

Article

Supplementary Material to “Analytical Determination of the Nucleation-Prone, Low-Density Fraction of Subcooled Water”

Olaf Hellmuth ^{1,*} and Rainer Feistel ²

¹ Leibniz Institute for Tropospheric Research (TROPOS), Permoserstraße 15, D-04318 Leipzig, Germany

² Leibniz Institute for Baltic Research (IOW), Seestraße 15, D-18119 Rostock-Warnemünde, Germany;
rainer.feistel@io-warnemuende.de

* Correspondence: olaf.hellmuth@tropos.de

Version August 25, 2020 submitted to Journal Not Specified

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²⁴ SM-1 The Thermodynamic Equation Of Seawater 2010 (TEOS-10)

²⁵ TEOS-10 is based on four independent thermodynamic potentials, defined as functions of the
²⁶ independent observables temperature, pressure, dry-air mass fraction, density, and salinity: (i) a
²⁷ Helmholtz function of fluid water (Wagner and Pruf², IAPWS R6-95 [3], known as “IAPWS-95”), (ii)

28 a Gibbs function of hexagonal ice (Feistel and Wagner [4], IAPWS R10-06 [5]), (iii) a Gibbs function
29 of seasalt dissolved in water (Feistel [67], IAPWS R13-08 [8]), and (iv) a Helmholtz function for dry
30 air (Lemmon *et al.* [9]). In combination with air–water cross-virial coefficients (Hyland and Wexler
31 [10], Harvey and Huang [11], Feistel *et al.* [12]) this set of thermodynamic potentials is used as the
32 primary standard for pure water (liquid, vapor, and solid), seawater and humid air from which all
33 other properties are derived by mathematical operations, i.e., without the need for additional empirical
34 functions.

35 The IAPWS-95 fluid-water formulation is based on the evaluation of a comprehensive and
36 consistent data set which was assembled from a total of about 20,000 experimental data of water.
37 Wagner and Prüß [2] took into account all available information given in the scientific articles which
38 described the data collection underlying the development of the thermal equation of state of water.
39 The authors critically reexamined the available data sets with respect to their internal consistency and
40 their basic applicability for the development of a new equation of state for water. Only those data
41 were incorporated into the final nonlinear fitting procedure, which were judged to be of high quality.
42 These selected data sets took into account experimental data which were available by the middle of
43 the year 1994 (Wagner and Prüß [2]). The availability of reliable experimental data on subcooled liquid
44 water (i.e., metastable with respect to the solid form of water) was restricted to a few data sets for
45 several properties only along the isobar $p=1013.25\text{ hPa}$, which set the lower limit of the temperature
46 range for the validity of IAPWS-95 for liquid water (and so of TEOS-10) to $T=236\text{ K}$. This temperature
47 is called the temperature of homogeneous ice nucleation (or homogeneous freezing temperature) at
48 $p=1013.25\text{ hPa}$ and represents the lower limit below which it is very difficult to subcool water at this
49 pressure. The assessment of the accuracy of the IAPWS-95 formulation in the temperature range of
50 subcooled liquid water (Wagner and Prüß [2], Section 7.3.2 therein) revealed that TEOS-10 fully satisfies
51 the meteorological needs with respect to accuracy down to this temperature. The IAPWS-95 fluid-water
52 formulation is valid in the entire *stable* fluid region of H_2O from the melting-pressure curve to 1273 K
53 at pressures up to 1000 MPa; the lowest temperature on the melting-pressure curve is 251.165 K (at
54 208.566 MPa) (IAPWS R6-95 [3], Section 5 therein). In the stable fluid region, the formulation can also
55 be extrapolated beyond these limits. Based on a comparison with experimental data, the formulation
56 was reported to behave reasonably when extrapolated into the metastable regions, i.e., for superheated
57 liquid at positive pressures (liquid-gas metastable region), and for subcooled liquid (solid-liquid
58 metastable region). The available data were reported to be in fair agreement with the Helmholtz free
59 energy formulation, but some recent high-pressure data are not represented within their uncertainties
60 (IAPWS R6-95 [3], Section 5 therein).

61 **SM-2 On the Relevance of the Two-State Character of Subcooled Water for Ice 62 Crystallization**

63 The two-state character of subcooled water has implications for ice crystallization which arise
64 from an empirical judgement of Ostwald [13] (pp. 306–309 therein), according to which “*in the*
65 *course of transformation of an unstable (or metastable) state into a stable one the system does not go directly*
66 *to the most stable conformation (corresponding to the modification with the lowest free energy) but prefers*
67 *to reach intermediate stages (corresponding to other possible metastable modifications) having the closest*
68 *free energy difference to the initial state*” (e.g., Schmelzer *et al.* [14][15], Schmelzer [16], Schmelzer *et al.*
69 [17], Gutzow and Schmelzer [18], Schmelzer and Abyzov [19]). Later, this perception has become
70 known as Ostwald’s rule of stages. However, with respect to phase transformation processes Schmelzer
71 *et al.* [14] and Gutzow and Schmelzer [18] emphasized the existence of exceptions from this rule,
72 leading to the conclusion that Ostwald’s rule of stages cannot be considered as a generally valid
73 thermodynamically founded law. This statement is in line with results from statistical mechanical
74 modelling of anisotropic nanoparticle crystallization carried out by Hedges and Whitelam [20], who
75 argued that although often upheld, the rule is without theoretical foundation and is not universally
76 obeyed.

⁷⁷ In advancing Ostwald's rule of stages Schmelzer *et al.* [15] (see also Schmelzer *et al.* [17], Gutzow
⁷⁸ and Schmelzer [18], Schmelzer and Abyzov [19], Schmelzer *et al.* [21]) proposed its generalization as
⁷⁹ follows: "In phase transformation processes, the structure and properties of the critical nucleus may differ
⁸⁰ qualitatively from the properties both of the ambient and the newly evolving macrophases. Those classes of critical
⁸¹ clusters determine the process of the transformation which correspond to a minimum of the work of critical
⁸² cluster formation (as compared with all other possible alternative structures and compositions which may be
⁸³ formed at the given thermodynamic constraints)." As emphasized by those authors, this generalization
⁸⁴ implies – as in Ostwald's formulation – that critical clusters with quite different compositions may be
⁸⁵ formed but does not restrict these possible cluster states to structures and compositions essentially
⁸⁶ determined by the evolving possibly stable or metastable macrophases. In Schmelzer *et al.* [15], [22],
⁸⁷ [21], [17], the generalized Ostwald's rule of stages was employed as a well-founded principle for
⁸⁸ a generalization of Gibbs' classical way of determination of the work of critical cluster formation
⁸⁹ (Gibbs [23]), known as generalized Gibbs' theory. In the latter, as reference states for the determination
⁹⁰ of the bulk contributions to the properties of the critical clusters, the authors did not choose the
⁹¹ quantities of the respective macrophase in equilibrium with the ambient phase; instead, they used
⁹² bulk contributions which correspond to the most appropriate structure and properties, i.e., to those
⁹³ structures and properties which result in a minimum of the work of critical cluster formation.

⁹⁴ Upon undercooling of water at sufficiently high pressure the character of the liquid changes
⁹⁵ by transformation from a dense, high-entropic phase to a less dense, low-entropic (more ordered)
⁹⁶ phase (Debenedetti and Stanley [24]). According to Ostwald's rule of stages, the low-entropic, more
⁹⁷ ordered phase can be thought as an intermediate stage (corresponding to other possible metastable
⁹⁸ modifications) having the closest free energy difference to the initial state. Following this perception,
⁹⁹ new ice embryos are expectable to be more likely formed from the low-density water fraction B
¹⁰⁰ rather than from the high-density fraction A. This would imply that the thermodynamic driving
¹⁰¹ force of ice crystallization (see, e.g., Hellmuth *et al.* [25]) should be scaled in terms of the difference
¹⁰² $\Delta G_{\beta\alpha}^B = G_{\beta}^B(T, p) - G_{\alpha}(T, p)$ between the Gibbs energies of low-density water B (represented by
¹⁰³ $G_{\beta}^B(T, p)$ with subscript β for subcooled water) and ice (represented by $G_{\alpha}(T, p)$ with subscript α for
¹⁰⁴ ice) rather than in terms of the difference $\Delta G_{\beta\alpha} = G_{\beta}(T, p, x) - G_{\alpha}(T, p)$ between mean-state water
¹⁰⁵ (represented by $G_{\beta}(T, p, x)$) and ice. Such perception of heterogeneity has some conceptual similarity
¹⁰⁶ to that employed in Abyzov *et al.* [26], who assumed an increase of the average size of the "structural
¹⁰⁷ units" of the maternal phase with decreasing temperature. This structural coarsening is identified
¹⁰⁸ with the cooperatively rearranging regions in the liquids, the increase of which is a consequence of a
¹⁰⁹ more complex kinetics as compared to a quasi-one-component description of the liquid commonly
¹¹⁰ employed in classical nucleation theory. As a consequence, crystal nucleation in glass-forming liquids
¹¹¹ is assumed to proceed with detectable rates only in the liquid-like (soft) regions and to be suppressed
¹¹² in solid-like (rigid) parts of the liquid. In their model, the fraction of liquid-like and solid-like regions
¹¹³ in dependence on temperature serves as a closure parameter, determined to achieve a comprehensive
¹¹⁴ agreement between classical nucleation theory and experiment not only at relatively high temperatures
¹¹⁵ but also at temperatures lower than that of the nucleation rate maximum.

An implication of these considerations is the determination of the nucleation rate as a mean value. Owing to the nonlinear dependence of the nucleation rate coefficient on temperature and pressure, the nucleation rate coefficient at mean-state conditions, J , differs from the mean-state nucleation rate coefficient, \bar{J} , tentatively defined by the following mixing rule:

$$J(\Delta G_{\beta\alpha}) \neq \bar{J} \approx \underbrace{xJ(\Delta G_{\beta\alpha}^B)}_{\text{from structure B}} + \underbrace{(1-x)J(\Delta G_{\beta\alpha}^A)}_{\text{from structure A}},$$

$$\Delta G_{\beta\alpha} = G_{\beta}(T, p, x) - G_{\alpha}(T, p),$$

$$\Delta G_{\beta\alpha}^A = G_{\beta}^A(T, p) - G_{\alpha}(T, p),$$

$$\Delta G_{\beta\alpha}^B = G_{\beta}^B(T, p) - G_{\alpha}(T, p).$$

- ¹¹⁶ The quantification of the differences $\Delta J_1 = J(\Delta G_{\beta\alpha}^B) - J(\Delta G_{\beta\alpha})$ and $\Delta J_2 = J(\Delta G_{\beta\alpha}) - \bar{J}$ is, however,
¹¹⁷ beyond the scope of the present analysis.

