# The International Association for the Properties of Water and Steam

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## Release on the IAPWS Formulation 2020 for the Viscosity of Heavy Water

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This release replaces the viscosity portion of the revised release of 2007 (IAPWS R4-84(2007)), and contains 9 pages, including this cover page.

This Revised Release has been authorized by the International Association for the Properties of Water and Steam (IAPWS) at its virtual meeting on 11 September, 2020. The members of IAPWS are: Australia, Britain and Ireland, Canada, the Czech Republic, Germany, Japan, New Zealand, Russia, Scandinavia (Denmark, Finland, Norway, Sweden), and the United States, and associate members Argentina and Brazil, China, Egypt, France, Greece, Israel, Italy, and Switzerland. The President at the time of adoption of this document was Dr. Jan Hrubý of the Czech Republic.

Summary

The formulation provided in this Release is recommended for calculating the viscosity of heavy water, which IAPWS defines as water whose hydrogen atoms are entirely the deuterium isotope ($^2$H or D) and whose oxygen isotopes have the same abundance as in ordinary water [1]. Further details about the formulation can be found in the article "New International Formulation for the Viscosity of Heavy Water" by M.J. Assael *et al.* [2]. This formulation provides the most accurate representation available at the time this Release was prepared for the viscosity of the fluid phases of heavy water over a wide range of conditions.

Further information about this Release and other documents issued by IAPWS can be obtained from the Executive Secretary of IAPWS (Dr. R.B. Dooley, bdooley@iapws.org) or from http://www.iapws.org.

**Contents**

## 1. Introductory Remarks

This release provides a correlating equation for the shear viscosity of pure heavy water, $D_2O$, over an extensive range of fluid states. A discussion of the background, development, and validation of this formulation is presented in Ref. [2].

Section 2 of this Release contains the correlating equation, necessary constants, range of validity of the equation, and estimates of the uncertainty of the correlation. Section 3 concerns the viscosity correlation for industrial use, and Section 4 presents selected values of the correlation at specific state points to enable computer verification of an implementation of the correlation.

## 2. Recommended Correlating Equation

2.1.    Nomenclature
        $T$ denotes absolute temperature on the International Temperature Scale of 1990
        $\rho$ denotes density
        $p$ denotes pressure
        $\mu$ denotes viscosity

2.2.    Reference constants
        The reference constants used in this formulation for temperature and density are the values of the critical temperature and density of heavy water recommended by IAPWS [3], while the reference pressure is the critical pressure given by the IAPWS reference equation of state [4] and the reference constant for viscosity has no physical significance.

| | | |
|---|---|---|
| reference temperature: | $T^* = 643.847$ K | (1) |
| reference pressure: | $p^* = 21.6618$ MPa | (2) |
| reference density: | $\rho^* = 356.0$ kg·m$^{-3}$ | (3) |
| reference viscosity: | $\mu^* = 1.00 \times 10^{-6}$ Pa·s | (4) |

2.3.  Dimensionless variables:

| | | |
|---|---|---|
| temperature: | $\bar{T} = T/T^*$ | (5) |
| pressure: | $\bar{p} = p/p^*$ | (6) |
| density: | $\bar{\rho} = \rho/\rho^*$ | (7) |
| viscosity: | $\bar{\mu} = \mu/\mu^*$ | (8) |

2.4.  Range of validity

Equation (10) below is recommended for computation of the viscosity for all thermodynamically stable fluid states in the following ranges of pressure $p$ and temperature $T$:

| | | |
|---|---|---|
| $0 < p \le p_t$ | and | $T_t \le T \le 775$ K |
| $p_t \le p \le 100$ MPa | and | $T_m(p) \le T \le 775$ K |
| $100$ MPa $< p \le 200$ MPa | and | $T_m(p) \le T \le 473$ K |
| $200$ MPa $< p \le 960$ MPa | and | $T_m(p) \le T \le 373$ K |

(9)

