Releases from the International Association for the Properties of Water and Steam for calculating properties of steam, ordinary and heavy water substance and seawater

A A Alexandrov¹, K A Orlov¹-² and M V Butakova¹

¹National Research University "Moscow Power Engineering Institute"
Russia, 111250 Moscow, Krasnokazarmennaya, 14
²Joint Institute for High Temperatures of the Russian Academy of Sciences
Russia, 125412 Moscow, Izhorskaya st. 13 Bd.2

Email: AlexandrovAA@mpei.ru

Abstract. An overview of the developed in recent years documents from the working group on thermophysical properties of water and steam from the International Association for the Properties of Water and Steam (www.iapws.org) is given. Not only brief description of each Formulation is given, but also information about relationship between them is provided. Most of listed documents are international and Russian state standards.

1. Introduction
The International Association for the Properties of Water and Steam (IAPWS) creating materials describing the properties of water in all its possible states. The documents developed used in all industrialized countries as international standards. The equations proposed for calculating the thermophysical properties during technical calculations in heat power engineering are considered in this article.

2. Ordinary water
The most accurate description of the thermodynamic properties of water is the equation IAPWS-95 [1], represented in the form of Helmholtz's energy as a function of the specific volume and temperature, i.e. \( A = f(v, T) \). Consequently, all other thermodynamic properties calculated through the derivatives of this quantity will be functions of the specific volume and temperature \( z = f(v, T) \). The equation is applicable in the temperature range from the melting line to 1273 K and at pressures up to 1000 MPa.

The representation of properties as a function of volume and temperature is very inconvenient for technical calculations, leads to a huge amount of iterative calculations and, accordingly, to large consumption of computer time. Therefore, for the implementation of industrial calculations, a system of equations of state IAPWS IF-97 was developed that describes the thermodynamic properties of water and steam in the pressure range up to 100 MPa for temperatures from 273 K to 1273 K and up to
50 MPa at temperatures up to 2273 K [2]. These equations are based on the data of [1] and the values calculated from them are consistent with these data within the limits of their error.

IAPWS IF-97 contains 5 basic equations for individual regions of water states (figure 1): 1 – liquid; 2 – superheated steam; 3 – near-critical states; 4 – saturation line; 5 – superheated steam. For regions 1, 2, and 5 equations have the form of the dependences of the Gibbs energy on pressure and temperature, i.e. $G = f(p, T)$, and only for region 3 the equation has the form $z = f(v, T)$. Application of equations with independent pressure, temperature variables on the form $h = f(p, T)$ substantially reduces the time for solving technical problems. However, in industrial calculations, it is often becomes necessary to determine the properties of steam for various other pairs of input parameters.

![Figure 1. Regions and equations of IAPWS IF-97](image)

For example, for calculation of the expansion in turbine stage, it is necessary to calculate the properties of the steam:

- Point 1 (start of expansion) – input parameters: pressure $p$, temperature $T$;
- Point 2 (end of adiabatic expansion) – input parameters: pressure $p$, specific entropy $s$;
- Point 3 (end of real expansion) – input parameters: pressure $p$, specific enthalpy $h$.

Therefore, IAPWS IF-97 includes a group of additional equations that allow to reduce the number of iterative calculations. Thus, for regions 1 and 2 there are equations in the form $T = f(p, s)$, as example:

$$T(p, s) = \sum_{i=1}^{20} n_i \cdot p_i \cdot (s + 2)^{i}$$  \hspace{1cm} (1)$$

and in the form $T = f(p, h)$:
\[ T(p, h) = \sum_{i=1}^{20} n_i \cdot p^{i_i} \cdot (h/2500 + 1)^{j_i} \]  

(2)

In the presence of these equations, if it is necessary to determine the properties for given \( p, s \), first the temperature is calculated from equation (1), and then all the properties from the basic equation \((p, T)\) for given region of IAPWS IF-97. The root-mean-square deviation of the temperature values calculated from the additional equations calculated from the base equations does not exceed \( \Delta T = 13.4 \text{ mK} \).