SM-3 IAPWS G12-15 Formulation for the Properties of Subcooled Water

SM-3.1 Equation of State

The EoS according to the IAPWS G12-15 [1] formulation (Equation (1) therein) is given by the dimensionless Gibbs energy ψ as function of temperature T and pressure p :

$$\begin{aligned}\psi(T, p) &= \frac{\hat{g}(T, p)}{R_W T_{LL}} \\ &= \psi^r(\tau, \pi) + (\tau + 1) \left[x_e L(\tau, \pi) + x_e \ln x_e + (1 - x_e) \ln(1 - x_e) + \omega(\pi) x_e (1 - x_e) \right].\end{aligned}\quad (\text{SM-3.1})$$

Here, $\hat{g}(T, p)$ denotes the specific Gibbs energy of subcooled water. The quantity x_e is the equilibrium mole fraction of the low-density structure of water in the two-state water mixture, and serves as a determinable parameter of the EoS. The other quantities are the temperature of the liquid-liquid critical point T_{LL} , the specific gas constant of water R_W , the dimensionless function of the ordering field L , the dimensionless interaction parameter ω , and the reduced temperature τ and the reduced pressure π defined as (IAPWS G12-15 [1], Equation (2) therein):

$$\tau = \frac{T}{T_{LL}} - 1, \quad \pi = \frac{p}{\hat{\rho}_0 R_W T_{LL}}.\quad (\text{SM-3.2})$$

The quantity $\hat{\rho}_0$ is the reference mass density of subcooled water. The values of T_{LL} , $\hat{\rho}_0$, and R_W are given in Table [SM-3.1.1](#). The dimensionless background Gibbs energy ψ^r reads (IAPWS G12-15 [1], Equation (3) therein):

$$\psi^r(\tau, \pi) = \sum_{i=1}^{20} c_i (\tau + 1)^{a_i} (\pi + \pi_0)^{b_i} \exp[-d_i(\pi + \pi_0)].\quad (\text{SM-3.3})$$

The reference dimensionless pressure π_0 is defined by

$$\pi_0 = \frac{p_0}{\hat{\rho}_0 R_W T_{LL}},\quad (\text{SM-3.4})$$

with p_0 given in Table [SM-3.1.1](#). The coefficients a_i , b_i , and c_i are presented in Table [SM-3.1.2](#). The order field $L(\tau, \pi)$ is defined by the following relations (IAPWS G12-15 [1], Equations (4) and (5) therein):

$$\begin{aligned}L(\tau, \pi) &= L_0 \left(\frac{K_2}{2k_1 k_2} \right) [1 + k_0 k_2 + k_1 (\pi + k_2 \tau) - K_1(\tau, \pi)], \\ K_1(\tau, \pi) &= \sqrt{[1 + k_0 k_2 + k_1 (\pi - k_2 \tau)]^2 - 4k_0 k_1 k_2 (\pi - k_2 \tau)}, \\ K_2 &= \sqrt{1 + k_2^2}.\end{aligned}\quad (\text{SM-3.5})$$

The values of L_0 , k_0 , k_1 , and k_2 are given in Table [SM-3.1.1](#). The quantity ω denotes the interaction parameter, which depends linearly on pressure (IAPWS G12-15 [1], Equation (6) therein):

$$\omega(\pi) = 2 + \omega_0 \pi.\quad (\text{SM-3.6})$$

The reference parameter ω_0 is given in Table [SM-3.1.1](#). The equilibrium mole fraction of the low-density structure of water is a function of temperature and pressure, $x_e = x_e(T, p)$, which is determined by minimizing the Gibbs energy in dependence on x_e at isothermal and isobaric conditions (IAPWS G12-15 [1], Equation (7) therein):

$$\left(\frac{\partial \psi(T, p, x)}{\partial x} \right)_{T, p} = 0.\quad (\text{SM-3.7})$$

Table SM-3.1.1. Parameter values for the equation of state given by Equations (SM-3.1)–(SM-3.8). Taken from IAPWS G12-15 [1] (Table 1 therein).

Parameter	Value	Parameter	Value	Unit
ω_0	0.521 226 9	p_0	300×10^6	Pa
L_0	0.763 179 54	T_{LL}	228.2	K
k_0	0.072 158 686	\hat{q}_0	1081.648 2	kg m^{-3}
k_1	-0.315 692 32	R_W	461.523 087	$\text{J kg}^{-1} \text{K}^{-1}$
k_2	5.299 260 8			

Table SM-3.1.2. Parameter values for the dimensionless regular background Gibbs energy ψ^r in Equation (SM-3.3). Taken from IAPWS G12-15 [1] (Table 2 therein).

i	c_i	a_i	b_i	d_i
1	$-8.157\ 068\ 138\ 165\ 5 \times 10^0$	0	0	0
2	$1.287\ 503\ 2 \times 10^0$	0	1	0
3	$7.090\ 167\ 359\ 801\ 2 \times 10^0$	1	0	0
4	$-3.277\ 916\ 1 \times 10^{-2}$	-0.2555	2.1051	-0.0016
5	$7.370\ 394\ 9 \times 10^{-1}$	1.5762	1.1422	0.6894
6	$-2.162\ 862\ 2 \times 10^{-1}$	1.6400	0.9510	0.0130
7	$-5.178\ 247\ 9 \times 10^0$	3.6385	0	0.0002
8	$4.229\ 351\ 7 \times 10^{-4}$	-0.3828	3.6402	0.0435
9	$2.359\ 210\ 9 \times 10^{-2}$	1.6219	2.0760	0.0500
10	$4.377\ 375\ 4 \times 10^0$	4.3287	-0.0016	0.0004
11	$-2.996\ 777\ 0 \times 10^{-3}$	3.4763	2.2769	0.0528
12	$-9.655\ 801\ 8 \times 10^{-1}$	5.1556	0.0008	0.0147
13	$3.759\ 528\ 6 \times 10^0$	-0.3593	0.3706	0.8584
14	$1.263\ 244\ 1 \times 10^0$	5.0361	-0.3975	0.9924
15	$2.854\ 269\ 7 \times 10^{-1}$	2.9786	2.9730	1.0041
16	$-8.599\ 494\ 7 \times 10^{-1}$	6.2373	-0.3180	1.0961
17	$-3.291\ 615\ 3 \times 10^{-1}$	4.0460	2.9805	1.0228
18	$9.001\ 961\ 6 \times 10^{-2}$	5.3558	2.9265	1.0303
19	$8.114\ 972\ 6 \times 10^{-2}$	9.0157	0.4456	1.6180
20	$-3.278\ 821\ 3 \times 10^0$	1.2194	0.1298	0.5213

Evaluation of Equation (SM-3.7) with $\psi(T, p, x_e)$ from Equation (SM-3.1) leads to the following transcendental equation $\mathcal{F}(x_e)=0$, the numerical root of which yields the sought-after value of x_e (IAPWS G12-15 [1], Equation (8) therein):

$$\mathcal{F}(x_e) = L(\tau, \pi) + \ln \left(\frac{x_e}{1 - x_e} \right) + \omega(\pi)(1 - 2x_e) = 0. \quad (\text{SM-3.8})$$

120

121 SM-3.2 Thermodynamic Properties

According to IAPWS G12-15 [1] (Equations (12)–(17) and Table 3 therein) the thermodynamic properties can be derived from the derivatives of $\psi(T, p)$ at the equilibrium mole fraction x_e . As a matter of convenience the corresponding dependencies are expressed in terms of the order parameter ϕ and the susceptibility χ (IAPWS G12-15 [1], Equation (12) therein):

$$\phi(x_e) = 2x_e - 1, \quad \chi(\pi, x_e) = \left(\frac{2}{1 - (\phi(x_e))^2} - \omega(\pi) \right)^{-1}. \quad (\text{SM-3.9})$$

Table SM-3.2.1. Derivatives of $L(\tau, \pi)$ and $\psi^r(\tau, \pi)$. To simplify the annotation of the derivatives of ψ^r (right column), the following shorthand definitions are used: $\bar{\tau} = \tau + 1$ and $\bar{\pi} = \pi + \pi_0$. Taken from IAPWS G12-15 [1] (Table 3 therein).

Derivatives of L	Derivatives of ψ^r
$L_\tau = \frac{L_0 K_2}{2} \left(1 + \frac{1 - k_0 k_2 + k_1 (\pi - k_2 \tau)}{K_1} \right)$	$\psi_\tau^r = \sum_{i=1}^{20} c_i a_i \bar{\tau}^{a_i-1} \bar{\pi}^{b_i} e^{-d_i \bar{\pi}}$
$L_\pi = \frac{L_0 K_2 (K_1 + k_0 k_2 - k_1 \pi + k_1 k_2 \tau - 1)}{2 k_2 K_1}$	$\psi_\pi^r = \sum_{i=1}^{20} c_i \bar{\tau}^{a_i} \bar{\pi}^{b_i-1} (b_i - d_i \bar{\pi}) e^{-d_i \bar{\pi}}$
$L_{\tau\tau} = -\frac{2 L_0 K_2 k_0 k_1 k_2^2}{K_1^3}$	$\psi_{\tau\tau}^r = \sum_{i=1}^{20} c_i a_i (a_i - 1) \bar{\tau}^{a_i-2} \bar{\pi}^{b_i} e^{-d_i \bar{\pi}}$
$L_{\tau\pi} = \frac{2 L_0 K_2 k_0 k_1 k_2}{K_1^3}$	$\psi_{\tau\pi}^r = \sum_{i=1}^{20} c_i a_i \bar{\tau}^{a_i-1} \bar{\pi}^{b_i-1} (b_i - d_i \bar{\pi}) e^{-d_i \bar{\pi}}$
$L_{\pi\pi} = -\frac{2 L_0 K_2 k_0 k_1}{K_1^3}$	$\psi_{\pi\pi}^r = \sum_{i=1}^{20} c_i \bar{\tau}^{a_i} \bar{\pi}^{b_i-2} \left[(d_i \bar{\pi} - b_i)^2 - b_i \right] e^{-d_i \bar{\pi}}$

¹²² In the following equations, the subscripts τ and π indicate partial derivatives with respect to the
¹²³ subscripted quantities τ and π . Expressions for the derivatives of $L(\tau, \pi)$ and $\psi^r(\tau, \pi)$ with respect
¹²⁴ to τ and π are presented in Table SM-3.2.1. As the equilibrium value of x_e is defined by Equation
¹²⁵ (SM-3.7), it is considered a function of τ and π .