In the inequalities above, $T_m$ is the pressure-dependent melting temperature, $p_t$ is the triple-point pressure and $T_t = 276.969$ K is the triple-point temperature as given in Ref. [4]. The equation of state in Ref. [4] should be used to determine the densities and density derivatives used as input to Eq. (10), 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 extrapolation of Eq. (10) outside the range of validity given above:
- For vapor states at temperatures below the triple-point temperature of 276.969 K and pressures less than or equal to the sublimation pressure, the viscosity calculation is dominated by the dilute-gas term, and this behaves in a physically reasonable manner down to at least 250 K.
- For stable fluid states outside the range of validity of Eq. (10) but within the range of validity of the Revised Release on the IAPWS Formulation 2017 for the Thermodynamic Properties of Heavy Water [3], the extrapolation behavior of Eq. (10) is physically reasonable.
- At high temperatures, the extrapolation of the dilute-gas portion of Eq. (10) is physically reasonable (for undissociated $D_2O$) up to at least 2500 K.
- For the metastable subcooled liquid at atmospheric pressure, Eq. (10) has an estimated uncertainty of 3.5 % down to 260 K, 7 % for 250 K to 260 K, rising to 13 % at 244 K when used with densities computed from Duška *et al.* [5]. When the density is computed from Herrig *et al.* [4], the uncertainties are the same except for the very lowest temperatures from 244 K to 250 K, where the uncertainty reaches 14 %.

## 2.5. Estimated uncertainty

The uncertainties in this formulation for thermodynamically stable states are summarized in Figure 1; they should be considered as estimates of an expanded uncertainty with a coverage factor of two.
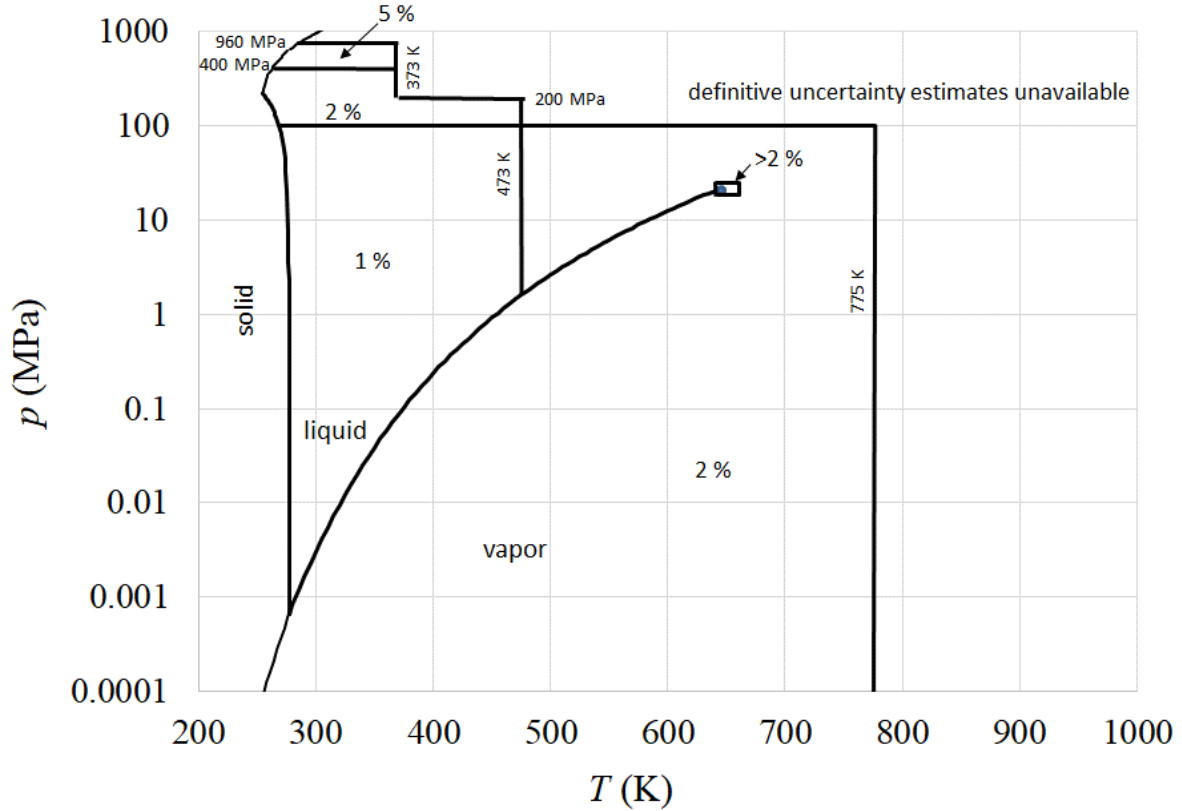


Figure 1. Estimated uncertainty of the correlating equation.