To calculate the properties of water and steam without iterations in a more complicated case with specific enthalpy and specific entropy as input parameters \((h, s)\), additional equations are given in another document [3]. This document contains equations of the form \( p = f(h, s) \) for regions 1 and 2, for example:

\[ \frac{p(h, s)}{p^*} = \left[ \sum_{i=1}^{20} n_i \cdot \left( \frac{h}{h^*} - 0.5 \right)^{i_i} \left( \frac{s}{s^*} - 1.2 \right)^{j_i} \right]^d \]  

(3)

where \( p^*, h^*, s^* \) are some constants for specific region of IAPWS IF-97.

When specifying \((h, s)\), the pressure \( p \) is first calculated from equation (3), then the temperature \( T \) is determined from equation (1) and all necessary properties are calculated from the basic equation with input parameters \((p, T)\). The use of such a calculation procedure in comparison with the 2-dimensional iteration Newton method for basic equations reduces the computer time by 20–30 times.

It should be noted that the IAPWS adopted a rule according to which the matching of quantities calculated by two different methods or by two different equations is considered satisfactory if the difference in their values does not exceed the tolerances:

\[ |v| = 0.05\%, |\Delta h| = 0.2 \text{ kJ·kg}^{-1}, |\Delta c_p| = 1\%, |\Delta s| = 0.1 \text{ kJ·kg}^{-1}·\text{K}^{-1}, |\Delta w| = 1\%. \]  

(4)

When using any additional equations, this rule is satisfied.

Additional equations necessary for non-iteration calculations also have been developed for the critical region (region 3) of the IAPWS IF-97 [4, 5]. In this area, the basic equation is represented in variables \((v, T)\). The specific volume \( v \) is extremely rarely used as an input variable in industrial calculations. Therefore, to determine it, additional equations of the form \( v = f(p, T) \) [4] are developed. The agreement of the quantities calculated by the iteration method or with the help of these equations, within the limits of: for specific enthalpy and specific entropy 0.001\%, isobaric heat capacity and sound velocity 0.01\%. Under these conditions, the error in calculating the specific volume by the additional equation should not exceed 0.001\%. To fulfill this requirement, the region 3 is divided into 20 sub-regions, each with its own equation. For a small part of the region 3 near to the critical point and determined by the parameters: temperature from 643.5 K to 650.97 K and pressure from 21.043 MPa to 22.5 MPa, 6 additional equations are used.

The additional equations for region 3 have the form

\[ \frac{v(p, T)}{v^*} = \left[ \sum_{i=1}^{N} n_i \cdot [(\frac{P}{P}) - a^i]^{I_i} \cdot [(\frac{T}{T^*}) - b^i]^{J_i} \right]^F \]  

(5)

where the constants \( v^*, p^*, T^*, N, n_i, a, b, c, d, e, I_i, J_i \) have their values for each sub-region.

In the main part of region 3, the specified requirements for the agreement of the calculated values are fulfilled. In the small near-critical part of the quantity \( \Delta v/v \) better than 0.1\% and only at pressures below 22.11 MPa this value increase to 2\%.

The use of additional equations for finding the properties of water and steam for given \((p, T)\) in region 3, in comparison with iterative calculation by the basic equation, reduces the computer time by 17 times.
Additional equations for region 3 are also developed to provide the possibility of carrying out non-iterative computation of properties for given values of \((p, h)\) and \((p, s)\) \([5]\). For this purpose, equations of the form and \(T(p, h)\), \(v(p, h)\) and \(T(h, s)\) and \(v(p, s)\). Calculations showed that in order to achieve consistency of the values of properties calculated by the two methods within the limits of the tolerances \((4)\), the errors in determining the temperature and the specific volume from these additional equations should not exceed \(\Delta T = 25 \text{ mK}, \Delta v/v = 0.01\%\). To fulfill these conditions, region 3 had to be divided into two subregions, each of which uses its own equations, but of the same structure

\[
\frac{T(p, h)}{T^*} = \sum_{i=1}^{N} n_i \cdot \left(\frac{p}{p^*} + a\right)^{\eta_i} \cdot \left(\frac{h}{h^*} - b\right)^{\eta_i}
\]  

\[
\frac{v(p, h)}{v^*} = \sum_{i=1}^{N} n_i \cdot \left(\frac{p}{p^*} + c\right)^{\eta_i} \cdot \left(\frac{h}{h^*} - d\right)^{\eta_i}
\]  