1. Specific volume $\hat{v} = 1/\hat{\rho}$ (with $\hat{\rho}$ denoting the mass density) (IAPWS G12-15 [1], Equation (13) therein):

$$\begin{aligned} \hat{v}(\tau, \pi) = & \frac{1}{\hat{\rho}_0(\tau, \pi)} \left\{ \frac{\tau+1}{2} \left[\frac{\omega_0}{2} \left(1 - \phi^2(x_e) \right) + L_\pi(\tau, \pi) \left(\phi(x_e) + 1 \right) \right] \right. \\ & \left. + \psi_\pi^r(\tau, \pi) \right\}. \end{aligned} \quad (\text{SM-3.10})$$

2. Specific entropy \hat{s} (IAPWS G12-15 [1], Equation (14) therein):

$$\begin{aligned} \hat{s}(\tau, \pi) = & -R_W \left\{ \frac{(\tau+1)L_\tau(\tau, \pi)}{2} \left(\phi(x_e) + 1 \right) \right. \\ & \left. + \left[x_e L(\tau, \pi) + x_e \ln x_e + (1-x_e) \ln(1-x_e) + \omega(\pi) x_e (1-x_e) \right] + \psi_\tau^r(\tau, \pi) \right\}. \end{aligned} \quad (\text{SM-3.11})$$

3. Isothermal compressibility, κ_T , thermal expansion coefficient, α_p , specific isobaric heat capacity, \hat{c}_p (IAPWS G12-15 [1], Equation (15) therein):

$$\begin{aligned} \kappa_T(\tau, \pi) = & \frac{\hat{\rho}(\tau, \pi)}{\hat{\rho}_0^2 R_W T_{LL}} \left\{ \frac{\tau+1}{2} \left[\chi \left(L_\pi(\tau, \pi) - \omega_0 \phi(x_e) \right)^2 \right. \right. \\ & \left. \left. - \left(\phi(x_e) + 1 \right) L_{\pi\pi}(\tau, \pi) \right] - \psi_{\pi\pi}^r(\tau, \pi) \right\}, \end{aligned}$$

$$\begin{aligned}\alpha_p(\tau, \pi) &= \frac{\hat{\varrho}(\tau, \pi)}{\hat{\varrho}_0 R_W T_{LL}} \left\{ \frac{L_{\tau\pi}(\tau, \pi)}{2} (\tau + 1) \left(\phi(x_e) + 1 \right) \right. \\ &\quad \left. + \frac{1}{2} \left[\frac{\omega_0 (1 - \phi^2(x_e))}{2} + L_\pi(\tau, \pi) \left(\phi(x_e) + 1 \right) \right] \right. \\ &\quad \left. - \frac{(\tau + 1)L_\tau(\tau, \pi)}{2} \chi \left(L_\pi(\tau, \pi) - \omega_0 \phi(x_e) \right) + \psi_{\tau\pi}^r(\tau, \pi) \right\}, \\ \hat{c}_p(\tau, \pi) &= -R_W(\tau + 1) \left\{ L_\tau(\tau, \pi) \left(\phi(x_e) + 1 \right) \right. \\ &\quad \left. + \frac{1}{2}(\tau + 1) \left[L_{\tau\tau}(\tau, \pi) \left(\phi(x_e) + 1 \right) - (L_\tau(\tau, \pi))^2 \chi \right] + \psi_{\tau\tau}^r(\tau, \pi) \right\}.\end{aligned}\tag{SM-3.12}$$

4. Specific isochoric heat capacity, \hat{c}_v (IAPWS G12-15 [1], Equation (16) therein):

$$\hat{c}_v(\tau, \pi) = \hat{c}_p(\tau, \pi) - \frac{T(\alpha_p(\tau, \pi))^2}{\hat{\varrho}(\tau, \pi)\kappa_T(\tau, \pi)}. \tag{SM-3.13}$$

5. Speed of sound, w (IAPWS G12-15 [1], Equation (17) therein):

$$\begin{aligned}w(\tau, \pi) &= \left[\hat{\varrho}(\tau, \pi)\kappa_T(\tau, \pi) \frac{\hat{c}_v(\tau, \pi)}{\hat{c}_p(\tau, \pi)} \right]^{-1/2} \\ &= \left[\hat{\varrho}(\tau, \pi)\kappa_T(\tau, \pi) - \frac{T(\alpha_p(\tau, \pi))^2}{\hat{c}_p(\tau, \pi)} \right]^{-1/2}.\end{aligned}\tag{SM-3.14}$$

¹²⁶ SM-3.3 Validity Range

The EoS of subcooled water given by Equations (SM-3.1)–(SM-3.14) is valid for metastable liquid water from the homogeneous ice nucleation temperature, $T_H(p)$, to the melting temperature, $T_M(p)$, at pressures in the interval $0 \leq p \leq 400$ MPa:

$$T_H(p) \leq T \leq T_M(p), \quad 0 \leq p \leq 400 \text{ MPa}.$$

The equation remains also valid for stable liquid states up to 300 K in the same pressure range, where IAPWS-95 remains the recommended formulation, and behaves reasonably when extrapolated to 1000 MPa. The homogeneous-ice nucleation curve can be approximated by the fits given in Equations (SM-3.15) and (SM-3.16) (IAPWS G12-15 [1], Equations (18) and (19) therein):

$$\begin{aligned}\frac{p_H}{\text{MPa}} &= 0.1 + 228.27 \left(1 - \theta^{6.243} \right) + 15.724 \left(1 - \theta^{79.81} \right), \\ \theta &= T/235.15 \text{ K}, \quad 0 \text{ MPa} \leq p \leq 198.9 \text{ MPa},\end{aligned}\tag{SM-3.15}$$

$$\begin{aligned}\frac{T_H}{\text{K}} &= 172.82 + 0.03718 \left(\frac{p}{\text{MPa}} \right) + 3.403 \times 10^{-5} \left(\frac{p}{\text{MPa}} \right)^2 \\ &\quad - 1.573 \times 10^{-8} \left(\frac{p}{\text{MPa}} \right)^3, \quad 198.9 \text{ MPa} \leq p \leq 1500 \text{ MPa}.\end{aligned}\tag{SM-3.16}$$

¹²⁷ The slope of the ice-nucleation curve exhibits a discontinuity at the break point $(T_{BP}, p_{BP}) = (181.4 \text{ K}, 198.9 \text{ MPa})$. At this point both curves intersect. Equation (SM-3.15) should be used for pressures $p < p_{BP}$, and Equation (SM-3.16) for pressures $p_{BP} < p$.

Table SM-3.3.1. Regression coefficients a_k , n_k for $p_M(T)$, Equation (SM-3.17), and b_k for the $T_M(p)$, Equation (SM-3.18). Taken from Feistel [27].

k	$p_M(T)$, Equation (SM-3.17)		$T_M(p)$, Equation (SM-3.18)
	a_k	n_k	b_k
1	0.119 539 337 · 10 ⁷	3	-1.663 561 044 845 51 · 10 ⁻⁷
2	0.808 183 159 · 10 ⁵	25.75	-2.135 192 419 794 06 · 10 ⁻¹³
3	0.333 826 860 · 10 ⁴	103.75	3.529 674 053 418 77 · 10 ⁻²⁰
4			-2.731 845 252 362 81 · 10 ⁻²⁶

Table SM-3.4.1. Subintervals for the numerical determination of the equilibrium mole fraction of low-density water, x_e , in dependence on $L(\tau, \pi)$ and $\omega(\pi)$. The “min” function returns the smallest value of its arguments. Taken from IAPWS G12-15 [1] (Table 4 therein).

ω interval	x_e subinterval	
	Lower bound	Upper bound
$\omega < \frac{10}{9} [\ln(19) - L]$	0.049	0.5
$\frac{10}{9} [\ln(19) - L] \leq \omega < \frac{50}{49} [\ln(99) - L]$	0.0099	0.051
$\frac{50}{49} [\ln(99) - L] \leq \omega$	$0.99 \exp\left[-\frac{50L}{49} - \omega\right]$	$\min\left[1.1 \exp(-L - \omega), 0.0101\right]$

To complete the specification of the validity range of the EoS, here we include also the determination of the melting curve, which is not part of the IAPWS G12-15 [1] formulation. The correlation equation for the melting pressure was developed by Wagner (2006) (cited in Feistel [27], Appendix 1 therein) on the base of the guidelines IAPWS [28] and IAPWS [29] and deviates from the melting curve less than its predecessor published in Wagner and Prüß [2] (Equation (2.16) therein):

$$\frac{p_M - p_{TP}}{p_{TP}} = \sum_{k=1}^3 a_k \left[1 - \left(\frac{T}{T_{TP}} \right)^{n_k} \right], \quad T_{TP} = 273.16 \text{ K}, \quad p_{TP} = 611.657 \text{ Pa}. \quad (\text{SM-3.17})$$

Here, T_{TP} and p_{TP} denote the temperature and pressure of the triple point. The correlation equation for the melting temperature was developed by Feistel [27] (Appendix 2 therein) also on the base of the guidelines IAPWS [28] and IAPWS [29] and deviates from the melting curve significantly less than its predecessor:

$$\frac{T_M - T_{TP}}{T_{TP}} = \sum_{k=1}^4 b_k \left[\frac{p - p_{TP}}{p_{TP}} \right]^k. \quad (\text{SM-3.18})$$

¹³⁰ The regression coefficients a_k , n_k and b_k are presented in Table SM-3.3.1.

¹³¹ SM-3.4 Constraints on the Numerical Solution of Equation (SM-3.8)

¹³² The numerical solution of Equation (SM-3.8) delivers the equilibrium mole fraction of low-density
¹³³ water, which is located in the interval $0 < x_e < 1$. Depending on the values of $L(\tau, \pi)$ and $\omega(\pi)$, IAPWS
¹³⁴ G12-15 [1] (Table 4 therein) distinguished three different subintervals, defined by lower and upper
¹³⁵ limits of the sought-after equilibrium value of x_e , which are presented in Table SM-3.4.1.

¹³⁶ SM-3.5 IAPWS G12-15 Thermodynamic Reference Values for the Check of the Correct Computer ¹³⁷ Implementation

¹³⁸ IAPWS G12-15 [1] (Table 5 therein) provides reference values for the check of the correct
¹³⁹ implementation of the EoS calculus. These values are listed in Table SM-3.5.1. In order to reproduce

¹⁴⁰ these table values to the number of given digits, the mole fraction x_e should be numerically determined
¹⁴¹ with a resolution of 10^{-10} .

Table SM-3.5.1. Thermodynamic reference values for check of the correct computer implementation. Taken from IAPWS G12-15 [1] (Table 5 therein).

