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Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance

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This release replaces the “Revised Release on the IAPWS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance,” issued in 2008.

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1. Introductory Remarks

This release provides a correlating equation for the thermal conductivity of pure water substance over an extended range of fluid states. A discussion of the background, development, and validation of this formulation is presented in Ref. [1].

Section 2 of this release contains the correlating equation, necessary constants, range of validity of the correlation, and estimates of the uncertainty of the correlation. Section 3 deals with the industrial application of the thermal-conductivity equation.

2. Recommended Correlating Equation

2.1. Nomenclature

T denotes absolute temperature on the International Temperature Scale of 1990

ρ denotes density

p denotes pressure

λ denotes thermal conductivity

μ denotes viscosity

c_p denotes isobaric specific heat capacity

c_v denotes isochoric specific heat capacity

2.2. Reference constants

The reference constants used in this formulation for temperature, pressure, and density agree with the presently accepted values of the critical temperature, pressure, and density of water recommended by IAPWS [2], and the specific gas constant is that used in the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use [3]. The reference constants for thermal conductivity and viscosity have no physical significance.

$$\text{reference temperature: } T^* = 647.096 \text{ K} \quad (1)$$

$$\text{reference pressure: } p^* = 22.064 \text{ MPa} \quad (2)$$

$$\text{reference density: } \rho^* = 322.0 \text{ kg} \cdot \text{m}^{-3} \quad (3)$$

$$\text{reference thermal conductivity: } \lambda^* = 1 \times 10^{-3} \text{ W} \cdot \text{K}^{-1} \cdot \text{m}^{-1} \quad (4)$$

$$\text{reference viscosity: } \mu^* = 1 \times 10^{-6} \text{ Pa} \cdot \text{s} \quad (5)$$

$$\text{specific gas constant: } R = 0.461 \, 518 \, 05 \text{ kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1} \quad (6)$$

2.3. Dimensionless variables

$$\text{temperature: } \bar{T} = T / T^* \quad (7)$$

$$\text{pressure: } \bar{p} = p / p^* \quad (8)$$

$$\text{density: } \bar{\rho} = \rho / \rho^* \quad (9)$$

$$\text{thermal conductivity: } \bar{\lambda} = \lambda / \lambda^* \quad (10)$$

$$\text{viscosity: } \bar{\mu} = \mu / \mu^* \quad (11)$$

$$\text{isobaric specific heat capacity: } \bar{c}_p = c_p / R \quad (12)$$

$$\text{heat-capacity ratio: } \kappa = c_p / c_v \quad (13)$$

2.4. Range of validity

Equation (15) below is recommended for computation of the thermal conductivity for all thermodynamically stable fluid states in the following ranges of pressure p and temperature T (see also Fig. 1):

$$\begin{aligned} 0 < p < p_t \text{ and } 273.16 \leq T \leq 1173.15 \text{ K,} \\ p_t \leq p \leq 100 \text{ MPa and } T_m(p) \leq T \leq 1173.15 \text{ K,} \\ 100 \text{ MPa} < p \leq 250 \text{ MPa for } T_m(p) \leq T \leq 874 \text{ K,} \\ 250 \text{ MPa} < p \leq 687 \text{ MPa for } T_m(p) \leq T \leq 573 \text{ K,} \\ 687 \text{ MPa} < p \leq 785 \text{ MPa for } T_m(p) \leq T \leq 403 \text{ K,} \\ 785 \text{ MPa} < p \leq 1000 \text{ MPa for } T_m(p) \leq T \leq 348 \text{ K.} \end{aligned} \quad (14)$$

In Eqs. (14), $p_t = 611.657 \text{ Pa}$ is the triple-point pressure and T_m is the pressure-dependent melting temperature as given in Ref. [4]. For general and scientific applications, the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use [3] should be used to determine the thermodynamic properties needed for the evaluation of Eq. (15). The IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water

Substance for General and Scientific Use should also be used to determine the densities as input to Eq. (15) when the state point under consideration is defined by pressure and temperature or by other thermodynamic variables instead of density and temperature.