\[
\frac{T(p, s)}{T^*} = \sum_{i=1}^{N} n_i \cdot \left(\frac{p}{p^*} + e\right)^{\eta_i} \cdot \left(\frac{s}{s^*} - q\right)^{\eta_i}
\]  

\[
\frac{v(p, s)}{v^*} = \sum_{i=1}^{N} n_i \cdot \left(\frac{p}{p^*} + f\right)^{\eta_i} \cdot \left(\frac{s}{s^*} - u\right)^{\eta_i}
\]

where the constants \(v^*, p^*, T^*, N, n_i, a, b, c, d, e, q, l, u, l_i, J_i\) have their values for each subdomain. The values for the critical point parameters by these equations are accurately transferred. When calculating water properties in the variables \((p, h)\) and \((p, s)\) in the critical region, the application of additional equations of the form \((6)–(9)\) allows to reduce the computer time of calculations by 20 times.

Additional equations have also been developed for calculating the properties of water in the critical region 3 when specifying the variables \((h, s)\) \([6]\). In this case, equations of the form \(p(h, s)\) were created for the same two subregions:

\[
\frac{p_{sa}(h, s)}{p^*} = \sum_{i=1}^{N} \left(\frac{h}{h^*} - a\right)^{l_i} \cdot \left(\frac{s}{s^*} - b\right)^{l_i}
\]

\[
\frac{p^*}{p_{sa}(h, s)} = \sum_{i=1}^{N} \left(\frac{h}{h^*} - c\right)^{l_i} \cdot \left(\frac{s}{s^*} - d\right)^{l_i}
\]

These equations allow to calculate pressure values with those determined by the basic equation better than 0.01\%. Then, the same algorithm is used as in the calculations in regions 1 and 2: using the obtained pressure \(p\), the temperature is calculated from the equation \(T(p, h)(6)\) and specific volume according to the equation \(v(p, s)(9)\). Then by the basic equation \((v, T)\) used for the necessary thermodynamic property calculation: \((h, s) \rightarrow p(h, s) \rightarrow T(p, h) \rightarrow v(p, s) \rightarrow z(v, T) = z(h, s)\)

Such calculation process for given \((h, s)\) in the near-critical region in comparison with the 2-dimensional iteration over the basic equation consume computer time 11 times less.

For the boundary curves in the critical region two additional equations for the saturation pressure are used:

\[
\frac{p_{sat}(h)}{p^*} = \sum_{i=1}^{N} n_i \left(\frac{h}{h^*} - a\right)^{l_i} \cdot \left(\frac{h}{h^*} - b\right)^{l_i}
\]
The following equations are proposed for calculating the pressure in the specific entropy range \( s' (623.15 \text{ K}) \leq s \leq s'' (623.15 \text{ K}) \) and ensure a complete coincidence of the values calculated from them. Additional equations are given in [6]. Here for the specific enthalpy of water on the saturation line \( h' \) two equations of the same form are proposed, but with different coefficients. The first of them is valid at temperature from 273.15 K to 623.15 K, the second from 623.15 K to the critical temperature:

\[
\frac{p_{\text{sat}}(s)}{p} = \sum_{i=1}^{N} n_i \left( \frac{s}{s} - c \right)^i \cdot \left( \frac{s}{s} - d \right)^i
\]  

(13)

These equations accurately reproduce the values of specific enthalpy at the triple and critical points, in other states provide discrepancies not higher than \( |\Delta h_{\text{max}}| = 0.0045 \text{ kJ} \cdot \text{kg}^{-1} \).

Specific enthalpy of saturated steam \( h'' \) depending on the specific entropy is also represented by two equations. The first is applicable from the triple point to \( s = 5.85 \text{ kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1} \) and has the form

\[
\frac{h''(s)}{h'} = \exp \sum_{i=1}^{N} n_i \left( \frac{s}{s} - c \right)^i \cdot \left( \frac{s}{s} + d \right)^i
\]  

(14)

The equation (15) accurately reproduce the specific enthalpy values at the triple point, in other states the difference does not exceed \( |\Delta h_{\text{max}}| = 0.0012 \text{ kJ} \cdot \text{kg}^{-1} \). The second equation of the form

\[
\frac{h''(s)}{h'} = \left[ \sum_{i=1}^{N} n_i \left( \frac{s}{s} - a \right)^i \cdot \left( \frac{s}{s} + b \right)^i \right]^4
\]  

(16)

is valid in the specific entropy range from \( s = 5.85 \text{ kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1} \) to the value of specific entropy at the critical point \( s_c = 4.412 \text{ kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1} \) and ensures matching of the calculated quantities with a discrepancy of not more than \( |\Delta h_{\text{max}}| = 0.0073 \text{ kJ} \cdot \text{kg}^{-1} \). When using these equations in determining the region in which the given states fall for different input parameters, the computer time decreases by a factor of 60.

