

### The International Association for the Properties of Water and Steam

## Kyoto, Japan September 2004

## Advisory Note No. 2

# **Roles of Various IAPWS Documents Concerning the Thermodynamic Properties of Ordinary Water Substance**

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This Advisory Note has been authorized by the International Association for the Properties of Water and Steam (IAPWS) at its meeting in Kyoto, Japan, 29 August to 3 September, 2004 for issue by its Secretariat. The members of IAPWS are: Britain and Ireland, Canada, the Czech Republic, Germany, Japan, New Zealand, Russia, Scandinavia (Denmark, Finland, Norway, Sweden), and the United States of America and associate members Argentina and Brazil, Australia, Egypt, France, Greece, Italy, and Switzerland. The President at the time of adoption of this document was Professor Koichi Watanabe of Japan.

This Advisory Note is reviewed annually and updated as required to reflect the issuance of new or revised IAPWS documents. Date of this revision September 2016.

#### Summary

IAPWS has issued several documents that give information on the thermodynamic properties of ordinary water substance. These documents are listed on the following pages. The first document, IAPWS-95, is considered by IAPWS to define the thermodynamic properties of water and steam. This advisory note has been prepared to explain the purpose of some of these documents, which might appear to give contradictory information. The name "ordinary water substance" is used to denote any phase or phases of water with normal naturally occurring isotopic abundances of hydrogen and oxygen. These abundances are those of Vienna Standard Mean Ocean Water as given in document 18. Other documents issued earlier by IAPWS have been superseded and are not considered in this note.

This Advisory Note contains 6 pages, including this cover page.

Further information about this Advisory Note 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.

# IAPWS documents containing information on the thermodynamic properties of ordinary water substance:

- 1. IAPWS R6-95(2016): Revised Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use. (Subsequently referred to as IAPWS-95). (Revised September 2016).
- 2. IAPWS G9-12: Guideline on a Low-Temperature Extension of the IAPWS-95 Formulation for Water Vapor. (October 2012).
- 3. IAPWS R10-06(2009): Revised Release on an Equation of State for H<sub>2</sub>O Ice Ih. (Revised September 2009).
- 4. IAPWS R7-97(2012): Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. (IAPWS-IF97). (Revised August 2007).
- 5. IAPWS AN1-03: Advisory Note No. 1: Uncertainties in Enthalpy for the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use (IAPWS-95) and the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (IAPWS-IF97). (August 2003).
- 6. IAPWS SR2-01(2014): Revised Supplementary Release on Backward Equations for Pressure as a Function of Enthalpy and Entropy p(h,s) to the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. (Revised June 2014).
- 7. IAPWS SR3-03(2014): Revised Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h) and T(p,s), v(p,s) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. (Revised June 2014).
- 8. IAPWS SR4-04(2014): Revised Supplementary Release on Backward Equations p(h,s) for Region 3, Equations as a Function of h and s for the Region Boundaries, and an Equation  $T_{\text{sat}}(h,s)$  for Region 4 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. (Revised June 2014).
- 9. IAPWS SR5-05(2016): Revised Supplementary Release on Backward Equations for Specific Volume as a Function of Pressure and Temperature v(p,T) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. (Revised September 2016).
- 10. IAPWS SR6-08(2011): Revised Supplementary Release on Properties of Liquid Water at 0.1 MPa. (Revised September 2011).
- 11. IAPWS SR7-09: Supplementary Release on a Computationally Efficient Thermodynamic Formulation for Liquid Water for Oceanographic Use. (September 2009).
- 12. IAPWS G6-03: Guideline on the Tabular Taylor Series Expansion (TTSE) Method for Calculation of Thermodynamic Properties of Water and Steam Applied to IAPWS-95 as an Example. (August 2003).

- 13. IAPWS G13-15: Guideline on the Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL). (July 2015)
- 14. IAPWS SR1-86(1992): Revised Supplementary Release on Saturation Properties of Ordinary Water Substance. (Revised September 1992).
- 15. IAPWS R14-08(2011): Revised Release on the Pressure along the Melting and Sublimation Curves of Ordinary Water Substance. (Revised September 2011).
- 16. IAPWS G12-15: Guideline on Thermodynamic Properties of Supercooled Water. (July 2015)
- 17. IAPWS R2-83(1992): Values of Temperature, Pressure and Density of Ordinary and Heavy Water Substances at their Respective Critical Points. (Revised September 1992).
- 18. IAPWS G5-01(2016): Guideline on the Use of Fundamental Constants and Basic Constants of Water. (Revised September 2016).
- 19. IAPWS AN4-09: Advisory Note No. 4: Roles of IAPWS and CIPM Standards for the Density of Water. (September 2009).
- 20. IAPWS R1-76(2014): Revised Release on the Surface Tension of Ordinary Water Substance. (Revised June 2014).

#### Notes on the listed documents and their application

a) IAPWS-95 (#1 above) is a fundamental equation of Helmholtz free energy as a function of temperature and density,  $f = f(T, \rho)$ , which yields other thermodynamic properties by differentiation and algebraic manipulation without the use of any other information. IAPWS-95 defines accurately the thermodynamic properties of the fluid phases of ordinary water substance, with complete thermodynamic consistency among these properties, over a wide range of states (pressures up to 1000 MPa and temperatures from the melting and sublimation temperatures to 1273 K). This definition of properties includes those on the liquid–vapor equilibrium line. The equation extrapolates sensibly to higher pressures and temperatures. Thus, IAPWS-95 is recommended as the source of the thermodynamic properties of water and steam. However, since the independent variables of IAPWS-95 are temperature and density, computing times for some applications may be excessive and alternatives are available as indicated below.