In addition, IAPWS makes the following statements about the extrapolation of Eq. (15) outside the range of validity given above:

- At high temperatures and low densities, Eq. (15) extrapolates in a physically reasonable manner above 1173.15 K. However, the extrapolation will become increasingly unrealistic above approximately 1500 K, where a contribution to the thermal conductivity due to the dissociation of H₂O becomes significant. See Ref. [1] for more details.
- Eq. (15) provides reasonable extrapolation behavior for pressures up to 4 GPa at temperatures up to 673 K. However, the recommended range of validity of the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use [3] only extends to up 1 GPa, although its extrapolation to higher pressures is physically reasonable (see [3]).
- 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 thermal conductivity calculation 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. (15) behaves in a physically reasonable manner down to 250 K.
- For stable fluid states outside the range of validity of Eq. (15), but within the range of validity of the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use [3], the extrapolation behavior of Eq. (15) is physically reasonable.

2.5. Estimated uncertainty

The uncertainties in this formulation are summarized in Figure 1; they can be considered as estimates of a combined expanded uncertainty with a coverage factor of two. Thus, the thermal conductivity at any state point can be expressed as $\lambda \pm \delta$, where δ is the applicable value in Figure 1. In the region for liquid water along the saturation line, the formulation agrees with the recommended values in Ref. [5] to within their estimated uncertainty of 0.7 %. Since the thermal conductivity diverges at the critical point, the uncertainty may become larger near the critical point.