The thermodynamic properties of water and steam on boundary lines at temperatures from the temperature of the triple point to 623.15 K (or at pressures up to 16.53 MPa) for any variables other than \((h, s)\) are calculated using the basic equations of region 4 and basic equations of regions 1 and 2. For calculations with the specification of \((h, s)\) in [6], an additional equation is proposed that is applicable in the region \( s \geq s'' (T = 623.15 \text{ K}) \) (figure 2).

\[
\frac{T(h, s)}{T''} = \sum_{i=1}^{N} n_i \left( \frac{h}{h'} - 0.119 \right)^i \cdot \left( \frac{s}{s'} - 1.07 \right)^i
\]  

(17)

The maximum deviation of the saturation temperature values calculated from this equation, calculated from the base one, is \( |\Delta T_{\text{max}}| = 0.86 \text{ mK} \). Next, pressure is calculated by using \( p_{\text{sat}} = f(T_{\text{sat}}) \) and all the necessary properties are calculated from the basic equations of regions 1 and 2. Calculating, for example, the degree of dryness of the steam \( x \) using equation (13) requires 11 times less computer time than by iteration and is characterized by discrepancies with the results of the exact calculation less than \( |\Delta x_{\text{max}}| = 0.64 \cdot 10^{-6} \).
Summarizing the results of considering additional equations of the IAPWS-IF97 system, we can show the following diagram on figure 3.

**Figure 2.** Division of region 3 into two subregions 3a and 3b for the backward equations $T(p,h)$, $v(p,h)$ and $T(p,s)$, $v(p,s)$
The use of these additional equations makes it possible to considerably reduce the computing time for carrying out industrial calculations.

Among other materials developed by IAPWS on the thermal properties of water and steam, the most important for heat power engineering are the equations for dynamic viscosity and thermal conductivity.

The dynamic viscosity of water and steam [6] is represented by a single equation applicable in a wide range of parameters:

- \( p \leq 1000 \text{ MPa for } 273.15 \text{ K} \leq T \leq 373.15 \text{ K} \)
- \( p \leq 500 \text{ MPa for } 273.15 \text{ K} \leq T \leq 433.15 \text{ K} \)
- \( p \leq 350 \text{ MPa for } 273.15 \text{ K} \leq T \leq 873.15 \text{ K} \)
- \( p \leq 300 \text{ MPa for } 273.15 \text{ K} \leq T \leq 1173.15 \text{ K} \)

The equation has the form

\[
\bar{\mu} = \frac{\mu}{\mu^*} = \bar{\mu}_0(\tau) \cdot \bar{\mu}_1(\tau, \delta) \cdot \bar{\mu}_2(\tau, \delta)
\]  
(18)

where \( \mu^* = 1.00 \cdot 10^{-6} \text{ Pa}\cdot\text{s} \); \( \tau = T/T^* \); \( T \) is the absolute temperature, \( \text{K} \); \( T^* = 647.096 \text{ K} \); \( \delta = \rho / \rho^* \); \( \rho \) is the density, \( \text{kg} \cdot \text{m}^{-3} \); \( \rho^* = 322.0 \text{ kg} \cdot \text{m}^{-3} \).

Here \( \bar{\mu}_0 = \frac{\mu_0}{\mu} \); \( \mu_0 \) – dynamic viscosity of steam in the limit of zero density

\[
\bar{\mu}_0(\tau) = \frac{100 \cdot \tau^{0.5}}{\sum_{i=0}^{3} H_i^j \cdot \tau^i}
\]  
(19)

And for the main part of the field of equation application:

\[
\bar{\mu}_1(\tau, \delta) = \exp\left[ \delta \cdot \sum_{i=0}^{5} \sum_{j=0}^{6} H_{i,j} \left( \frac{1}{\tau} - 1 \right)^i \left( \delta - 1 \right)^j \right]
\]  
(20)

where the density \( \rho \) is calculated by the equation IAPWS 95 [1].