## 2.6. Correlating equation

The viscosity is represented by the equation

$$\bar{\mu} = \bar{\mu}_0(\bar{T}) \times \bar{\mu}_1(\bar{T}, \bar{\rho}) \times \bar{\mu}_2(\bar{T}, \bar{\rho}). \tag{10}$$

The first factor $\bar{\mu}_0$ of the product represents the viscosity in the dilute-gas limit and is given by

$$\bar{\mu}_0(\bar{T}) = \sqrt{\bar{T}}\, \frac{0.889754 + 61.22217\,\bar{T} - 44.8866\,\bar{T}^2 + 111.5812\,\bar{T}^3 + 3.547412\,\bar{T}^4}{0.79637 + 2.38127\,\bar{T} - 0.33463\,\bar{T}^2 + 2.669\,\bar{T}^3 + 0.000211366\,\bar{T}^4}. \tag{11}$$

The second factor $\bar{\mu}_1$ of the product represents the contribution to viscosity due to finite density:

$$\bar{\mu}_1(\bar{T},\bar{\rho}) = \exp\left[\bar{\rho}\sum_{i=0}^{6}\left(\frac{1}{\bar{T}}-1\right)^i\sum_{j=0}^{6}H_{ij}(\bar{\rho}-1)^j\right], \tag{12}$$

with coefficients $H_{ij}$ given in Table 1. The third factor $\bar{\mu}_2$ of the product represents the critical enhancement of the viscosity.

Table 1. Coefficients $H_{ij}$ for $\bar{\mu}_1(\bar{T},\bar{\rho})$.

| $i$ | $j$ | $H_{ij}$ | $i$ | $j$ | $H_{ij}$ |
|---|---|---|---|---|---|
| 0 | 0 | $H_{00} = 0.510\,953$ | 0 | 3 | $H_{03} = 0.066\,103\,5$ |
| 2 | 0 | $H_{20} = -0.558\,947$ | 1 | 3 | $H_{13} = 0.044\,939\,3$ |
| 3 | 0 | $H_{30} = -2.718\,820$ | 2 | 3 | $H_{23} = 1.466\,670$ |
| 4 | 0 | $H_{40} = 0.480\,990$ | 5 | 3 | $H_{53} = 0.938\,984$ |
| 5 | 0 | $H_{50} = 2.404\,510$ | 6 | 3 | $H_{63} = -0.108\,354$ |
| 6 | 0 | $H_{60} = -1.824\,320$ | 0 | 4 | $H_{04} = -0.004\,812\,65$ |
| 0 | 1 | $H_{01} = 0.275\,847$ | 2 | 4 | $H_{24} = -1.545\,710$ |
| 1 | 1 | $H_{11} = 0.762\,957$ | 3 | 4 | $H_{34} = -0.057\,093\,8$ |
| 3 | 1 | $H_{31} = 1.760\,340$ | 5 | 4 | $H_{54} = -0.075\,378\,3$ |
| 4 | 1 | $H_{41} = 0.081\,908\,6$ | 2 | 5 | $H_{25} = 0.553\,080$ |
| 6 | 1 | $H_{61} = 1.417\,750$ | 2 | 6 | $H_{26} = -0.065\,020\,1$ |
| 0 | 2 | $H_{02} = -0.228\,148$ | | | |
| 1 | 2 | $H_{12} = -0.321\,497$ | | | |
| 5 | 2 | $H_{52} = -2.302\,500$ | | | |

Note: Coefficients $H_{ij}$ omitted from the table are identically equal to zero.

2.7    Critical enhancement

The critical enhancement is only significant in a very small region in density and temperature around the critical point. Although exactly at the critical point the viscosity is infinite, the enhancement term contributes an amount greater than 2 % of the full viscosity only within the following boundaries:

$$641.428 \text{ K} < T < 652.259 \text{ K}, \qquad 243.393 \text{ kg·m}^{-3} < \rho < 481.819 \text{ kg·m}^{-3}. \tag{13}$$

Thus, the critical enhancement is significant only within the boundaries specified by (13); outside this region, the enhancement is always less than the uncertainty in the formulation. This allows simplification for certain industrial calculations (see Sections 2.8 and 3).