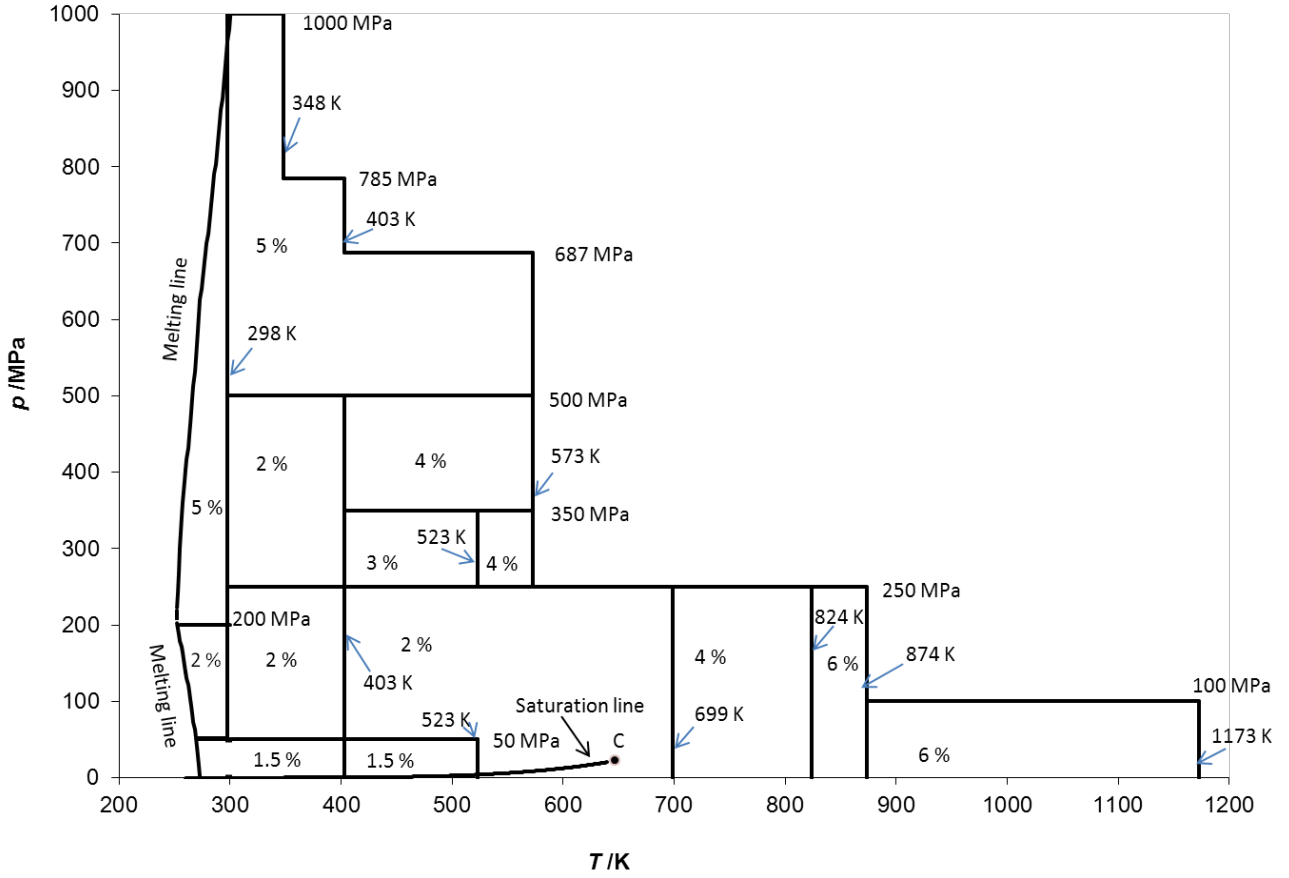


Figure 1. Estimated uncertainty of the correlating equation.

2.6. Correlating equation

The thermal conductivity is represented by the equation

$$\bar{\lambda} = \bar{\lambda}_0(\bar{T}) \times \bar{\lambda}_1(\bar{T}, \bar{\rho}) + \bar{\lambda}_2(\bar{T}, \bar{\rho}). \quad (15)$$

The first factor $\bar{\lambda}_0$ of the product in Eq. (15) represents the thermal conductivity in the dilute-gas limit and is given by

$$\bar{\lambda}_0(\bar{T}) = \frac{\sqrt{\bar{T}}}{\sum_{k=0}^4 \frac{L_k}{\bar{T}^k}}, \quad (16)$$

with coefficients L_k given in Table 1.

Table 1. Coefficients L_k in Eq. (16) for $\bar{\lambda}_0(\bar{T})$

| 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 | $4.096\,266 \times 10^{-4}$ |

The second factor $\bar{\lambda}_1$ of the product in Eq. (15) represents the contribution to thermal conductivity due to finite density:

$$\bar{\lambda}_1(\bar{T}, \bar{\rho}) = \exp \left[\bar{\rho} \sum_{i=0}^4 \left(\left(\frac{1}{\bar{T}} - 1 \right)^i \sum_{j=0}^5 L_{ij} (\bar{\rho} - 1)^j \right) \right] , \quad (17)$$

with coefficients L_{ij} given in Table 2.

Table 2. Coefficients L_{ij} in Eq. (17) for $\bar{\lambda}_1(\bar{T}, \bar{\rho})$

| j i | 0 | 1 | 2 | 3 | 4 | 5 |
|------------|---------------|----------------|----------------|-----------------|------------------|-------------------|
| 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 |

2.7. Critical enhancement

The additive contribution $\bar{\lambda}_2$ in Eq. (15) represents the critical enhancement of the thermal conductivity. This additive contribution is defined over the entire range of states by

$$\bar{\lambda}_2(\bar{T}, \bar{\rho}) = \Lambda \frac{\bar{\rho} c_p \bar{T}}{\bar{\mu}} Z(y), \quad (18)$$

where Λ is a numerical constant. The function $Z(y)$ is defined by

$$Z(y) = \frac{2}{\pi y} \left\{ \left[(1 - \kappa^{-1}) \arctan(y) + \kappa^{-1} y \right] - \left[1 - \exp\left(\frac{-1}{y^{-1} + y^2 / 3\bar{\rho}^2}\right) \right] \right\}, \quad (19)$$