Component \( \bar{\mu}_2(\tau, \delta) \) of equation (18) represent anomalous behaviour of dynamic viscosity and contributes more than 2% only in a small region near the critical point determined by the parameters \( 645.91 \text{ K} < T < 650.77 \text{ K} \), \( 245.8 \text{ kg} \cdot \text{m}^{-3} < \rho < 405.3 \text{ kg} \cdot \text{m}^{-3} \). According to [7], technical calculations can be use value \( \bar{\mu}_2(\tau, \delta) = 1 \), and the density values necessary for computations according to (16) can be determined from the IAPWS-IF97 [2], since the changes in the viscosity values caused by this change nowhere exceed the established tolerances.

The uncertainty of the dynamic viscosity values calculated from equation (18) is shown in figure 4.

A single equation [7] for a wide range of parameters was created for the thermal conductivity of water and steam. This region is defined by the following parameters

\[
0 < p < p_{\text{triple}} \text{ at } 273.16 \text{ K} \leq T \leq 1173.15 \text{ K}
\]

\[
p_{\text{triple}} \leq p \leq 100 \text{ MPa at } T_{\text{melt}}(p) \leq T \leq 1173.15 \text{ K}
\]
100 MPa < \( p \leq 250 \) MPa at \( T_{\text{melt}}(p) \leq T \leq 874 \) K
250 MPa < \( p \leq 687 \) MPa at \( T_{\text{melt}}(p) \leq T \leq 573 \) K
687 MPa < \( p \leq 785 \) MPa at \( T_{\text{melt}}(p) \leq T \leq 403 \) K
785 MPa < \( p \leq 1000 \) MPa at \( T_{\text{melt}}(p) \leq T \leq 348 \) K

Here \( T_{\text{melt}}(p) \) is the melting point of ice at a pressure \( p \) and \( p_{\text{triple}} \) is the pressure at the triple point of water.

The uncertainty of the dynamic viscosity

![Figure 4](image-url)

The structure of the equation is similar to the structure of the equation for dynamic viscosity

\[
\tilde{\lambda} = \tilde{\lambda}_0(T) \times \tilde{\lambda}_1(T, \rho) + \tilde{\lambda}_2(T, \rho)
\]  

(21)
where \( \tilde{\lambda}_0(T) \) is the coefficient of thermal conductivity of steam in a dilute-gas limit; \( \tilde{\lambda}_1(T, \bar{\rho}) \) – factor that represents the contribution to thermal conductivity due to finite density; the additive contribution \( \tilde{\lambda}_2(T, \bar{\rho}) \) represents the critical enhancement of the thermal conductivity.

Equations for components from (21) have the form

\[
\tilde{\lambda}_0(T) = \frac{\sqrt{T}}{\sum_{k=0}^{4} L_k}
\]

\[
\tilde{\lambda}_1(T, \bar{\rho}) = \exp \left[ \bar{\rho} \sum_{j=0}^{4} \left( \frac{1}{T} - 1 \right)^j \sum_{j=0}^{4} L_j (\bar{\rho} - 1)^j \right]
\]

Here the thermal conductivity \( \tilde{\lambda} = \frac{\tilde{\lambda}}{\tilde{\lambda}^*} \), where \( \tilde{\lambda}^* = 10^{-3} \text{ W·K}^{-1}·\text{m}^{-1} \).

The third component of equation (21) used in calculating the coefficient of thermal conductivity in the near-critical region, where in critical point the value of the thermal conductivity increases to infinity. The ranges of the parameters in which its contribution is an essential quantity are shown in figure 5.

![Figure 5](image)

**Figure 5.** The boundaries of the parameter regions, where the contribution of the near-critical component in the total value of the thermal conductivity exceeds 5%, 1%, 0.5%, 0.1%.

Function \( \tilde{\lambda}_2(T, \bar{\rho}) \) is defined in the entire range of application of equation (21) as
\[
\tilde{\lambda}_2(T, \rho) = \lambda \frac{\partial c_p}{\partial T} Z(y)
\]  

(24)

For calculation of (24) the dynamic viscosity \(\mu\) is calculated by (18), and the isobaric heat capacity \(c_p\), the density \(\rho\) and its derivatives needed to determine the function \(Z(y)\), should be calculated using the equation IAPWS-95 [1]. An estimate of the uncertainty in the values of the thermal conductivity, calculated from (21), is shown in figure 6.