$\frac{T}{\text{K}}$	$\frac{p}{\text{MPa}}$	$\frac{\hat{q}}{\text{kg m}^{-3}}$	$\frac{\alpha_p}{10^{-4}\text{K}^{-1}}$	$\frac{\kappa_T}{10^{-4}\text{MPa}^{-1}}$	$\frac{\hat{c}_p}{\text{J kg}^{-1}\text{K}^{-1}}$	$\frac{w}{\text{m s}^{-1}}$	x	L
273.15	0.101325	999.842 29	-0.683 042	5.088 499	4218.3002	1402.3886	0.096 654 7155	0.621 204 74
235.15	0.101325	968.099 99	-29.633 816	11.580 785	5997.5632	1134.5855	0.255 102 8587	0.091 763 68
250	200	1090.456 77	3.267 768	3.361 311	3708.3902	1668.2020	0.030 429 2667	0.723 770 81
200	400	1185.028 00	6.716 009	2.567 237	3338.5250	1899.3294	0.007 170 080 9	1.155 396 5
250	400	1151.715 17	4.929 927	2.277 029	3757.2144	2015.8782	0.005 358 836 6	1.434 5145

¹⁴² SM-4 Analytical Solution of a Cubic Equation

Starting point of the analytical solution is the following general form of the cubic equation:

$$Ax^3 + Bx^2 + Cx + D = 0, \quad x \in \mathbb{C}; \quad A, B, C \in \mathbb{R}. \quad (\text{SM-4.1})$$

Here, x denotes the sought-after root of the equation, which is element of the complex numbers. The parameters A, B, C , and D are real numbers. Equation (SM-4.1) can be solved by means of *Cardano's method*, the rationale of which can be found, e.g., in Gellert *et al.* [30] (pp. 104–207 therein). Employing the transformations

$$r = \frac{B}{A}, \quad s = \frac{C}{A}, \quad t = \frac{D}{A}, \quad A \neq 0,$$

one arrives at the normal form of the cubic equation:

$$x^3 + rx^2 + sx + t = 0, \quad x \in \mathbb{C}; \quad r, s, t \in \mathbb{R}. \quad (\text{SM-4.2})$$

In the set of complex numbers, each cubic equation has three solutions, which can coincide. One of these solutions is real, the other two are either real too or conjugate complex. According to Cardano's formula, the application of the transformation

$$x = y - \frac{r}{3} \quad (\text{SM-4.3})$$

to the normal form yields the reduced form, in which the quadratic term is absent:

$$y^3 + py + q = 0, \quad p = s - \frac{r^2}{3}, \quad q = \frac{2r^3}{27} - \frac{sr}{3} + t. \quad (\text{SM-4.4})$$

For the sought-after solution y the following ansatz is used:

$$y = u + v.$$

This ansatz results in the following equation:

$$(u + v)^3 + p(u + v) + q = 0 \quad \text{or, equivalently} \quad u^3 + v^3 + q + (u + v)(3uv + p) = 0.$$

This is one equation for the two unknown variables u and v . To satisfy the remaining degree of freedom, a side condition is employed which removes the term $(u + v)(3uv + p)$:

$$3uv + p = 0.$$

Therewith, one obtains the following two equations for the determination of u and v :

$$u^3 + v^3 = -q \quad \rightsquigarrow \text{quadratization} \rightsquigarrow \quad u^6 + 2u^3v^3 + v^6 = q^2, \quad (\text{SM-4.5})$$

$$uv = -\frac{p}{3} \quad \rightsquigarrow \text{four times the third power} \rightsquigarrow \quad 4u^3v^3 = -4\left(\frac{p}{3}\right)^3. \quad (\text{SM-4.6})$$

Subtraction of Equation (SM-4.6) from Equation (SM-4.5) yields:

$$(u^3 - v^3)^2 = q^2 + 4\left(\frac{p}{3}\right)^3 = 4\underbrace{\left[\left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3\right]}_{=\Delta} \quad \rightsquigarrow \quad u^3 - v^3 = \pm 2\sqrt{\Delta}. \quad (\text{SM-4.7})$$

Combining the first form in Equation (SM-4.5) with the second form in Equation (SM-4.7),

$$u^3 + v^3 = -q, \quad u^3 - v^3 = \pm 2\sqrt{\Delta},$$

one arrives at the following solutions for u and v :

$$u^3 = -\frac{q}{2} \pm \sqrt{\Delta}, \quad v^3 = -\frac{q}{2} \mp \sqrt{\Delta}. \quad (\text{SM-4.8})$$

- ¹⁴³ Upon interchanging the upper signs in front of the roots with the lower ones the quantity u^3 migrates
¹⁴⁴ to v^3 , while the equations $u^3 + v^3 + q = 0$ and $uv = -p/3$ remain unchanged. Therefore it is sufficient,
¹⁴⁵ to consider only one pair of signs, e.g., the upper one.

Each third root of a complex number has three values; next to x_1 there are two further solutions x_2 and x_3 with

$$x_2 = \varepsilon_2 x_1, \quad x_3 = \varepsilon_3 x_1, \quad \varepsilon_2 = \frac{1}{2}(-1 + i\sqrt{3}), \quad \varepsilon_3 = \frac{1}{2}(-1 - i\sqrt{3}).$$

Therewith, one obtains the following solutions for u and v :

$$\begin{aligned} u_1 &= \sqrt[3]{-\frac{q}{2} + \sqrt{\Delta}}, & u_2 &= \varepsilon_2 u_1, & u_3 &= \varepsilon_3 u_1, \\ v_1 &= \sqrt[3]{-\frac{q}{2} - \sqrt{\Delta}}, & v_2 &= \varepsilon_2 v_1, & v_3 &= \varepsilon_3 v_1. \end{aligned} \quad (\text{SM-4.9})$$

For $y = u_i + v_j$ with $i = 1, 2, 3$ and $j = 1, 2, 3$ one would obtain nine solutions of the cubic equation. However, the number of solutions reduces to the following three only,

$$y_1 = u_1 + v_1, \quad y_2 = u_2 + v_3, \quad y_3 = u_3 + v_2,$$

because the side constraint $u_i v_j = -p/3$ is fulfilled only for $u_1 v_1$, $u_2 v_3$ and $u_3 v_2$ by virtue of

$$\varepsilon_2 \varepsilon_3 = \frac{1}{2}(-1 + i\sqrt{3}) \cdot \frac{1}{2}(-1 - i\sqrt{3}) = \frac{1}{4}(1 + 3) = 1.$$

Presuming that the radicand of the square root is nonnegative,

$$\Delta = \left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3 \geq 0,$$

the solution y_1 is real,

$$y_1 = u_1 + v_1 = \sqrt[3]{-\frac{q}{2} + \sqrt{\Delta}} + \sqrt[3]{-\frac{q}{2} - \sqrt{\Delta}}, \quad (\text{SM-4.10})$$

while y_2 and y_3 are conjugate complex, as can be seen below:

$$\begin{aligned} y_2 &= u_2 + v_3 = u_1 \varepsilon_2 + v_1 \varepsilon_3 = -\frac{1}{2}(u_1 + v_1) + \left[\frac{1}{2}(u_1 - v_1)\right] \cdot i\sqrt{3}, \\ y_3 &= u_3 + v_2 = u_1 \varepsilon_3 + v_1 \varepsilon_2 = -\frac{1}{2}(u_1 + v_1) - \left[\frac{1}{2}(u_1 - v_1)\right] \cdot i\sqrt{3}. \end{aligned} \quad (\text{SM-4.11})$$

- ¹⁴⁶ The solution given by Equation (SM-4.10) is known as Cardano's formula.

For the case that the radicand of the square root is negative ("casus irreducibilis"),

$$\Delta = \left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3 < 0,$$

there exist three real trigonometric solutions for y in Equation(SM-4.3). Introducing the auxiliary variables

$$r_0 = \sqrt{-\left(\frac{p}{3}\right)^3}, \quad \cos \varphi = -\frac{q}{2\sqrt{-\left(\frac{p}{3}\right)^3}},$$

these three real solutions read:

$$\begin{aligned} y_1 &= 2\sqrt[3]{r_0} \cos\left(\frac{\varphi}{3}\right), \\ y_2 &= 2\sqrt[3]{r_0} \cos\left(\frac{\varphi}{3} + \frac{2\pi}{3}\right), \\ y_3 &= 2\sqrt[3]{r_0} \cos\left(\frac{\varphi}{3} + \frac{4\pi}{3}\right). \end{aligned} \tag{SM-4.12}$$

- ¹⁴⁷ The back transformation from the solutions of the reduced form, y_i , to the solutions of the normal form, x_i , is carried out using Equation (SM-4.3).
- ¹⁴⁸

SM-5 Table Values of the Computer-Program Verification

Table SM-5.1. Deviations of the numerically determined values of mass density $\hat{\varrho}$, thermal expansion coefficient α_p , isothermal compressibility κ_T , isobaric heat capacity c_p , speed of sound w , equilibrium mole fraction of low-density water, x_e , and the ordering field L using the root finder of Press *et al.* [31] (Section 9.1 therein) from the IAPWS G12-15 [1] reference values (subscript *, Table SM-3.5.1). Integer n denotes the number of equally spaced segments of the root interval of x_e . Relative deviations are given in parts per billion (ppb). Bold-style values denote extrema.

$\frac{T}{K}$	$\frac{p}{MPa}$	$\frac{\hat{\varrho} - \hat{\varrho}_*}{\hat{\varrho}_*}$	$\frac{\alpha_p - \alpha_{p,*}}{10^{-4} K^{-1}}$	$\frac{\kappa_T - \kappa_{T,*}}{K_{T,*}}$	$\frac{\hat{c}_p - \hat{c}_{p,*}}{\hat{c}_{p,*}}$	$\frac{w - w_*}{w_*}$	$\frac{x_e - x_{e*}}{x_{e,*}}$	$\frac{L - L_*}{L_*}$
$n = 10^9$								
273.15	0.101325	-3.23	-0.49·10 ⁻⁶	91.40	-7.36	-25.29	0.65	-4.24
235.15	0.101325	-1.88	-0.28·10 ⁻⁶	34.53	8.01	-29.12	0.09	-45.23
250	200	-2.64	0.11·10 ⁻⁶	-45.28	-10.95	-21.75	1.14	-3.61
200	400	2.32	-0.42·10 ⁻⁶	-135.49	-7.67	-0.18	3.32	-29.13
250	400		0.31·10 ⁻⁶	109.62	9.59	-20.41	3.30	-11.59
$n = 10^8$								
273.15	0.101325	2.21	-0.31·10 ⁻⁶	82.11	-10.15	-21.20	-12.53	
235.15	0.101325	-2.87	0.36·10 ⁻⁷	29.06	3.03	-29.00	-3.28	
250	200	-1.70	0.14·10 ⁻⁶	-49.39	-10.98	-19.60	-5.46	
200	400	-2.64	-0.42·10⁻⁶	-135.41	-7.67	-0.23	3.62	
250	400	2.32	0.31·10 ⁻⁶	109.65	9.58	-20.42	3.40	
$n = 10^7$								
273.15	0.101325	3.63	0.93·10 ⁻⁸	65.78	-15.04	-14.01	-35.71	
235.15	0.101325	9.44	-0.56·10⁻⁵	127.69	92.79	31.16	57.56	
250	200	-2.21	0.70·10 ⁻⁷	-37.68	-10.90	-25.73	13.32	
200	400	-2.66	-0.42·10 ⁻⁶	-134.63	-7.67	-0.65	6.35	
250	400	2.33	0.31·10 ⁻⁶	109.08	9.59	-20.12	0.93	
$n = 10^6$								
273.15	0.101325	17.92	0.32·10 ⁻⁵	-98.61	-64.31	58.32	-269.00	
235.15	0.101325	57.40	0.52·10⁻⁴	-875.69	-820.26	-9.13	-561.33	
250	200	-0.37	0.31·10 ⁻⁶	-79.81	-11.19	-3.70	-54.21	
200	400	-2.23	-0.41·10 ⁻⁶	-150.79	-7.54	8.11	-50.74	
250	400	1.95	0.29·10 ⁻⁶	122.99	9.46	-27.61	61.19	

Continuation of Table SM-5.1.