where $\kappa = c_p / c_v$ and

$$y = \bar{q}_D \xi(\bar{T}, \bar{\rho}). \quad (20)$$

In Eq. (20), \bar{q}_D is a reference wave number and ξ a correlation length, so that y is a dimensionless variable. To avoid numerical truncation issues in Eq. (19) for small values of y , the function $Z(y)$ is subject to the condition

$$Z(y) = 0 \quad \text{for } y < 1.2 \times 10^{-7}. \quad (21)$$

The correlation length ξ in Eq. (20) is to be calculated by the same procedure as that defined in the IAPWS Formulation for the Viscosity of Ordinary Water Substance [6,7]. Specifically,

$$\xi = \xi_0 \left(\frac{\Delta\bar{\chi}}{\Gamma_0} \right)^{v/\gamma} \quad (22)$$

in terms of $\Delta\bar{\chi}$ (≥ 0) defined by

$$\Delta\bar{\chi}(\bar{T}, \bar{\rho}) = \bar{\rho} \left[\zeta(\bar{T}, \bar{\rho}) - \zeta(\bar{T}_R, \bar{\rho}) \frac{\bar{T}_R}{\bar{T}} \right] \quad (23)$$

with

$$\zeta = \left(\frac{\partial \bar{\rho}}{\partial \bar{p}} \right)_{\bar{T}}, \quad (24)$$

where ξ_0, Γ_0, v , and γ are constants.

When $\Delta\bar{\chi}$ calculated from Eq. (23) is less than zero, it must be set to zero for calculations to proceed.¹

The constants needed to compute the critical enhancement, $\bar{\lambda}_2$, are provided in Table 3.

Table 3. Critical-region constants

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

For general and scientific use, the dimensionless isobaric specific heat capacity, \bar{c}_p , in Eq. (18), the heat-capacity ratio, κ , in Eq. (19), and the dimensionless isothermal compressibility, ζ , in Eq. (23) are to be calculated from the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use [3], while the dimensionless viscosity, $\bar{\mu}$, in Eq. (18) is to be calculated from Eq. (10) in the IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance [6].

¹Due to the numerical implementation of the equation of state, the calculated singularity in the first derivative in Eq. (23) 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 $0.01 \text{ kg}\cdot\text{m}^{-3}$ of ρ_c on the critical isotherm). The formulation should be used with caution in this very small region.

Figure 2 shows the significance of the critical-enhancement contribution to the thermal conductivity at various temperatures and densities.