For the technical calculations carried out in the field of parameters \(p \leq 100\) MPa for \(273.15 \leq T \leq 1073.15\) K, \(p \leq 50\) MPa for \(1073.15 \leq T \leq 1173.15\) K it is possible to calculate the density and its derivatives using IAPWS-IF97 system equations. The only substitution is the use of an additional equation for \(\zeta\) used in the determination of the function \(Z(y)\):

\[
\zeta(T, \rho) = \frac{1}{\sum_{j=0} A_{ij} \cdot \rho^j}
\]  

(25)

The uncertainty estimate of the calculated thermal conductivity values coincides with the values shown in figure 5, with the exception of a narrow region immediately near to the critical point.

3. Sea water

Until 2010, a set of International EOS-80 equations, representing individual properties in function of temperature, pressure and salinity, expressed in units of the Practical Salinity Scale of 1978 (PPS-78) was used to describe the thermodynamic properties of sea water [8]. In 2010, the Intergovernmental Oceanographic Commission adopted the document TEOS-10 [8], replacing EOS-80 with the IAPWS-
developed equation for Gibbs energy from which thermodynamically consistent expressions can be obtained for all other properties of sea water. In this case, the absolute salinity of $S_A$ [9] is used to characterize the concentration of solute $s$ [9]. Absolute salinity refers to the mass fraction of dissolved salts in seawater $S_A \text{ kg kg}^{-1}$.

The relationship between the different salinity scales can be established on the basis that the salinity of the standard mean oceanic water (SMOW) at 14.996 °C (ITS-90) and $p_0 = 0.101325 \text{ MPa}$ on a practical scale is $S_p = 35$, and absolute salinity at the same parameters $S_A = 0.03516504 \text{ kg kg}^{-1}$. Hence,

$$S_p = 0.03516504/35 = 1.004715 \cdot 10^{-3} \text{ kg kg}^{-1} \quad (26)$$

The equation of state of sea water [10] is represented in the form of the Gibbs energy $G = f(S, T, p)$, which is composed of Gibbs energies of pure water and dissolved substances

$$g(S, T, p) = g^W(T, p) + g^S(S, T, p) \quad (27)$$

The Gibbs energy of pure water, $g^W(T, p)$, should be calculated from the equation of state IAPWS-95 [1], and the Gibbs energy of salts in the above form is represented by the expression

$$g^S(S, T, p) / g^* = \sum_{k=0}^{5} \sum_{j=0}^{6} \left( g_{jkb} \cdot \xi^2 \cdot \ln \xi + \sum_{i=2}^{7} g_{ijk} \xi^j \right) \cdot \tau^k \cdot \pi^k \quad (28)$$

Here $g^* = 1 \text{ kJ kg}^{-1}$, $\tau = (T - T_0)/T^*$, $T_0 = 273.15 \text{ K}$, $T^* = 40 \text{ K}$, $\pi = (p - p_0)/p^*$, $p_0 = 0.101325 \text{ MPa}$, $p^* = 10^3 \text{ Pa}$, $\xi = \sqrt{S / S^*}$, $S^* = 0.040188617 \text{ kg kg}^{-1}$. Equations for other thermodynamic properties of sea water are derived from equation (27).

The range of validity of the equation (27) is determined by the parameters $0 \leq S \leq 0.12 \text{ kg kg}^{-1}$, $261 \text{ K} \leq T \leq 353 \text{ K}$, $0 < p \leq 100 \text{ MPa}$ and includes the entire area of existence of the water of the World Ocean (Neptunian region): $0 \leq S \leq 0.042 \text{ kg kg}^{-1}$, $T_f \leq T \leq 313 \text{ K}$, $0.101325 \text{ MPa} \leq p \leq 100 \text{ MPa}$, where $T_f$ is the freezing temperature.

