Fast and Accurate Calculation of Transport Properties of Water and Steam Using the Tabular Taylor Series Expansion (TTSE) Method (TTSEtrans)

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A set of computer programs and data tables of TTSE method to calculate the transport properties of water and steam has been developed. Its accuracy and computing speed were compared to those widely used in current industrial applications. The computing time was found to be half of the current method in the compressed-water and superheated-steam regions, and one-tenth in the supercritical region. The accuracy is comparable to or better than that of current method.

Nomenclature

Variables

c_p	Specific isobaric heat capacity
h	Specific enthalpy
p	Pressure
Pr	Prandtl number = $c_p\mu$ / λ
s	Specific entropy
T	Absolute temperature
v	Specific volume
z	General variable for properties
Δ	Deviation
λ	Thermal conductivity
μ	Dynamic viscosity
ρ	Density

Indices

i	Index for specific enthalpy
j	Index for pressure

Subscripts

c	Critical point
max	Maximum
rms	Root mean square
IA	Values calculated from equations specified in IAPWS releases
TT	Values calculated from TTSEtrans
97	Values calculated from IAPWS equations but IAPWS-IF97 is used as input

Introduction

The advantage of the tabular Taylor series expansion (TTSE) method is that it enables rapid calculation of properties without sacrificing accuracy. The calculations are fast since fewer numerical computations are required when tables of stored properties and their derivatives are used. The stored properties and derivatives are exactly determined from the basic equations so that the accuracy of the TTSE method depends on the grid spacing of the storage tables.

The author had developed a set of computer programs and data tables, named TTSE-95 [1], based on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use (IAPWS-95) [2]. The International Association for the Properties of Water and Steam (IAPWS) had adopted the TTSE method as an IAPWS Guideline [3].

Transport properties are key to calculations in heat transfer and fluid mechanics. Because the numerical routines for calculating transport properties are repeatedly called, its computing time is an important issue for industrial applications.

The objective of this paper is to introduce a new set of TTSE programs and data tables, named TTSEtrans, as an extension to TTSE-95 for calculating transport properties of water and steam.

Overview of TTSE-95 for Thermodynamic Properties

The basic equation in TTSE-95 is taken from IAPWS-95. Pressure p and enthalpy h are the independent variables. The computational domain ranges from 0 to 4000 kJ kg^{-1} in enthalpy and the triple point to 100 MPa in pressure. The range is divided into 200 by 200 cells by uniform spacing 20 kJ kg^{-1} in the direction of enthalpy and geometrical spacing in the direction of pressure

with the ratio of 1.06215. The cells are indexed with integers i for the direction of h, and j for the direction of p, which are defined as:

$h = 20(i - 104) + h_c$ and $p = 1.06215^{(j - 174)}p_c$,

where, h_c denotes specific enthalpy at the critical point 2084.2562631 kJ kg^{-1} and p_c denotes the critical pressure 22.064 MPa.

The primitives $T(p,h)$, $v(p,h)$, $s(p,h)$, and its (first-, second-, and cross) derivatives are evaluated at a node point in each cell. The evaluated values are stored in coefficient tables. The thermodynamic properties are calculated by quadratic equation using the stored coefficients. Special cell-finding logic is employed to achieve high computing speed. The accuracy and computing speed have been tested by IAPWS [4]. The test results on business applications for power industries, such as power cycle design and boiler transient simulation, showed that TTSE-95 is useful to reduce the computing time without sacrificing accuracy.

