\rho/\partial p)_T$ at ρ, T$_R$ (kg m^3 MPa^1)	$0.311\,832\,789 \times 10$	$0.275\,192\,511 \times 10$
ξ (nm)	$0.158\,223\,683 \times 10$	$0.124\,722\,016 \times 10^2$
c_p (kJ kg^{-1} K^{-1})	$0.101\,054\,488 \times 10^3$	$0.312\,090\,124 \times 10^4$
c_V (kJ kg^{-1} K^{-1})	$0.437\,466\,458 \times 10$	$0.452\,163\,449 \times 10$
$Z(y)$	$0.217\,577\,777$	$0.322\,306\,729 \times 10^{-1}$
μ (μPa s)	$0.312\,204\,749 \times 10^2$	$0.393\,455\,495 \times 10^2$

to the critical point, exhibiting discontinuities and taking large positive and negative values. To avoid this problem, if the value of ζ computed from Eq. (19) with IAPWS-IF97 is negative, or if it is greater than 1×10^{13}, ζ should be set equal to 1×10^{13}. Similarly, if the value of $\bar{c}_p$ computed with IAPWS-IF97 is negative, or if it is greater than 1×10^{13}, $\bar{c}_p$ should be set equal to 1×10^{13}. In addition, due to some numerical implementations of the equation of state, the calculated singularity in the first derivative in Eq. (18) may not occur exactly at $T_c = T^*$ and $\rho_c = \rho^*$ as it should. Therefore, calculated values of $\bar{\lambda}_2$ may behave unphysically at points extremely close to the critical point (approximately within 0.01 kg m^{-3} of ρ_c on the critical isotherm). The formulation should be used with caution in this region. Tables 12–14 correspond to Region 1, Region 2, and Region 3, respectively, as defined in IAPWS-IF97.[3] In Region 5, $\bar{\lambda}_2 = 0$.

6. Discussion

The international task group, comprising members affiliated with IAPWS and IATP, has completed its examination of the data, theory, and models most appropriate for describing the thermal conductivity of water over broad ranges of temperature and pressure. The resulting Eq. (2), with subsidiary equations and the accompanying tables of coefficients and parameters, should allow calculation of the thermal conductivity of water for most purposes according to international consensus and within uncertainty bounds achievable with current information. As evidenced by Fig. 17, there are still regions (for example, at pressures above 500 MPa or temperatures above about 800 K) where new experimental data with low uncertainties could lead to improvements in future representations of the thermal-conductivity surface of water. Furthermore, improvements in theory may better elucidate the high-temperature extrapolation behavior.

The form of Eq. (2) and the general forms of the constituent factors are very similar to those established in the earlier standard formulation described in Ref. 29. However, the new equation provides an improved theoretical description of the critical region, allows calculations in a broader range of state variables, considers an expanded set of experimental data, and is consistent with the more recent consensus document for the thermodynamic properties of water. The comparisons of Sec. 4 provide support for the uncertainty estimates over the full range of applicability of the correlation.

The current IAPWS Release on the Thermal Conductivity of Ordinary Water Substance[6] provides a concise description of the correlating equations for potential users. This paper provides a more detailed explanation of the formulation.

thermal conductivity of supercooled water. We are greatly indebted to R. Mareš of the University of West Bohemia, Czech Republic for directing an international effort to check the proposed thermal-conductivity formulation. Finally, we are much indebted to A. H. Harvey (NIST, Boulder) for many helpful suggestions and discussions.

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