The uncertainties of the quantities calculated by (27) vary significantly depending on the range of parameters. So for the main region $0.005 \leq S \leq 0.042 \text{ kg kg}^{-1}$, $273 \text{ K} \leq T \leq 313 \text{ K}$, the relative uncertainty of the density at a pressure of $p = 0.1 \text{ MPa}$ is $4 \cdot 10^{-6}$, and at a pressures up to $100 \text{ MPa}$ – $1 \cdot 10^{-5}$. The uncertainty of the isobaric heat capacity in this region at a pressure $p = 0.1 \text{ MPa}$ is $0.5 \text{ J kg}^{-1} \text{ K}^{-1}$, and at the same pressure for all temperature and salinity range is $4 \text{ J kg}^{-1} \text{ K}^{-1}$.

Calculation of the Gibbs energy of pure water at given temperature and pressure $g^W(T, p)$ in (23) using the equation of state IAPWS-95 [1], as provided in [10], leads to large computer time. This is due to the fact that equation from [1] has the form of the Helmholtz free energy with input variables temperature and specific volume. And calculations for the given variables temperature and pressure $(p, T)$ requires a large number of iterations. Therefore, IAPWS, in conjunction with the International Ocean Physical Sciences Association (IAPSO) Working Group No. 127, has developed an equation $g^W(T, p)$ for pure water in oceanographic studies [11]. The equation has the form

$$g^W(T, p) / g^* = \sum_{j=0}^{7} \sum_{k=0}^{6} g_{jkb} \cdot \tau^j \cdot \pi^k \quad (29)$$

and is valid for the parameter range $100 \text{ Pa} \leq p \leq 1000 \text{ Pa}$ $T_f \leq T \leq 313.15 \text{ K}$ where $T_f = (270.15 - p \cdot 7.43 \cdot 10^{-8} \text{ Pa} \cdot \text{K})$. The change in the values of the thermodynamic properties caused by the replacement of the equation IAPWS-95 by equation (29) is slightly less than the established tolerances, and its usage significantly reduces computer computation time.

The problem of computer time is also relevant for industrial calculations of processes with sea water. Therefore, in [13] in (23) proposed for calculation the properties of pure water use IAPWS-IF-97 [2] region 1 equation except equation from IAPWS-95 [1]. The analysis performed in [13] showed
that such a replacement does not lead to an increase in the uncertainty of the computed values, and the calculation time is reduced by more than 100 times. The results of calculating the change in the temperature of phase transitions (boiling and freezing) are also presented in [13], with an increase in the salinity of sea water. It should be noted that an increase in salinity to 0.012 kg·kg$^{-1}$ at atmospheric pressure leads to decreasing for 8 K of the freezing point.

Among all other thermophysical properties of sea water, recommendations have so far been developed only for thermal conductivity [14]. An equation has been created that corresponds to the thermal conductivity of ordinary water [7]:

\[
(\lambda - \lambda_w) / \lambda_0 = a \cdot (1000 \cdot S)^{1+b}
\]

here \(a = a_1 \cdot \exp [a_2 \cdot (T - T_0) / 1 \cdot K] \); \(b = b_1 \cdot \exp [b_2 \cdot (T - T_0) / 1 \cdot K] \); \(\lambda_0 = 1 \text{ W m}^{-1} \text{ K}^{-1}, T_0 = 273.15 \text{ K}; a_n \) and \(b_n \) – linear functions on pressure. Thermal conductivity of ordinary water \(\lambda_w\) is calculated from equation (21).

The equation is applicable in the range of parameters \(273.15 \leq T \leq 313.1, 0 \leq S \leq 0.017 \text{ kg kg}^{-1}, 0 \leq p \leq 140 \text{ MPa}\).

The uncertainty of calculated values of thermal conductivity is estimated by 0.44%.

In the whole range of parameters, the thermal conductivity of sea water is less than normal, and this decrease does not exceed 3%.