IAPWS Equations for Transport Properties and Calculation Method in Industrial Applications

The equation for the dynamic viscosity μ is given in Appendix A of the IAPWS release "The IAPS Formulation 1985 for the Viscosity of Ordinary Water Substance" [5]. It is represented as a function of T and ρ. To reproduce the values of $\mu(p,T)$ in Table C in the release, ρ is to be calculated from the IAPWS-95 as

$$\mu_{IA}(p,T) = \mu(T,\rho_{95}(p,T)).$$

However, its computational speed is very low because of IAPWS-95. Instead, it is a common practice to use ρ calculated from the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (IAPWS-IF97) [6] as:

$$\mu_{97}(p,T) = \mu(T,\rho_{97}(p,T)).$$

While the difference between $\mu_{IA}(p,T)$ and $\mu_{97}(p,T)$ is acceptable for general applications, the deviation is considerably large in the vicinity of the critical point. Although the computing time is reduced by IAPWS-IF97, the calculation is still time-consuming, because the equation for μ includes an exponential function.

For the thermal conductivity λ, two different equations are currently recommended by the IAPWS release "The IAPS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance, IAPWS Release"[7]. They are represented as functions of T and ρ. Both of them are widely used in industrial applications, but the equation in Appendix C is more accurate than that in Appendix B. The input value ρ for the former equation is to be calculated from the IAPWS-95, but IAPWS-IF97 is commonly used to reduce computing time with sacrifice of accuracy. The equation for λ is much more time-consuming than that for μ, because it includes three exponential functions, an exponentiation by non-integer value, and two function calls of derivatives of thermodynamic properties.

Design Concept of TTSEtrans

The aim of TTSEtrans is to reproduce the transport property values with shorter computing time, and comparable or higher accuracy relative to the common practice.

In this paper, the accuracy of TTSEtrans is evaluated by deviation Δz_{TT} as defined by

$$\Delta z_{TT} = |(z_{TT} - z_{IA})/z_{IA}|.$$

There is no established industrial requirement for the accuracy of transport properties. However, the deviations of the common practice using the IAPWS-IF97 input are good references to assess the accuracies of TTSEtrans. The reference deviation Δz_{97} is defined as

$$\Delta z_{97} = |(z_{97} - z_{IA})/z_{IA}|.$$

The deviations Δz_{TT} and Δz_{97} are evaluated in single-phase equilibrium region and not in metastable region.

As long as Δz_{TT} remains comparable to or better than the reference, the cell structure of TTSE-95 is applied to TTSEtrans. Using the common structure, TTSE-95 and TTSEtrans can compute both thermodynamic- and transport properties at a point of state without repeating the cell-finding process.

Behavior of Dynamic Viscosity and $\Delta\mu_{TT}(p,h)$

Figure 1 shows the behavior of μ on the p-h plane. It is smooth, and TTSEtrans easily simulates it. Figures 2, 3, and 4 are plots of the maximum

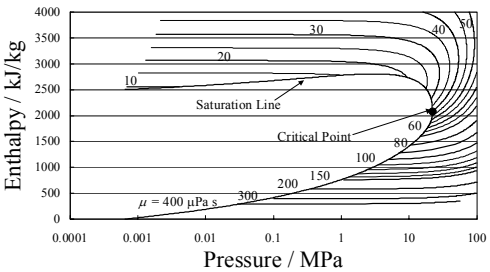

Figure 1. Dynamic viscosity on p-h plane

deviation $\Delta\mu_{TT}(p,h)$ in each cell along selected isobars. As seen, the deviations are lower than 0.1 % except in high-pressure and very low-enthalpy region where the IAPWS equation is not valid.

Behavior of Thermal Conductivity and $\Delta\mu_{TT}(p,h)$

Figure 5 shows the behavior of λ. In contrast to μ, it shows a steep peak at the critical point. Its detail is seen in Figure 6. Dotted lines in Figure 6 show the boundaries of cells and suggest that the cell size is too large to simulate the behavior by quadratic

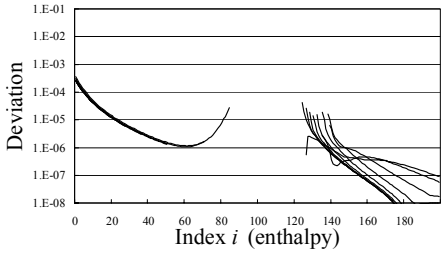

Figure 2. Maximum $\Delta\mu_{TT}$ of cells along selected isobars $p < 17.33$ MPa