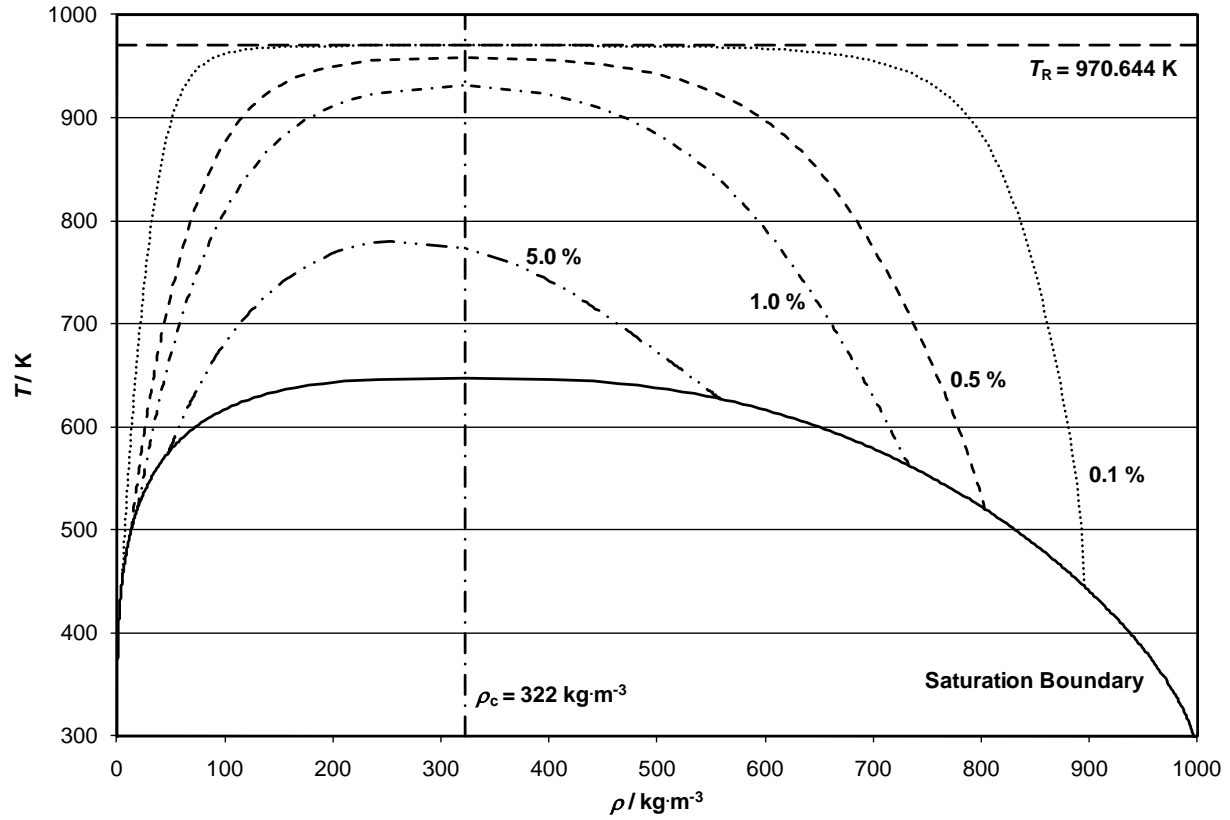


Figure 2. Contours in the temperature-density plane where the contribution from the critical enhancement $\bar{\lambda}_2$ to the total thermal conductivity $\bar{\lambda}$ equals 5 %, 1 %, 0.5 %, and 0.1 %.

2.8. Computer-program verification

The following tables 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.

Table 4. Sample points for computer-program verification of the correlating equation, Eq. (15). 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 |

Note: Some derivatives from the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use [3] diverge at $\rho = 0$; for those points in Table 4 $\bar{\lambda}_2$ must be set to zero. For the liquid points at 298.15 K, $\Delta\bar{\chi}$ calculated from Eq. (23) is less than zero, so (as stated in Sec. 2.7) it must be set to zero for calculations to proceed and $\bar{\lambda}_2 = 0$.

Table 5. Sample points for computer-program verification of the correlating equation, Eq. (15), including the critical-enhancement contribution $\bar{\lambda}_2$. For all points, $\bar{\lambda}_0$ (647.35 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 |

3. Recommendations for Industrial Use

3.1. Industrial application of correlating equation

For industrial applications where greater computing speed is needed, the dimensionless isobaric specific heat capacity, \bar{c}_p , in Eq. (18), the heat-capacity ratio, κ , in Eq. (19), and the dimensionless isothermal compressibility, ζ , in Eq. (23) should be calculated from the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam [8], while the dimensionless viscosity, $\bar{\mu}$, in Eq. (18) 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 [6], with one exception:

The function $\zeta(\bar{T}_R, \bar{\rho})$ in Eq. (23) is to be calculated from

$$\zeta(\bar{T}_R, \bar{\rho}) = \frac{1}{\sum_{i=0}^5 A_{ij} \bar{\rho}^i}, \quad (25)$$

with coefficients A_{ij} given in Table 6.