$\frac{T}{K}$	$\frac{p}{\text{MPa}}$	$\frac{\hat{q} - \hat{q}_*}{\hat{q}_*}$	$\frac{\alpha_p - \alpha_{p,*}}{10^{-4}\text{K}^{-1}}$	$\frac{\kappa_T - \kappa_{T,*}}{\kappa_{T,*}}$	$\frac{\hat{c}_p - \hat{c}_{p,*}}{\hat{c}_{p,*}}$	$\frac{w - w_*}{w_*}$	$\frac{x_e - x_{e*}}{x_{e,*}}$	$\frac{L - L_*}{L_*}$
$n = 10^5$								
273.15	0.101325	-124.98	-0.29:10 ⁻⁴	1545.41	428.40	-665.03	2064.05	
235.15	0.101325	-801.76	-0.68:10 ⁻³	12022.59	10916.90	-292.31	7394.27	
250	200	17.99	0.27:10 ⁻⁵	-501.08	-14.16	216.56	-729.56	
200	400	-3.66	-0.44:10 ⁻⁶	-96.93	-7.98	-21.07	139.56	
250	400	2.37	0.31:10 ⁻⁶	107.56	9.60	-19.30	-5.67	
$n = 10^4$								
273.15	0.101325	4162.02	0.93:10 ⁻³	-47775.34	-14352.32	21036.79	-67927.36	
235.15	0.101325	7790.13	0.67:10 ⁻²	-116951.57	-106440.33	2543.51	-72161.87	
250	200	1670.25	0.22:10 ⁻³	-38414.77	-281.40	20040.61	-61509.86	
200	400	39.29	0.46:10 ⁻⁶	-1712.79	5.15	854.42	-5569.52	
250	400	-10.22	-0.40:10 ⁻⁶	570.43	5.18	-268.67	1999.93	
$n = 10^3$								
273.15	0.101325	47036.98	0.11:10 ⁻¹	-540984.39	-162098.23	238206.89	-767841.48	
235.15	0.101325	93738.95	0.80:10 ⁻¹	-1405616.97	-1278231.17	31390.30	-867723.32	
250	200	-165.60	-0.21:10 ⁻⁴	3711.58	15.53	-1986.04	6023.81	
200	400	373.38	0.74:10 ⁻⁵	-14280.55	107.24	7663.89	-49973.49	
250	400	-52.19	-0.28:10 ⁻⁵	2113.33	-9.56	-1099.92	8685.26	
$n = 10^2$								
273.15	0.101325	190018.18	0.42:10 ⁻¹	-2185035.19	-653781.33	964106.57	-3100888.54	
235.15	0.101325	380627.98	0.32	-5687105.11	-5160921.64	133965.74	-3519594.82	
250	200	165107.11	0.22:10 ⁻¹	-3785627.41	-26483.21	1998581.69	-6072006.33	
200	400	850.66	0.17:10 ⁻⁴	-32234.42	253.09	17391.91	-113407.72	
250	400	-3829.77	-0.22:10 ⁻³	140976.82	-1336.42	-75904.32	610364.54	
$n = 10^1$								
273.15	0.101325	-12287514.62	-2.95	145898351.27	48896156.92	-53603509.82	206873347.01	
235.15	0.101325	1341300.94	1.13	-19805072.01	-17848920.22	547357.55	-12359166.48	
250	200	1823017.78	0.24	-41455907.74	-266681.45	22491481.74	-66852307.68	
200	400	-32557.06	-0.68:10 ⁻³	1224714.96	-9955.36	-662964.78	4326988.81	
250	400	-8027.03	-0.46:10 ⁻³	295274.11	-2810.64	-159002.41	1278897.07	

¹⁴⁹ **SM-6 Table Values of the Deviations of the Analytical from the IAPWS G12-15**
¹⁵⁰ **[1] Reference Formulation**

Table SM-6.1. Deviation of the analytically determined mass density $\hat{\rho}$, thermal expansion coefficient α_p , isothermal compressibility κ_T , isobaric heat capacity c_p , speed of sound w , equilibrium mole fraction of low-density water, x_e , and the ordering field L according to Section [SM-3.1](#) from the IAPWS G12-15 [1] reference values (subscript \star , Table [SM-3.5.1](#)). Relative deviations are given in parts per billion (ppb). Bold-styled values denote extrema.

T K	p MPa	$\frac{\hat{\rho} - \hat{\rho}_\star}{\hat{\rho}_\star}$	$\frac{\alpha_p - \alpha_{p,\star}}{10^{-4} \text{ K}^{-1}}$	$\frac{\kappa_T - \kappa_{T,\star}}{\kappa_{T,\star}}$	$\frac{\hat{c}_p - \hat{c}_{p,\star}}{\hat{c}_{p,\star}}$	$\frac{w - w_\star}{w_\star}$	$\frac{x_e - x_{e\star}}{x_{e,\star}}$	$\frac{L - L_\star}{L_\star}$
$n = 10^9$								
273.15	0.101325	2.20	$-0.31 \cdot 10^{-6}$	82.19	-10.13	-21.23	-12.43	-4.24
235.15	0.101325	0.172 · 10⁶	0.15	-2.58 · 10⁶	-2.34 · 10⁶	0.059 · 10⁶	-1.596 · 10⁶	-45.23
250	200	-1.88	$0.11 \cdot 10^{-6}$	-45.26	-10.95	-21.76	1.16	3.61
200	400	-2.64	$-0.42 \cdot 10^{-6}$	-135.50	-7.67	-0.17	3.28	29.13
250	400	2.32	$0.31 \cdot 10^{-6}$	109.63	9.59	-20.41	3.31	-11.59

151 SM-7 Table Values of the Deviation of the Analytically from the Numerically
152 Determined Thermodynamic Properties of Subcooled Water

153 SM-7.1 Mass Density

Table SM-7.1.1. Relative deviation, $(\hat{\varrho} - \hat{\varrho}_{\text{num}}) / \hat{\varrho}_{\text{num}}$ in parts per billion (ppb), of the mass density $\hat{\varrho}$ using the analytically determined low-density water fraction from the mass density $\hat{\varrho}_{\text{num}}$ using the numerically determined low-density water fraction at $p=0.101325 \text{ MPa}$.

T K	$\frac{\hat{\varrho} - \hat{\varrho}_{\text{num}}}{\hat{\varrho}_{\text{num}}}$
235.15	172468.89
240.15	19920.96
245.15	3096.26
250.15	573.01
255.15	119.43
260.15	26.98
265.15	6.44
270.15	1.78
275.15	0.38
280.15	0.13
285.15	0.03
290.15	-0.03
295.15	-0.06
300.15	0.13

Table SM-7.1.2. As Table SM-7.1.1, but for $0.1 \leq p/\text{MPa} \leq 400$ and $253.15 \leq T/\text{K} \leq 303.15$.

$\frac{p}{\text{MPa}}$	T/K									293.15	298.15	303.15
	253.15	255.65	258.15	260.65	263.15	265.65	268.15	270.65	273.15			
0.1	220.99	102.65	48.57	23.44	11.49	5.61	2.95	1.54	0.79	-0.10	-0.13	0.05
5.0	152.68	71.77	34.23	16.71	8.19	4.22	2.09	1.14	0.49	0.12	0.03	0.00
10.0	104.40	49.70	23.89	11.95	5.94	2.97	1.52	0.76	0.52	-0.15	0.10	0.12
15.0	71.10	34.15	16.66	8.43	4.05	2.00	1.18	0.57	0.29	-0.02	-0.15	-0.00
20.0	48.26	23.40	11.72	5.86	3.10	1.59	0.66	0.38	0.29	-0.11	0.00	-0.01
25.0	32.52	16.07	8.06	4.13	2.07	1.03	0.44	0.24	0.26	-0.02	-0.09	-0.01
30.0	22.14	10.94	5.66	2.70	1.55	0.68	0.28	0.19	0.07	0.08	-0.01	-0.01
35.0	14.96	7.38	3.78	1.91	1.15	0.50	0.35	0.04	0.01	0.01	0.01	-0.00
40.0	9.99	5.17	2.63	1.45	0.79	0.27	0.24	0.14	0.14	-0.12	-0.01	-0.01
45.0	6.75	3.33	1.70	0.86	0.54	0.42	0.26	0.00	-0.07	-0.01	-0.01	-0.01
50.0	4.56	2.30	1.13	0.51	0.21	0.19	0.02	0.09	0.10	0.01	0.01	0.00
55.0	2.98	1.55	0.84	0.30	0.24	0.19	0.20	0.15	-0.13	-0.01	0.00	0.01
60.0	2.04	1.05	0.52	0.24	0.08	0.12	-0.07	0.05	-0.08	0.00	-0.01	-0.01
65.0	1.48	0.87	0.53	0.36	0.22	0.10	0.12	0.12	-0.09	-0.01	0.01	-0.01
70.0	0.76	0.36	0.34	0.25	0.18	0.15	-0.01	0.12	-0.08	-0.01	-0.01	-0.01
75.0	0.66	0.24	0.11	0.03	-0.02	-0.04	0.14	0.14	0.01	-0.01	-0.01	-0.01
80.0	0.47	0.07	0.13	0.02	0.19	0.02	-0.05	0.14	0.14	-0.02	-0.01	0.01
85.0	0.12	0.23	0.19	0.21	-0.13	0.10	0.01	-0.11	-0.16	0.01	-0.02	-0.00
90.0	0.18	0.02	0.02	-0.08	-0.05	0.09	-0.07	0.17	-0.12	-0.01	-0.02	-0.00
95.0	-0.04	0.03	0.09	-0.13	0.14	-0.11	0.05	-0.03	-0.00	-0.01	-0.01	0.00
100.0	0.13	0.00	0.15	0.04	0.03	0.15	-0.05	0.00	-0.01	0.01	-0.01	0.01
105.0	-0.00	-0.06	0.04	0.03	0.17	0.12	-0.00	0.00	0.02	0.01	-0.00	-0.00
110.0	0.05	-0.04	-0.10	-0.12	0.10	-0.01	0.00	-0.01	-0.01	-0.01	-0.01	0.01

Continuation of Table SM-7.1.2.