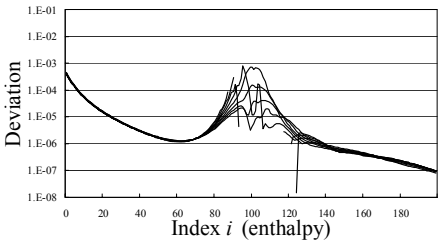

Figure 3. Maximum $\Delta\mu_{TT}$ of cells along selected isobars $17.33 \le p \le 28.08$ MPa

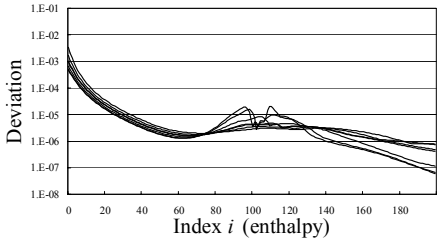

Figure 4. Maximum $\Delta\mu_{TT}$ of cells along selected isobars $28.08 < p < 100$ MPa

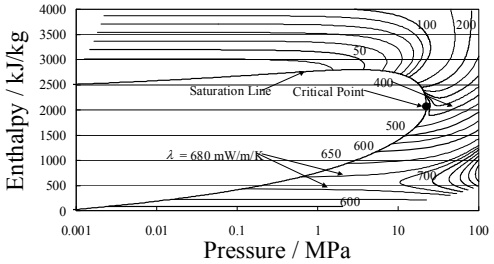

Figure 5. Thermal conductivity on *p*-*h* plane

it shows a steep peak at the critical point. Its detail is seen in Figure 6. Dotted lines in Figure 6 show the boundaries of cells and suggest that the cell size is too large to simulate the behavior by quadratic

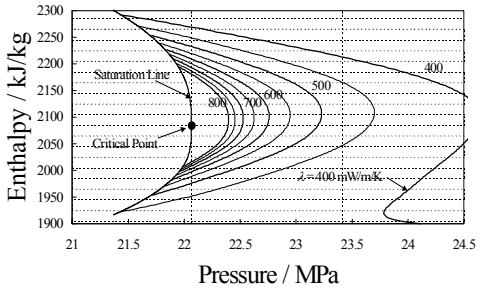

Figure 6. Thermal conductivity on *p*-*h* plane, detail of near the critical point

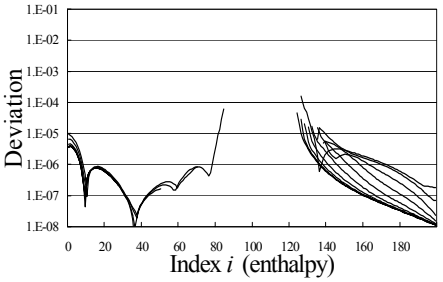

Figure 7. Maximum $\Delta\lambda_{TT}$ of cells along selected isobars $p < 17.33$ MPa

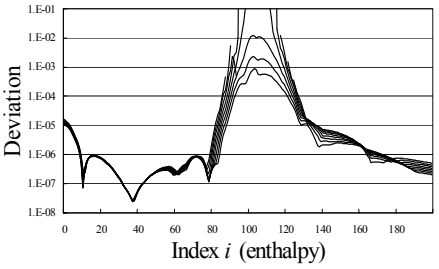

Figure 8. Maximum $\Delta\lambda_{TT}$ of cells along isobars $17.33 \le p \le 28.08$ MPa

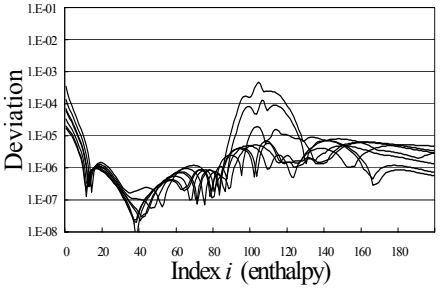

Figure 9. Maximum $\Delta\lambda_{TT}$ of cells along selected isobars $28.08 < p < 100$ MPa