For the gas phase, the low-temperature limit of IAPWS-95 can be reduced from 130 K to 50 K with the low-temperature extension described in (#2).

- b) The IAPWS Revised Release on an Equation of State for Ice Ih (#3 above) defines the thermodynamic properties of the solid phase, when the ice form Ih is the equilibrium state, at temperatures below the melting and sublimation curves.
- c) IAPWS-IF97 (#4 above) is a set of equations designed to give accurate thermodynamic properties of liquid and gas with short computing times. The equations have been fitted to properties calculated from IAPWS-95 and therefore should not be considered as definitive for the thermodynamic properties. In order to achieve fast computing times, this formulation covers a smaller range of states than IAPWS-95 and this smaller range is divided into regions. Some of these regions have backward equations with different independent variables from the basic equation for the particular region. These backward equations may give directly a required property from the user's independent variables or provide a very close initial value for an iterative solution.
- d) Advisory Note No. 1 (#5 above) provides information on the uncertainties of the enthalpies obtained from IAPWS-95 and IAPWS-IF97 in addition to the information given in the releases on IAPWS-95 and IAPWS-IF97.
- e) The supplementary releases numbered 6, 7, 8, and 9 above provide additional backward equations for use with IAPWS-IF97 or for use in their own right. They are intended to reduce computing times further when using IAPWS-IF97.
- f) The supplementary release on liquid water near 0.1 MPa (#10 above), contains simple equations for thermodynamic and other properties of the liquid at or close to atmospheric pressure to save the user the task of writing code for IAPWS-95 or IAPWS-IF97. The equations for thermodynamic properties have been fitted to values generated from IAPWS-95 and they reproduce IAPWS-95 within its uncertainties.
- g) The Supplementary Release numbered 11 above is intended for use with the IAPWS Formulation 2008 for the Thermodynamic Properties of Seawater. It provides properties for pure liquid water with sufficient accuracy and has the advantage of the independent variables temperature and pressure, thus eliminating the necessity of iteration that would be required if IAPWS-95 were used. This equation was fitted to data from IAPWS-95.

- h) Tabular Taylor Series Expansion (TTSE) is a method of providing fast calculations for thermodynamic properties with an accuracy dependent on the grid size selected for the table of look-up properties used in the computation. The TTSE method can be applied to any property, with the values in the look-up table taken from an appropriate source. The guideline (#12 above), uses properties computed from IAPWS-95 for the look-up table.
- The Spline-Based Table Lookup (SBTL) is another method for providing fast, accurate, and consistent thermodynamic property calculations. It can be applied to any property formulation; the guideline (#13 above) demonstrates its application to both IAPWS-95 (#1 above) and IAPWS-IF97 (#4).
- j) The equations described in the supplementary release numbered 14 above, for the saturation properties, can be used to calculate saturation pressure, and density, specific enthalpy, and specific entropy of the coexisting liquid and vapor phases directly as a function of temperature. The range is from the triple point to the critical point. Although IAPWS-95 defines these properties, the equations from this supplementary release can be more quickly applied. The differences between a property obtained from these equations and from IAPWS-95 are generally negligible.
- k) The release for the pressures along the melting and sublimation curves (#15 above) gives, as the title indicates, equations for the pressures as functions of temperature for equilibrium between liquid water and ice Ih, ice III, ice V, ice VI, and ice VII, and for equilibrium between water vapor and ice Ih. The equations thus give the lower temperature bounds for the range of equilibrium fluid states to which IAPWS-95 applies. For the equilibria with ice Ih, the equations were fitted to values obtained by equating chemical potentials from the IAPWS-95 release for fluid water (#1 above) and that for ice Ih (#3 above), giving results that are negligibly different from those obtained from the full phase-equilibrium calculation employing IAPWS-95 and the ice Ih formulation.
- The guideline numbered 16 above provides a formulation for calculating thermodynamic properties of supercooled water. Here, "supercooled" refers to metastable liquid states where the equilibrium phase would be ice. While it is possible to calculate properties from extrapolating IAPWS-95 in most of this region, the values calculated according to this guideline are believed to be more accurate.

- m) The release on values at the critical point (#17 above) gives values recommended by IAPWS for the critical temperature, pressure, and density. These values are used as parameters in many IAPWS formulations.
- n) Document number 18 gives the recommendations of IAPWS for the best current values of fundamental physical constants of water (such as its molar mass, isotopic composition, and dipole moment). This document is reviewed (and updated if necessary) annually, so values of these constants used in older IAPWS documents may differ slightly from the latest values given in this document.
- Advisory Note No. 4 (#19 above) explains the relative roles of an equation of the CIPM (intended for use in metrology and covering a limited range of temperature) and IAPWS-95, with recommendations for the appropriate use of each.
- p) Document number 2 providing information on surface tension is included to complete the list of thermodynamic property formulations.