$\frac{p}{\text{MPa}}$	T / K						
	253.15	255.65	258.15	260.65	263.15	265.65	268.15
115.0	-0.08	0.03	0.14	-0.05	0.02	0.01	-0.00
120.0	0.15	0.00	0.16	-0.01	0.00	-0.01	-0.01
125.0	-0.16	-0.07	0.01	0.00	0.01	-0.02	-0.01
130.0	-0.07	0.00	-0.01	0.00	-0.01	-0.01	0.01
135.0	0.02	0.00	-0.01	0.01	-0.01	0.00	-0.01
140.0	0.00	0.00	-0.01	0.00	0.00	-0.02	0.00
145.0	-0.00	-0.01	0.01	-0.01	0.00	0.00	-0.01
150.0	-0.01	-0.00	-0.01	-0.02	0.01	-0.01	-0.00
155.0	0.01	0.01	-0.01	0.02	0.01	-0.01	0.02
160.0	0.00	-0.00	-0.01	-0.01	0.00	0.00	-0.01
165.0	0.01	0.01	0.00	0.02	-0.01	0.00	0.01
170.0	-0.01	-0.01	-0.00	0.01	-0.01	0.02	0.00
175.0	-0.01	-0.02	-0.01	-0.01	0.01	0.01	-0.01
180.0	0.01	-0.02	-0.01	0.01	0.01	0.01	-0.01
185.0	-0.02	0.01	0.00	-0.00	0.00	-0.02	0.01
190.0	0.01	-0.00	0.00	0.01	-0.00	0.00	-0.01
195.0	0.01	0.02	0.01	-0.01	-0.02	0.01	0.01
200.0	-0.01	0.01	-0.01	0.01	-0.02	0.01	-0.01
205.0	0.02	-0.01	0.01	0.00	0.00	-0.00	0.02
210.0	-0.01	0.01	-0.00	-0.01	0.01	-0.00	-0.01
215.0	-0.00	-0.01	0.01	-0.01	0.02	0.02	0.00
220.0	-0.00	0.01	0.01	-0.00	0.02	0.01	0.01
225.0	-0.01	0.00	0.01	0.00	-0.02	0.01	-0.01
230.0	-0.01	-0.01	-0.01	-0.01	-0.02	0.02	0.00
235.0	0.02	-0.01	0.01	-0.00	-0.01	-0.02	0.01
240.0	-0.01	-0.00	0.01	0.01	-0.00	0.02	-0.01
245.0	-0.01	0.00	-0.00	-0.01	-0.00	-0.02	0.02
250.0	0.02	-0.00	-0.00	0.02	-0.01	0.02	-0.01

Continuation of Table SM-7.1.2.

$\frac{p}{\text{MPa}}$	T / K						
	253.15	255.65	258.15	260.65	263.15	265.65	268.15
255.0	-0.02	0.02	-0.02	-0.00	-0.01	0.01	0.02
260.0	-0.02	-0.00	0.02	-0.00	-0.02	-0.00	-0.02
265.0	0.02	-0.01	0.00	0.01	-0.01	-0.00	0.02
270.0	0.02	-0.02	-0.01	0.00	0.01	-0.02	0.01
275.0	-0.01	-0.02	-0.02	0.02	-0.00	0.02	-0.01
280.0	0.00	-0.00	0.02	-0.01	-0.01	0.02	-0.00
285.0	-0.01	-0.01	-0.00	-0.01	-0.01	0.02	-0.00
290.0	0.01	-0.00	0.01	-0.01	0.02	0.00	-0.01
295.0	-0.01	-0.01	0.01	-0.00	0.01	-0.02	0.02
300.0	-0.02	0.02	0.01	0.01	-0.01	0.00	-0.02
305.0	-0.02	-0.02	0.01	-0.01	0.01	-0.01	0.00
310.0	-0.00	-0.01	-0.01	0.02	-0.00	-0.02	-0.00
315.0	0.02	0.01	-0.02	0.01	-0.01	0.00	-0.01
320.0	-0.01	0.02	-0.01	-0.00	0.00	0.00	-0.01
325.0	0.00	0.00	-0.00	0.00	0.00	-0.00	0.00
330.0	0.00	-0.00	0.00	-0.00	0.00	-0.00	0.00
335.0	0.00	-0.00	0.00	0.00	-0.00	0.00	-0.00
340.0	0.00	-0.00	-0.00	0.00	-0.00	-0.00	0.00
345.0	-0.00	0.00	0.00	0.00	0.00	0.00	-0.00
350.0	-0.00	-0.00	0.00	0.00	-0.00	0.00	-0.00
355.0	-0.00	0.00	0.00	0.00	-0.00	0.00	-0.00
360.0	-0.00	0.00	0.00	0.00	0.00	-0.00	0.00
365.0	0.00	0.00	0.00	-0.00	0.00	0.00	0.00
370.0	-0.00	-0.00	0.00	-0.00	0.00	-0.00	0.00
375.0	-0.00	-0.00	0.00	0.00	-0.00	0.00	0.00
380.0	0.00	-0.00	0.00	-0.00	0.00	0.00	-0.00

Continuation of Table SM-7.1.2.

$\frac{p}{\text{MPa}}$	T / K						
385.0	253.15	255.65	258.15	260.65	263.15	265.65	268.15
385.0	0.00	-0.00	0.00	0.00	0.00	-0.00	0.00
390.0	0.00	-0.00	0.00	-0.00	0.00	-0.00	0.00
395.0	0.00	0.00	-0.00	0.00	-0.00	0.00	-0.00
400.0	-0.00	0.00	-0.00	-0.00	0.00	0.00	-0.00

Table SM-7.1.3. As Table [SM-7.1.1](#), but for $0.1 \leq p/\text{MPa} \leq 1000$ and $235.15 \leq T/\text{K} \leq 303.15$.

p/MPa	T/K			
	273.15	293.15	298.15	303.15
0.1	0.79	-0.10	-0.13	0.05
50.0	0.10	0.01	0.01	0.00
100.0	-0.01	0.01	-0.01	0.01
150.0	-0.00	-0.01	-0.01	-0.01
200.0	0.01	-0.01	-0.01	-0.01
250.0	0.01	-0.01	-0.02	0.01
300.0	-0.02	0.00	-0.00	-0.00
350.0	-0.00	-0.00	0.00	0.00
400.0	-0.00	-0.00	-0.00	0.00
450.0	0.00	-0.00	-0.00	0.00
500.0	-0.00	0.00	-0.00	-0.00
550.0	-0.00	0.00	-0.00	-0.00
600.0	-0.00	0.00	-0.00	0.00
650.0	0.00	0.00	0.00	0.00
700.0	-0.00	0.00	0.00	-0.00
750.0	-0.00	0.00	-0.00	-0.00
800.0	-0.00	-0.00	0.00	-0.00
850.0	0.00	-0.00	-0.00	0.00
900.0	0.00	-0.00	0.00	0.00
950.0	-0.00	0.00	-0.00	-0.00
1000.0	-0.00	0.00	-0.00	0.00

Table SM-7.1.4. As Table SM-7.1.1, but for $200 \leq p/\text{hPa} \leq 1000$ and $235.15 \leq T/K \leq 300.15$.

T/K	p/hPa						200
	1000	900	800	700	600	500	
235.15	172494.11	172684.18	172874.63	173065.06	173255.86	173446.84	173638.00
240.15	19923.63	19942.33	19961.02	19979.90	19998.77	20017.41	20036.25
245.15	3096.52	3099.25	3101.81	3104.41	3107.06	3109.77	3112.29
250.15	572.97	573.37	573.85	574.42	574.82	575.31	575.64
255.15	119.34	119.46	119.59	119.47	119.60	119.73	119.87
260.15	26.97	27.21	27.03	27.22	27.27	27.17	27.18
265.15	6.54	6.59	6.56	6.47	6.57	6.59	6.54
270.15	1.72	1.58	1.71	1.82	1.63	1.71	1.78
275.15	0.31	0.57	0.58	0.33	0.40	0.50	0.34
280.15	0.09	0.05	0.08	0.18	0.05	-0.01	0.01
285.15	-0.10	-0.01	0.18	0.17	-0.03	0.17	0.17
290.15	0.13	-0.12	0.08	0.10	-0.06	-0.09	0.02
295.15	-0.13	-0.02	-0.08	0.03	-0.03	0.07	0.02
300.15	-0.14	-0.03	-0.06	0.09	0.09	-0.04	0.00

¹⁵⁴ **SM-7.2 Thermal Expansivity**

Table SM-7.2.1. Deviation, $(\alpha_p - \alpha_{p,\text{num}}) / (10^{-4} \text{ K}^{-1})$, of the thermal expansivity α_p using the analytically determined low-density water fraction from the thermal expansivity $\alpha_{p,\text{num}}$ using the numerically determined low-density water fraction for $0.1 \leq p/\text{MPa} \leq 600$ and $245.5 \leq T/\text{K} \leq 288.0$.

p MPa	T/K					
	245.5	253.2	262.8	273.8	281.3	288.0
0.1	0.11E-02	0.68E-04	0.32E-05	0.16E-06	0.16E-07	0.65E-08
10.0	0.44E-03	0.31E-04	0.16E-05	0.81E-07	0.91E-08	0.31E-08
20.0	0.17E-03	0.14E-04	0.79E-06	0.49E-07	0.11E-07	0.14E-07
30.0	0.67E-04	0.59E-05	0.39E-06	0.24E-07	0.24E-07	-0.12E-07
40.0	0.26E-04	0.25E-05	0.18E-06	-0.14E-07	-0.52E-08	-0.84E-09
50.0	0.99E-05	0.10E-05	0.11E-06	-0.15E-07	-0.23E-07	0.98E-09
60.0	0.38E-05	0.47E-06	0.17E-07	0.16E-07	-0.29E-07	0.24E-08
70.0	0.15E-05	0.23E-06	0.20E-08	-0.35E-08	0.30E-07	-0.25E-08
80.0	0.54E-06	0.71E-07	0.10E-07	0.49E-08	-0.11E-08	0.14E-08
90.0	0.21E-06	0.70E-08	0.35E-07	0.27E-07	0.18E-08	-0.48E-09
100.0	0.12E-06	0.43E-07	-0.13E-08	-0.18E-09	-0.82E-09	0.24E-09
110.0	0.21E-07	-0.24E-07	-0.18E-08	0.12E-08	-0.19E-08	-0.24E-08
120.0	0.26E-07	-0.11E-07	0.25E-08	0.22E-08	0.68E-09	0.14E-09
130.0	-0.21E-09	-0.18E-07	0.77E-10	-0.96E-09	0.21E-09	-0.17E-08
140.0	0.73E-08	0.92E-09	-0.77E-10	-0.22E-08	0.71E-09	-0.20E-08
150.0	0.18E-08	0.19E-08	-0.80E-09	0.47E-10	0.25E-08	0.80E-09
160.0	-0.42E-09	-0.15E-09	-0.26E-08	-0.20E-08	-0.19E-08	0.25E-08
170.0	-0.18E-08	0.18E-08	-0.21E-08	0.23E-08	-0.24E-08	0.22E-08
180.0	0.22E-08	-0.32E-09	-0.20E-08	-0.22E-08	-0.26E-08	-0.19E-09
190.0	-0.13E-08	0.18E-08	-0.65E-09	-0.22E-09	-0.86E-09	0.11E-08
200.0	-0.38E-09	-0.13E-08	0.79E-09	-0.21E-08	0.76E-09	-0.14E-08
210.0	0.21E-08	0.33E-09	-0.16E-08	0.22E-09	0.18E-08	0.10E-09
220.0	-0.21E-08	-0.21E-08	0.16E-08	0.99E-09	0.34E-09	-0.17E-08
230.0	0.63E-09	-0.20E-08	-0.20E-08	-0.18E-08	0.13E-08	0.16E-08
240.0	-0.49E-09	0.22E-08	0.19E-08	0.61E-09	0.25E-08	0.16E-08
250.0	-0.45E-09	0.32E-09	0.19E-08	-0.57E-10	-0.77E-09	0.20E-08
260.0	-0.15E-09	0.29E-09	-0.10E-08	0.99E-10	0.68E-09	-0.68E-09
270.0	0.18E-08	0.50E-09	-0.18E-08	-0.23E-08	-0.19E-08	-0.18E-08
280.0	-0.12E-08	0.11E-08	-0.19E-08	-0.10E-08	-0.14E-08	-0.12E-08
290.0	-0.11E-08	0.15E-08	0.27E-09	-0.12E-08	-0.23E-08	-0.47E-10
300.0	0.17E-08	-0.64E-09	-0.67E-09	-0.35E-09	0.54E-10	0.43E-10
310.0	0.48E-09	-0.12E-08	-0.66E-09	-0.16E-10	0.62E-11	0.45E-10
320.0	-0.70E-09	-0.12E-08	0.22E-10	-0.24E-10	-0.50E-10	-0.29E-10
330.0	-0.38E-09	-0.51E-10	-0.38E-10	-0.52E-10	-0.43E-11	0.35E-10
340.0	-0.65E-11	-0.43E-10	0.47E-10	0.49E-10	-0.42E-10	0.38E-10
350.0	0.22E-11	0.45E-11	-0.30E-10	-0.88E-11	-0.30E-10	0.39E-11
360.0	0.69E-11	-0.31E-10	0.12E-10	-0.24E-10	-0.52E-11	0.24E-10
370.0	0.13E-10	0.13E-10	0.31E-10	0.45E-11	-0.12E-10	0.39E-11
380.0	-0.26E-10	-0.23E-10	-0.23E-10	0.17E-10	-0.28E-10	-0.31E-10
390.0	0.13E-11	-0.18E-10	0.23E-10	-0.25E-10	-0.64E-11	-0.14E-11
400.0	0.47E-11	0.19E-10	0.20E-10	0.36E-11	0.99E-11	0.32E-11
410.0	-0.68E-11	-0.12E-10	-0.18E-10	0.63E-11	0.14E-10	0.33E-11
420.0	0.15E-10	-0.16E-10	-0.77E-11	0.15E-10	-0.14E-10	-0.12E-10
430.0	-0.53E-11	-0.11E-10	-0.43E-11	0.12E-10	0.31E-11	0.10E-11
440.0	0.11E-10	0.10E-10	0.14E-10	-0.57E-11	-0.17E-10	0.88E-11
450.0	0.55E-11	0.79E-11	0.68E-11	0.68E-11	0.19E-11	0.57E-11
460.0	-0.22E-11	-0.90E-11	-0.54E-11	0.12E-10	0.10E-10	0.14E-10
470.0	0.44E-13	-0.38E-11	-0.43E-11	0.13E-10	0.81E-11	-0.10E-10
480.0	-0.32E-11	-0.86E-11	-0.12E-11	0.28E-11	-0.95E-11	0.68E-11
490.0	-0.62E-11	-0.72E-11	-0.27E-11	0.81E-11	0.10E-10	-0.11E-10