TTSE function. Figures 7, 8, and 9 are plots of the maximum deviation $\Delta\lambda_{TT}(p,h)$ in each cell along selected isobars. The deviations are smaller than 0.1 % except near the critical point. Figure 10 illustrates the location of the cells where the maximum deviation exceeds 0.1 %. Figure 11 shows the detail of such cells and illustrates the grid refinement applied to TTSEtrans. The grid refinement is 101 × 101 fine mesh shown with broken line. Since it is still not sufficient, TTSEtrans directly uses the basic IAPWS equation in the region very close to the critical point. The basic equation is time-consuming but it does not degrade the average computing speed in usual commercial applications. By these countermeasures the deviation in λ is reduced to lower than 10 %.

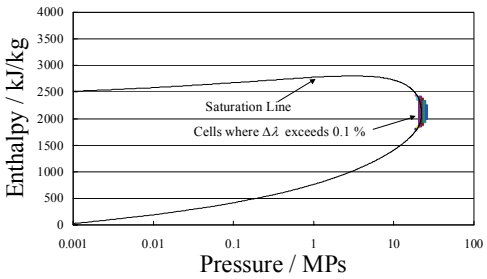

Figure 10. Cells where maximum $\Delta\lambda_{TT}$ exceeds 0.1 %

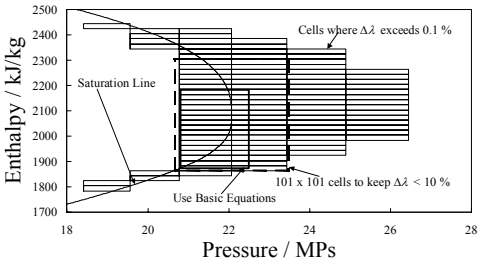

Figure 11. Countermeasures to reduce $\Delta\lambda_{TT}$ in critical region

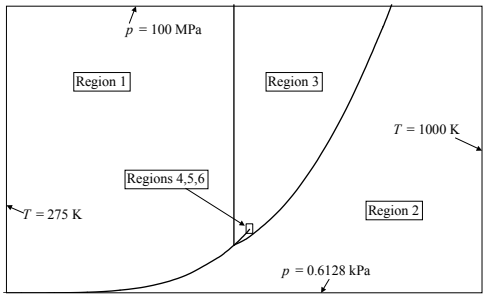

Figure 12. Definition of test regions

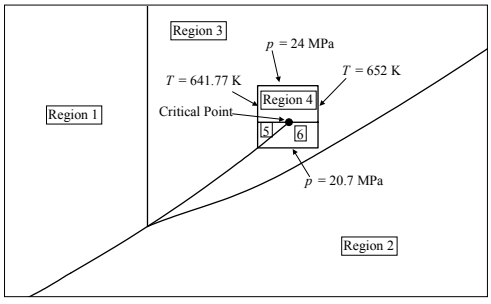

Figure 13. Definition of test regions, detail of regions 4, 5, and 6

Specific Isobaric Heat Capacity c_p

Equation for c_p is already included in TTSE-95, but it is linear equation and its accuracy is not sufficient to use in the vicinity of the critical point. TTSEtrans provides a table for c_p. In addition, the similar treatment as used for λ is applied to achieve higher accuracy in this region.

Accuracy test

To demonstrate the accuracy of TTSEtrans in determining the functions $\lambda(p,T)$, $\mu(p,T)$, $c_p(p,T)$, and $Pr(p,T)$, random access tests were performed. For reference, the same functions using the IAPWS-IF97 inputs were tested. The tests were performed over 6 regions defined by

Region 1: p = 0.0006128 to 100 MPa, T = 275 to 623.15 K, stable liquid,
(almost equal to Region 1 of IAPWS-IF97)

Region 2: p = 0.0006128 to 100 MPa, T = 275 to 1000 K, stable vapor,
(almost equal to Region 2 of IAPWS-IF97)

Region 3: Region 3 of IAPWS-IF97, except regions defined below,

Region 4: p = 22.064 to 24 MPa, T = 641.77 to 652 K,

Region 5: p = 20.7 to 22.064 MPa, T = 641.77 K to saturation temperature, and

Region 6: p = 20.7 to 22.064 MPa, T from saturation temperature to 652 K.