Table 6. Coefficients A_{ij} in Eq. (25) for $\zeta(\bar{T}_R, \bar{\rho})$

| | $j = 0$ | $j = 1$ | $j = 2$ |
|---------|--------------------|--------------------|-------------------|
| $i = 0$ | 6.53786807199516 | 6.52717759281799 | 5.35500529896124 |
| $i = 1$ | -5.61149954923348 | -6.30816983387575 | -3.96415689925446 |
| $i = 2$ | 3.39624167361325 | 8.08379285492595 | 8.91990208918795 |
| $i = 3$ | -2.27492629730878 | -9.82240510197603 | -12.0338729505790 |
| $i = 4$ | 10.2631854662709 | 12.1358413791395 | 9.19494865194302 |
| $i = 5$ | 1.97815050331519 | -5.54349664571295 | -2.16866274479712 |
| | $j = 3$ | $j = 4$ | |
| $i = 0$ | 1.55225959906681 | 1.11999926419994 | |
| $i = 1$ | 0.464621290821181 | 0.595748562571649 | |
| $i = 2$ | 8.93237374861479 | 9.88952565078920 | |
| $i = 3$ | -11.0321960061126 | -10.3255051147040 | |
| $i = 4$ | 6.16780999933360 | 4.66861294457414 | |
| $i = 5$ | -0.965458722086812 | -0.503243546373828 | |

The subscript j denotes ranges defined as:

$$\begin{aligned}
 j = 0: & \quad \bar{\rho} \leq 0.310559006 \\
 j = 1: & \quad 0.310559006 < \bar{\rho} \leq 0.776397516 \\
 j = 2: & \quad 0.776397516 < \bar{\rho} \leq 1.242236025 \\
 j = 3: & \quad 1.242236025 < \bar{\rho} \leq 1.863354037 \\
 j = 4: & \quad 1.863354037 < \bar{\rho}
 \end{aligned} \tag{26}$$

3.2. Range of validity of industrial equation

$$\begin{aligned}
 p &\leq 100 \text{ MPa for } 273.15 \text{ K} \leq T \leq 1073.15 \text{ K}, \\
 p &\leq 50 \text{ MPa for } 1073.15 \text{ K} \leq T \leq 1173.15 \text{ K}.
 \end{aligned} \tag{27}$$

3.3. Estimated uncertainty of industrial equation

The uncertainty of the industrial equation results from two contributions:

1. The uncertainty of the recommended correlating equation for general and scientific use, illustrated in Figure 1.
2. Deviation caused by using industrial formulations 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 Figure 1 are applicable to the industrial equation except for a small region near the critical point, where deviations of the industrial equation become larger.

3.4. Computer-program verification of industrial equation

The following tables are provided to assist the user in computer-program verification for industrial use.² Tables 7, 8, and 9 correspond to Region 1, Region 2, and Region 3, respectively, as defined in the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam [8].³

²The IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam [8] exhibits unphysical behavior for ζ and \bar{c}_p very close 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. (24) 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} . See also footnote 1 on page 8.

³In Region 5, $\bar{\lambda}_2 = 0$.

Table 7. Program-verification table for $\lambda(p, T)$ in Region 1

| p (MPa) | 20 | 50 |
|---|---------------------------|---------------------------|
| T (K) | 620 | 620 |
| λ (mW·m ⁻¹ ·K ⁻¹) | 0.481485195×10^3 | 0.545038940×10^3 |
| $\bar{\lambda}_0$ | 0.484911627×10^2 | 0.484911627×10^2 |
| $\bar{\lambda}_1$ | 0.966869008×10 | 0.111212177×10^2 |
| $\bar{\lambda}_2$ | 0.126391714×10^2 | 0.575816285×10 |
| ρ (kg·m ⁻³) | 0.613227777×10^3 | 0.699226043×10^3 |
| $(\partial\rho/\partial p)_T$ at ρ, T (kg·m ⁻³ ·MPa ⁻¹) | 0.520937820×10 | 0.184869007×10 |
| $(\partial\rho/\partial p)_T$ at ρ, T_R (kg·m ⁻³ ·MPa ⁻¹) | 0.935037951 | 0.639306277 |
| ξ (nm) | 0.377694973 | 0.189692422 |
| c_p (kJ·kg ⁻¹ ·K ⁻¹) | 0.763433705×10 | 0.532047725×10 |
| c_v (kJ·kg ⁻¹ ·K ⁻¹) | 0.303793441×10 | 0.291692653×10 |
| $Z(y)$ Eq. (19) | 0.166942638 | 0.113592223 |
| μ (μPa·s) | 0.709051068×10^2 | 0.841527945×10^2 |