The function $\bar{\mu}_2$ is defined over the entire range of states by:

$$\bar{\mu}_2 = \exp\left(x_\mu Y\right), \tag{14}$$

where $x_\mu$ is the critical exponent for viscosity and the function $Y$ is defined for two ranges of correlation length $\xi$. For $0 \le \xi \le 0.030\,218\,066\,92$ nm

$$Y = \frac{1}{5} q_{\mathrm{C}} \xi \left( q_{\mathrm{D}} \xi \right)^5 \left( 1 - q_{\mathrm{C}} \xi + \left( q_{\mathrm{C}} \xi \right)^2 - \frac{765}{504} \left( q_{\mathrm{D}} \xi \right)^2 \right), \tag{15}$$

while for $\xi > 0.030\ 218\ 066\ 92$ nm

$$Y = \frac{1}{12} \sin \left( 3 \psi_{\mathrm{D}} \right) - \frac{1}{4 q_{\mathrm{C}} \xi} \sin \left( 2 \psi_{\mathrm{D}} \right) + \frac{1}{\left( q_{\mathrm{C}} \xi \right)^2} \left[ 1 - \frac{5}{4} \left( q_{\mathrm{C}} \xi \right)^2 \right] \sin \left( \psi_{\mathrm{D}} \right)$$
$$- \frac{1}{\left( q_{\mathrm{C}} \xi \right)^3} \left\{ \left[ 1 - \frac{3}{2} \left( q_{\mathrm{C}} \xi \right)^2 \right] \psi_{\mathrm{D}} - \left| \left( q_{\mathrm{C}} \xi \right)^2 - 1 \right|^{3/2} L(w) \right\} \tag{16}$$

with

$$\psi_{\mathrm{D}} = \arccos \left( 1 + q_{\mathrm{D}}^2 \xi^2 \right)^{-\frac{1}{2}} \tag{17}$$

and with the function $L(w)$ given by

$$L(w) = \begin{cases} \ln \dfrac{1+w}{1-w}, & \text{for } q_{\mathrm{C}} \xi > 1 \\ 2 \arctan |w|, & \text{for } q_{\mathrm{C}} \xi \leq 1 \end{cases}. \tag{18}$$

The variable $w$ is defined by

$$w = \left| \frac{q_{\mathrm{C}} \xi - 1}{q_{\mathrm{C}} \xi + 1} \right|^{\frac{1}{2}} \tan \left( \frac{\psi_{\mathrm{D}}}{2} \right). \tag{19}$$

The critical enhancement of viscosity given by Eqs. (14) – (19) is a function of the correlation length $\xi$:

$$\xi = \xi_0 \left( \frac{\overline{\Delta \chi}}{\Gamma_0^+} \right)^{\frac{\nu}{\gamma}} \tag{20}$$

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

$$\overline{\Delta \chi} = \overline{\rho} \left[ \left( \frac{\partial \overline{\rho}(\overline{T}, \overline{\rho})}{\partial \overline{p}} \right)_{\overline{T}} - \left( \frac{\partial \overline{\rho}(\overline{T}_{\mathrm{R}}, \overline{\rho})}{\partial \overline{p}} \right)_{\overline{T}} \frac{\overline{T}_{\mathrm{R}}}{\overline{T}} \right]. \tag{21}$$

When $\overline{\Delta\chi}$ calculated by Eq. (21) is less than zero, it must be set to zero for calculations to proceed.[1]

The constants needed to compute the critical enhancement, $\overline{\mu}_2$, in Eqs. (14) – (21) are provided in Table 2.

Table 2. Critical-Region Constants.

| | |
|---|---|
| $x_\mu$ | 0.068 |
| $q_{\mathrm{C}}^{-1}$ | 1.9 nm |
| $q_{\mathrm{D}}^{-1}$ | 0.4 nm |
| $\upsilon$ | 0.630 |
| $\gamma$ | 1.239 |
| $\xi_0$ | 0.13 nm |
| $\Gamma_0^+$ | 0.06 |
| $\overline{T}_{\mathrm{R}}$ | 1.5 |

2.8    Simplified use outside the critical region

Because the critical enhancement is insignificant except in a small region around the critical point (described approximately by Eq. (13)), complexity and computing time may be reduced by omitting the critical enhancement for applications outside this region.[2]  This can be done by setting $\overline{\mu}_2 = 1$.