Continuation of Table [SM-7.2.1](#).

$\frac{p}{\text{MPa}}$	T/K					
	245.5	253.2	262.8	273.8	281.3	288.0
500.0	0.51E-11	-0.18E-11	-0.60E-11	-0.20E-11	-0.66E-11	0.68E-11
510.0	-0.12E-11	-0.48E-11	0.21E-11	-0.37E-11	0.41E-11	0.71E-11
520.0	0.30E-11	-0.41E-11	-0.54E-12	-0.42E-11	0.59E-11	-0.33E-11
530.0	0.29E-11	-0.34E-11	0.48E-13	-0.81E-12	0.25E-11	0.21E-11
540.0	-0.14E-11	0.34E-11	0.65E-14	0.40E-11	0.29E-11	0.34E-11
550.0	0.89E-12	0.98E-12	-0.38E-11	-0.46E-11	-0.37E-11	0.28E-11
560.0	0.14E-11	-0.24E-11	-0.32E-11	-0.98E-12	-0.44E-11	0.47E-11
570.0	-0.10E-11	-0.75E-13	-0.66E-12	-0.20E-11	-0.30E-11	0.35E-11
580.0	-0.11E-14	-0.47E-12	0.27E-12	-0.23E-11	-0.11E-11	-0.26E-11
590.0	-0.96E-12	0.21E-12	-0.16E-11	0.97E-12	0.15E-11	-0.58E-12
600.0	-0.88E-12	-0.12E-11	-0.93E-12	-0.69E-12	-0.32E-12	0.17E-11

¹⁵⁵ **SM-7.3 Compressibility**

Table SM-7.3.1. Relative deviation, $(\kappa_T - \kappa_{T,\text{num}}) / \kappa_{T,\text{num}}$ in parts per billion (ppb), of the isothermal compressibility κ_T using the analytically determined low-density water fraction from the thermal expansivity $\kappa_{T,\text{num}}$ using the numerically determined low-density water fraction for $0.1 \leq p/\text{MPa} \leq 190$ and $235.15 \leq T/\text{K} \leq 300.15$.

T/K	p/MPa					
	0.101325	10.0	50.0	100.0	150.0	190.0
235.15	-2583606.23	-868662.57	-12123.11	-86.13	-3.93	-0.25
240.15	-257131.42	-104712.54	-2534.75	-23.65	1.62	-0.25
245.15	-37519.10	-16968.92	-589.71	-6.69	0.17	-0.01
250.15	-6743.93	-3268.78	-149.13	-5.37	-0.30	-0.37
255.15	-1386.73	-705.53	-40.33	-2.79	-0.31	-0.03
260.15	-311.39	-165.93	-9.89	-2.20	0.15	0.36
265.15	-74.12	-40.47	-4.30	2.64	0.30	0.30
270.15	-20.46	-9.19	0.30	0.13	0.01	0.20
275.15	-4.39	-2.04	-0.40	0.25	-0.30	0.16
280.15	-1.45	-1.92	-0.75	-0.24	0.09	0.13
285.15	-0.36	1.46	2.08	0.07	0.00	-0.17
290.15	0.38	-1.44	1.76	0.13	0.25	-0.19
295.15	0.70	1.35	0.17	-0.01	-0.22	0.31
300.15	-1.50	0.38	-0.12	0.20	-0.12	-0.22

¹⁵⁶ SM-7.4 Isobaric Heat Capacity

Table SM-7.4.1. Relative deviation, $(\hat{c}_p - \hat{c}_{p,\text{num}}) / \hat{c}_{p,\text{num}}$ in parts per billion (ppb), of the isobaric heat capacity \hat{c}_p using the analytically determined low-density water fraction from the isobaric heat capacity $\hat{c}_{p,\text{num}}$ using the numerically determined low-density water fraction for $0.1 \leq p/\text{MPa} \leq 190$ and $235.15 \leq T/\text{K} \leq 300.15$.

T/K	p/MPa								
	0.101325	19.6	29.4	39.2	49.0	68.6	98.1	150.0	190.0
235.15	-2348083.25	-173405.05	-48054.63	-13614.26	-3938.60	-348.45	-10.17	-0.11	-0.00
240.15	-180561.64	-19872.54	-6502.75	-2131.01	-700.89	-76.96	-2.72	0.05	-0.00
245.15	-21310.20	-2984.89	-1091.15	-395.69	-142.83	-18.92	-1.09	0.01	-0.00
250.15	-3219.47	-533.75	-211.66	-83.07	-32.67	-4.87	-0.45	-0.01	-0.00
255.15	-574.24	-108.00	-45.56	-18.96	-8.24	-1.08	-0.30	-0.01	-0.00
260.15	-114.81	-24.04	-10.42	-4.96	-1.92	-0.35	-0.15	0.01	0.01
265.15	-24.87	-5.47	-2.52	-1.63	-0.60	0.20	0.06	0.01	0.01
270.15	-6.37	-1.77	-1.12	0.06	-0.27	-0.01	0.03	0.00	0.00
275.15	-1.29	-0.23	-0.34	-0.45	-0.08	-0.02	-0.01	-0.01	0.00
280.15	-0.41	0.25	0.23	-0.31	-0.33	-0.28	-0.03	0.00	0.00
285.15	-0.10	-0.11	0.34	0.04	-0.38	-0.00	0.02	0.00	-0.01
290.15	0.10	-0.17	0.37	0.01	0.12	-0.01	0.00	0.01	-0.01
295.15	0.18	-0.05	0.34	0.02	0.00	0.03	0.02	-0.01	0.01
300.15	-0.39	0.06	0.00	-0.01	-0.02	0.01	-0.00	-0.01	-0.01

Table SM-7.4.2. As Table SM-7.4.1, but for $200 \leq p/\text{hPa} \leq 1000$ and $235.15 \leq T/\text{K} \leq 300.15$.

T/K	p/hPa								
	1000	900	800	700	600	500	400	300	200
235.15	-2348501.21	-2351652.63	-2354810.49	-2357969.59	-2361135.13	-2364304.50	-2367477.70	-2370657.33	-2373838.17
240.15	-180590.11	-180791.41	-180992.64	-181195.73	-181398.75	-181599.77	-181802.65	-182007.38	-182210.10
245.15	-21312.37	-21334.25	-21354.89	-21375.87	-21397.20	-21418.86	-21439.30	-21461.65	-21482.76
250.15	-3219.34	-3221.96	-3225.06	-3228.62	-3231.30	-3234.44	-3236.69	-3239.42	-3242.61
255.15	-573.79	-574.47	-575.15	-574.62	-575.31	-576.01	-576.71	-577.42	-578.13
260.15	-114.80	-115.80	-115.05	-115.90	-116.11	-115.67	-115.73	-116.26	-116.16
265.15	-25.26	-25.46	-25.37	-25.00	-25.39	-25.49	-25.30	-25.88	-25.12
270.15	-6.14	-5.65	-6.11	-6.51	-5.85	-6.13	-6.37	-6.54	-5.65
275.15	-1.05	-1.94	-1.95	-1.10	-1.33	-1.67	-1.14	-1.69	-1.37
280.15	-0.30	-0.16	-0.25	-0.57	-0.16	0.02	-0.03	-0.30	-0.81
285.15	0.32	0.04	-0.56	-0.54	0.09	-0.53	-0.54	0.06	0.35
290.15	-0.39	0.35	-0.23	-0.29	0.19	0.27	-0.05	0.16	-0.02
295.15	0.37	0.07	0.23	-0.08	0.09	-0.22	-0.05	-0.35	-0.18
300.15	0.40	0.08	0.17	-0.26	-0.28	0.12	-0.00	0.29	0.06

157 SM-7.5 Sound Speed

Table SM-7.5.1. Relative deviation, $(w - w_{\text{num}}) / w_{\text{num}}$ in parts per billion (ppb), of the sound speed w using the analytically determined low-density water fraction from the sound speed w_{num} using the numerically determined low-density water fraction for $0.1 \leq p/\text{MPa} \leq 400$ and $253.15 \leq T/\text{K} \leq 303.15$.