Table 8. Program-verification table for $\lambda(p, T)$ in Region 2

| p (MPa) | 0.3 | 50 |
|---|------------------------------|---------------------------|
| T (K) | 650 | 800 |
| λ (mW·m ⁻¹ ·K ⁻¹) | 0.522311024×10^2 | 0.177709914×10^3 |
| $\bar{\lambda}_0$ | 0.518787461×10^2 | 0.698329394×10^2 |
| $\bar{\lambda}_1$ | 0.100678943×10 | 0.244965343×10 |
| $\bar{\lambda}_2$ | $0.129246457 \times 10^{-3}$ | 0.664341394×10 |
| ρ (kg·m ⁻³) | 0.100452141×10 | 0.218030012×10^3 |
| $(\partial\rho/\partial p)_T$ at ρ, T (kg·m ⁻³ ·MPa ⁻¹) | 0.336351419×10 | 0.661484493×10 |
| $(\partial\rho/\partial p)_T$ at ρ, T_R (kg·m ⁻³ ·MPa ⁻¹) | 0.223819386×10 | 0.312182530×10 |
| ξ (nm) | $0.104305448 \times 10^{-2}$ | 0.193491903 |
| c_p (kJ·kg ⁻¹ ·K ⁻¹) | 0.207010035×10 | 0.590718707×10 |
| c_v (kJ·kg ⁻¹ ·K ⁻¹) | 0.159675313×10 | 0.252343426×10 |
| $Z(y)$ Eq. (19) | $0.121437275 \times 10^{-2}$ | 0.137263826 |
| μ (μPa·s) | 0.234877453×10^2 | 0.393727534×10^2 |

Table 9. Program-verification table for $\lambda(\rho, T)$ in Region 3

| T (K) | 647.35 | 647.35 |
|---|---------------------------|------------------------------|
| ρ (kg·m ⁻³) | 222 | 322 |
| λ (mW·m ⁻¹ ·K ⁻¹) | 0.366879411×10^3 | 0.124182415×10^4 |
| $\bar{\lambda}_0$ | 0.515764797×10^2 | 0.515764797×10^2 |
| $\bar{\lambda}_1$ | 0.348407362×10 | 0.496819532×10 |
| $\bar{\lambda}_2$ | 0.187183159×10^3 | 0.985582122×10^3 |
| $(\partial\rho/\partial p)_T$ at ρ, T (kg·m ⁻³ ·MPa ⁻¹) | 0.177778595×10^3 | 0.692651138×10^4 |
| $(\partial\rho/\partial p)_T$ at ρ, T_R (kg·m ⁻³ ·MPa ⁻¹) | 0.311832789×10 | 0.275192511×10 |
| ξ (nm) | 0.158223683×10 | 0.124722016×10^2 |
| c_p (kJ·kg ⁻¹ ·K ⁻¹) | 0.101054488×10^3 | 0.312090124×10^4 |
| c_v (kJ·kg ⁻¹ ·K ⁻¹) | 0.437466458×10 | 0.452163449×10 |
| $Z(y)$ Eq. (19) | 0.217577777 | $0.322306729 \times 10^{-1}$ |
| μ (μPa·s) | 0.312204749×10^2 | 0.393455495×10^2 |

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