4. Heavy water (D$_2$O)

The thermodynamic properties of heavy water are represented by a single equation of state in the form of the dependence of Helmholtz's free energy as function of temperature and density [15]. This dependence is given in a dimensionless form

\[
\tilde{f}(\tilde{T}, \tilde{\rho}) = \tilde{f}_0(\tilde{T}, \tilde{\rho}) + \tilde{f}_1(\tilde{T}, \tilde{\rho})
\]

Here

\[
\tilde{f}_0(\tilde{T}, \tilde{\rho}) = (A_{00} + A_{01} \cdot \tilde{T}) \cdot \ln \tilde{T} + \sum_{j=2}^{7} A_{0j} \cdot \tilde{T}^{j-2} + A_{08} \cdot \tilde{T} \ln \tilde{\rho}
\]

\[
\tilde{f}_1(\tilde{T}, \tilde{\rho}) = \tilde{T} \cdot \tilde{\rho} \cdot (1 / \tilde{T} - 1 / \tilde{T_0}) \times \sum_{j=1}^{5} \left(1 / \tilde{T} - 1 / \tilde{T_0}\right)^{j-2} \cdot \sum_{j=1}^{8} A_{ij} \cdot (\tilde{\rho} - \tilde{\rho}_i)^{-1} + \exp (-1.5394 \cdot \tilde{\rho}) \cdot \sum_{j=9}^{10} A_{ij} \cdot \tilde{\rho}^{j-9}\]

where \(\tilde{f} = f / f^*, \quad f^* = \rho^* / \rho^*, \quad \tilde{T} = T / T^*, \quad \tilde{\rho} = \rho / \rho^*, \quad T^* = 643.847 \text{ K}, \quad \rho^* = 358 \text{ kg m}^{-3}, \quad p^* = 21.671 \text{ MPa}\).

The equation is valid in the parameters range: 276.95 K \(\leq T \leq 800 \text{ K}, 0 \leq p \leq 100 \text{ MPa}, \) except for a small region near the critical point \(|T - T^*| \leq 10 \text{ K}, |\rho - 1| \leq 0.3\). The equation for the critical region is given in [16].

Estimates of the uncertainty of the density calculated by the equation (31) vary from 0.015% to 0.07% in the liquid region and from several hundredths of a percent at moderate steam pressures to 0.5% and higher at pressures above 50 MPa.

Along with the equation of state for thermodynamic properties, there are also equations for the dynamic viscosity and thermal conductivity [17].

For dynamic viscosity, the equation has a form similar to that for the dynamic viscosity of ordinary water, but without a term corresponding to the critical region:

\[
\tilde{\mu}(\tilde{T}, \tilde{\rho}) = \tilde{\mu}_0(\tilde{T}) \cdot \tilde{\mu}_1(\tilde{T}, \tilde{\rho}),
\]
Where $\bar{\mu} = \frac{\mu}{\mu'}$, $\mu' = 55.2651$ mPa s, and the factors $\bar{\mu}(\bar{T})$ and $\bar{\mu}(\bar{T}, \bar{\rho})$ have the same analytical form as for ordinary water (19) and (20). The equation is applicable in the region defined by the parameters $277 \, K \leq T \leq 775 \, K$, $0 \leq p \leq 100 \, MPa$. Uncertainty of calculated values of viscosity is estimated at 1% for liquid, 2% in the main steam region, and increases to 5% in near-critical region. Immediately near the critical point in the temperature range $0.995 \leq \bar{T} \leq 1.005$ and densities $0.9 \leq \bar{\rho} \leq 1.1$ it is impossible to estimate the uncertainty, since the equation does not provide for the existence of a critical viscosity anomaly.

Thermal conductivity of heavy water is represented by the equation

$$\bar{\lambda}(\bar{T}, \bar{\rho}) = \lambda_0 + \Delta \lambda + \Delta \lambda_c + \Delta \lambda_z$$

(35)

where $\bar{\lambda} = \lambda / \lambda'$, $\lambda' = 0.742128$ mW·m⁻¹·K⁻¹. Here $\lambda_0$ is a function of temperature, and all other terms are complex functions of temperature and density. The equation (35) designed to calculate the thermal conductivity in the parameter region $277 \, K \leq T \leq 825 \, K$, $0 \leq p \leq 100 \, MPa$. Estimates of the values calculated from it are: 2% in the liquid region, and from 2% to 5% in the main steam region, and 10% in the near-critical region. Just as for viscosity, but over a wider temperature range of $0.99 \leq \bar{T} \leq 1.05$ and densities $0.8 \leq \bar{\rho} \leq 1.1$ it is impossible to give an estimate of the uncertainty immediately near the critical point, since the equation does not provide for the existence of a critical anomaly of thermal conductivity.

All equations for the thermophysical properties of heavy water created more than 30 years ago. Currently, IAPWS is working to improve them.

5. References

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