p/MPa	T/K											
	253.15	255.65	258.15	260.65	263.15	268.15	273.15	278.15	288.15	293.15	298.15	303.15
0.1	821.07	404.34	201.15	101.40	51.64	14.15	3.99	0.56	0.57	-0.58	-0.80	0.31
10.0	448.92	223.04	111.30	57.55	29.48	7.95	2.86	-0.01	-0.21	-0.95	0.61	0.75
20.0	234.26	117.26	60.43	31.02	16.78	3.72	1.70	-0.38	-0.77	-0.71	0.01	-0.06
30.0	119.03	60.25	31.89	15.52	9.10	1.67	0.41	-0.19	-0.64	0.51	-0.07	-0.10
40.0	58.63	30.90	15.99	8.99	4.99	1.56	0.91	0.58	-0.99	-0.86	-0.08	-0.08
50.0	28.91	14.82	7.36	3.36	1.42	0.12	0.70	-0.97	0.25	0.05	0.10	0.01
60.0	13.87	7.19	3.63	1.70	0.60	-0.47	-0.58	-0.15	-0.00	0.02	-0.09	-0.11
70.0	5.50	2.65	2.53	1.83	1.35	-0.10	-0.62	-0.03	0.02	-0.05	-0.05	-0.05
80.0	3.58	0.52	0.98	0.13	1.48	-0.36	1.09	0.07	0.10	-0.13	-0.10	0.09
90.0	1.46	0.20	0.18	-0.68	-0.39	-0.56	-0.99	-0.01	-0.10	-0.09	-0.14	-0.00
100.0	1.06	0.02	1.31	0.31	0.24	-0.46	-0.08	0.09	0.01	0.07	-0.07	0.05
110.0	0.43	-0.39	-0.92	-1.03	0.85	0.02	-0.05	0.13	0.10	-0.08	-0.09	0.12
120.0	1.41	0.03	1.43	-0.06	-0.07	-0.06	-0.10	0.09	-0.04	0.04	0.15	0.02
130.0	-0.68	0.04	-0.05	0.02	-0.12	-0.13	-0.09	-0.08	-0.12	0.00	-0.12	0.11
140.0	0.01	0.04	-0.13	0.01	0.02	-0.11	0.11	-0.05	-0.03	0.13	0.13	0.12
150.0	-0.15	-0.03	-0.08	-0.16	0.06	-0.14	-0.02	0.14	0.15	-0.06	-0.15	-0.08
160.0	0.01	-0.05	-0.09	-0.13	-0.02	0.02	-0.05	-0.12	0.02	-0.09	0.07	0.13
170.0	-0.13	-0.13	-0.00	0.07	-0.08	0.16	0.05	-0.09	-0.17	0.09	-0.08	-0.01
180.0	0.15	-0.20	-0.14	0.06	0.11	0.14	-0.17	-0.03	0.15	0.18	-0.08	0.12

Continuation of Table SM-7.5.1.

p/MPa	T/K											
	253.15	255.65	258.15	260.65	263.15	268.15	273.15	278.15	288.15	293.15	298.15	303.15
190.0	0.15	-0.01	0.04	0.08	-0.05	0.08	-0.05	-0.01	0.03	0.15	0.10	-0.01
200.0	-0.16	0.14	-0.12	-0.16	0.14	0.10	0.11	0.10	0.20	-0.13	-0.14	-0.12
210.0	-0.07	0.16	-0.03	-0.16	0.14	-0.04	-0.03	-0.23	0.12	0.10	0.06	-0.04
220.0	-0.01	0.09	0.13	-0.03	0.24	0.09	-0.09	0.02	0.16	-0.05	0.20	-0.23
230.0	-0.15	-0.19	-0.15	-0.13	-0.17	0.20	0.01	-0.10	0.09	-0.16	-0.11	-0.02
240.0	-0.07	-0.01	0.14	0.07	-0.05	0.20	-0.12	-0.11	0.01	0.23	0.13	-0.08
250.0	0.26	-0.02	-0.00	0.21	-0.12	-0.13	0.15	-0.25	0.19	-0.09	-0.23	0.08
260.0	-0.27	-0.01	0.23	-0.04	-0.24	-0.01	-0.23	-0.03	-0.11	0.05	0.03	-0.00
270.0	0.27	-0.25	-0.09	0.06	0.17	0.17	-0.21	0.08	-0.14	0.27	-0.01	-0.00
280.0	0.07	-0.04	0.25	-0.09	-0.16	-0.04	-0.08	-0.01	-0.22	0.00	0.01	-0.00
290.0	0.16	0.15	-0.02	0.17	-0.15	0.06	-0.17	0.24	-0.01	-0.00	-0.00	-0.01
300.0	-0.26	0.31	0.15	0.14	-0.13	-0.27	-0.31	0.00	0.01	0.00	-0.00	-0.00
310.0	-0.00	-0.10	-0.10	0.27	-0.07	-0.35	0.01	0.00	-0.00	0.00	0.01	-0.01
320.0	-0.16	0.28	-0.22	-0.01	-0.01	0.01	0.00	0.01	-0.00	0.00	0.00	-0.00
330.0	0.00	-0.01	-0.01	0.01	-0.01	0.00	0.01	0.01	0.00	-0.01	-0.00	-0.00
340.0	0.01	0.00	-0.00	-0.01	0.01	-0.01	-0.01	-0.00	0.01	-0.00	-0.00	-0.00
350.0	-0.00	0.00	-0.01	0.00	0.00	0.01	-0.01	-0.01	0.00	-0.00	0.00	0.00
360.0	-0.00	-0.00	0.01	0.00	0.01	-0.00	0.01	-0.01	-0.01	-0.00	0.00	0.01
370.0	-0.00	-0.00	-0.01	0.00	-0.00	-0.01	0.00	-0.01	-0.01	0.00	-0.00	0.00
380.0	0.00	-0.00	0.01	-0.01	-0.00	0.00	0.01	-0.00	-0.01	-0.00	0.00	0.00
390.0	0.00	-0.00	0.01	-0.00	0.00	-0.01	0.01	0.00	0.00	-0.00	-0.00	-0.00
400.0	-0.00	0.00	-0.00	-0.00	-0.00	0.00	-0.01	-0.00	-0.00	-0.00	-0.00	0.00

Table SM-7.5.2. As in Table SM-7.5.1, but for $0.1 \leq p/\text{MPa} \leq 1000$ and $273.15 \leq T/\text{K} \leq 303.15$.

p/MPa	T/K			
	273.15	283.15	293.15	303.15
0.1	3.99	-0.37	-0.58	0.31
50.0	0.70	-0.92	0.05	0.01
100.0	-0.08	-0.04	0.07	0.05
150.0	-0.02	-0.00	-0.06	-0.08
200.0	0.11	0.12	-0.13	-0.12
250.0	0.15	-0.04	-0.09	0.08
300.0	-0.31	-0.01	0.00	-0.00
350.0	-0.01	0.00	-0.00	0.00
400.0	-0.01	-0.00	-0.00	0.00
450.0	0.01	0.00	-0.00	0.00
500.0	-0.00	-0.00	0.00	-0.00
550.0	-0.00	0.00	0.00	-0.00
600.0	-0.00	0.00	0.00	0.00
650.0	0.00	-0.00	0.00	0.00
700.0	-0.00	-0.00	0.00	-0.00
750.0	-0.00	0.00	0.00	-0.00
800.0	-0.00	0.00	-0.00	-0.00
850.0	0.00	0.00	-0.00	0.00
900.0	0.00	0.00	-0.00	0.00
950.0	-0.00	-0.00	0.00	-0.00
1000.0	-0.00	-0.00	0.00	0.00

¹⁵⁸ **SM-7.6 Gibbs Energy and Entropy**

Table SM-7.6.1. Relative deviation, $(\hat{g} - \hat{g}_{\text{num}}) / \hat{g}_{\text{num}}$ in units of parts per billion (ppb), of the specific Gibbs energy \hat{g} using the analytically determined low-density water fraction (Section 3.2) from the specific Gibbs energy \hat{g}_{num} using the numerically determined low-density water fraction for $200 \leq p/\text{hPa} \leq 1000$ and $235.15 \leq T/K \leq 300.15$.

T/K	p/hPa								
	1000	900	800	700	600	500	400	300	200
235.15	-945.79	-946.99	-948.19	-949.39	-950.60	-951.81	-953.02	-954.23	-955.45
240.15	-21.86	-21.87	-21.89	-21.90	-21.92	-21.93	-21.95	-21.96	-21.98
245.15	-0.89	-0.89	-0.89	-0.89	-0.89	-0.90	-0.90	-0.90	-0.90
250.15	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05	-0.05
255.15	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
260.15	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
265.15	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.00
270.15	0.00	0.00	0.00	-0.04	-0.00	-0.00	-0.00	0.00	-0.00
275.15	0.00	0.00	-0.00	-0.00	0.00	0.00	0.00	0.03	-0.00
280.15	0.00	-0.00	-0.00	-0.00	-0.00	0.00	-0.00	-0.00	-0.00
285.15	0.00	-0.00	-0.00	-0.00	0.00	-0.00	0.00	0.00	-0.00
290.15	-0.00	0.00	-0.00	-0.00	-0.00	-0.00	0.00	-0.00	0.00
295.15	-0.00	-0.00	-0.00	-0.00	0.00	-0.00	-0.00	0.00	0.00
300.15	-0.00	0.00	-0.00	-0.00	-0.00	0.00	-0.00	-0.00	0.00

Table SM-7.6.2. Relative deviation, $(\hat{s} - \hat{s}_{\text{num}}) / \hat{s}_{\text{num}}$ in parts per billion (ppb), of the specific entropy \hat{s} using the analytically determined low-density water fraction from the specific entropy \hat{s}_{num} using the numerically determined low-density water fraction for $200 \leq p / \text{hPa} \leq 1000$ and $235.15 \leq T / \text{K} \leq 300.15$.

T / K	p / hPa					
	1000	900	800	700	600	500
235.15	-856729.10	-857726.22	-858725.32	-859724.49	-860725.64	-861727.81
240.15	-110411.71	-110520.32	-110628.86	-110738.51	-110848.08	-110956.40
245.15	-19971.77	-19990.14	-20007.34	-20024.87	-20042.71	-20060.87
250.15	-4485.25	-4488.50	-4492.40	-4496.96	-4500.27	-4504.24
255.15	-1196.76	-1198.08	-1199.41	-1198.21	-1199.56	-1200.92
260.15	-376.89	-380.17	-377.66	-380.42	-381.08	-379.64
265.15	-149.70	-150.88	-150.34	-148.10	-150.40	-150.99
270.15	-105.74	-97.25	-105.11	-112.00	-100.59	-105.53
275.15	29.42	54.17	54.67	30.89	37.33	46.74
280.15	2.52	1.36	2.13	4.81	1.37	-0.15
285.15	-1.66	-0.21	2.90	2.81	-0.48	2.77
290.15	1.48	-1.35	0.89	1.10	-0.72	-1.02
295.15	-1.14	-0.20	-0.69	0.23	-0.26	0.65
300.15	-1.02	-0.20	-0.43	0.66	0.70	-0.32

159

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