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[1] Due to the numerical implementation of the equation of state, the calculated singularity in the first derivative in Eq. (21) may not occur exactly at $T_c$ and $\rho_c$ as it should.  Therefore, calculated values of $\overline{\mu}_2$ may behave unphysically at points extremely close to the critical point (approximately within 0.01 kg·m$^{-3}$ of $\rho_c$ on the critical isotherm).  The formulation should be used with caution in this very small region.

[2] If a calculation is performed that uses the critical enhancement, Eq. (14), near the critical point but omits it far from the critical point, some discontinuity is inevitable.  This discontinuity is less than 0.052 % for single-phase states outside a region near the critical point bounded by the equation

$$T/(1\,\mathrm{K}) = \sum_{i=0}^{3} a_i \left(\rho/(1\,\mathrm{kg}\cdot\mathrm{m}^{-3})\right)^i,$$

where $a_0 = 447.555$, $a_1 = 1.73284$, $a_2 = -3.02766\times10^{-3}$, and $a_3 = 1.24296\times10^{-6}$.

## 3. Recommendation for Industrial Application

For industrial uses where greater computing speed and/or reduced complexity are needed, or when conditions remain outside of the region specified by Eq. (13), the factor $\bar{\mu}_2$ in Eq. (10) may be set to unity everywhere:

$$\bar{\mu}_2 = 1. \qquad\qquad \text{(for simplified industrial use)} \qquad\qquad (22)$$

## 4. Computer-Program Verification

The following tables are provided to assist the user in computer-program verification. The viscosity calculations are based on the tabulated temperatures and densities.

Table 3. Sample points for computer-program verification of the interpolating equation, Eq. (10) with Eq. (22).

| $T$ (K) | $\rho$ (kg·m$^{-3}$) | $\mu$ (µPa·s) |
|---|---|---|
| 298.15 | 0.00 | 10.035 938 |
| 298.15 | 1105 | 1092.642 4 |
| 298.15 | 1130 | 1088.362 6 |
| 373.15 | 1064 | 326.637 91 |
| 775.00 | 1 | 29.639 474 |
| 775.00 | 100 | 31.930 085 |
| 775.00 | 400 | 53.324 172 |

Table 4. Sample points for computer-program verification of the correlating equation, Eq. (10), in the region near the critical point.[3]

| $T$ (K) | $\rho$ (kg·m$^{-3}$) | $\xi$ (nm) | $\bar{\mu}_2$ | $\mu$ (µPa·s) |
|---|---|---|---|---|
| 644.101 | 145 | 0.358 588 | 1.000 359 | 26.640 959 |
| 644.101 | 245 | 1.612 131 | 1.014 771 | 32.119 967 |
| 644.101 | 295 | 5.034 205 | 1.050 059 | 36.828 275 |
| 644.101 | 345 | 15.100 542 | 1.106 000 | 43.225 017 |
| 644.101 | 395 | 9.678 686 | 1.080 915 | 47.193 530 |
| 644.101 | 445 | 2.903 437 | 1.030 066 | 50.241 640 |

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[3] Due to the numerical implementation of the critical enhancement, calculated values may differ by ±0.000 001 nm for $\xi$ or ±0.000 001 µPa·s for $\mu$.

## 5. References

[1]   International Association for the Properties of Water and Steam, IAPWS G5-01(2020), Guideline on the Use of Fundamental Physical Constants and Basic Constants of Water, available from http://www.iapws.org.

[2]   Assael, M.J., Monogenidou, S.A., Huber, M.L., Perkins, R.A., and Sengers, J.V., New International Formulation for the Viscosity of Heavy Water, *J. Phys. Chem. Ref. Data*, submitted (2021).

[3]   International Association for the Properties of Water and Steam, IAPWS R16-17(2018), Revised Release on the IAPWS Formulation 2017 for the Thermodynamic Properties of Heavy Water, available at http://www.iapws.org/relguide/Heavy.html

[4]   Herrig, S., Thol, M., Span, R., Harvey, A.H., and Lemmon, E.W., A Reference Equation of State for Heavy Water, *J. Phys. Chem. Ref. Data* **47**, 043102 (2018).

[5]   Duška, M., Hrubý, J., Caupin, F., and Anisimov, M.A., Communication: Two-structure thermodynamics unifying all scenarios for water anomalies, arXiv: 1708.04054v1 (2017).