Figures 12 and 13 illustrate the regions.

Deviations were evaluated using 1,000,000 random inputs with uniform distribution in p and T. The maximum and root-mean-square of deviations Δz_{TT} and Δz_{97} are seen in Figures 14-1 to 14-8. The test results show that the deviation of TTSEtrans is much smaller than that of the calculation with the IAPWS-IF97 input except in the region 1. The maximum deviation in μ is nearly 0.1 % in the

region 1, but it occurs in high-pressure and very low-temperature areas not used in the industrial applications.

Computing Time Test

Computing times of Prandtl number $Pr_{TT}(p,T)$, $Pr_{97}(p,T)$, and $Pr_{IA}(p,T)$ that includes subroutine calls for c_p, λ, and μ, were tested. The tests were performed on a PC with Pentium III/1.2GHz. Figure 15 shows the test results.

The computing time of TTSEtrans is about half of that of the calculation with the IAPWS-IF97 input in the regions 1 and 2, and about one-tenth in other regions.

Discontinuity at Cell Boundaries

The value calculated from TTSE method is not continuous at cell boundaries. The maximum

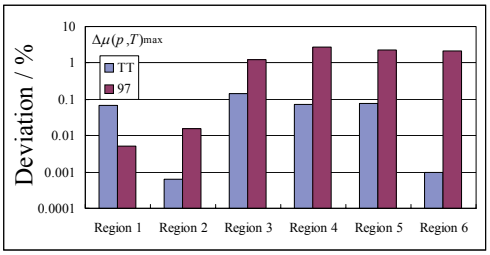

Figure 14-1. Maximum values of $\Delta\mu(p,T)_{TT}$ and $\Delta\mu(p,T)_{97}$ in each test region

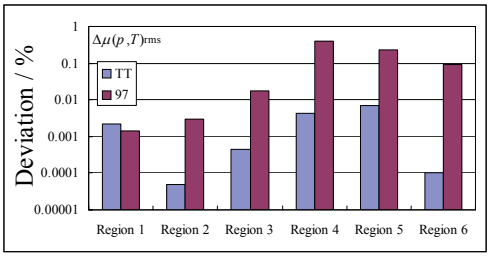

Figure 14-2. Root-mean-square of $\Delta\mu(p,T)_{TT}$ and $\Delta\mu(p,T)_{97}$ in each test region

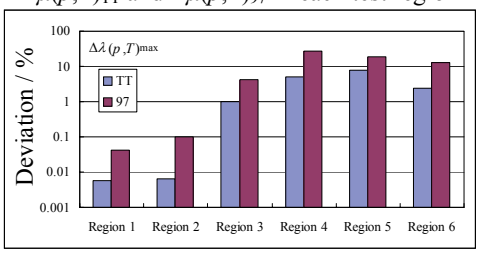

Figure 14-3. Maximum values of $\Delta\lambda(p,T)_{TT}$ and $\Delta\lambda(p,T)_{97}$ in each test region

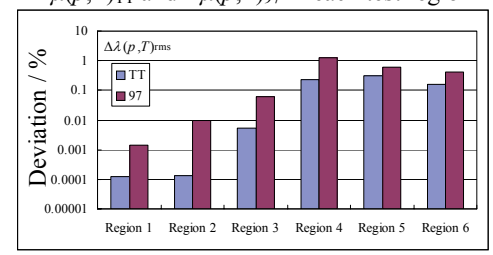

Figure 14-4. Root-mean-square of $\Delta\lambda(p,T)_{TT}$ and $\Delta\lambda(p,T)_{97}$ in each test region

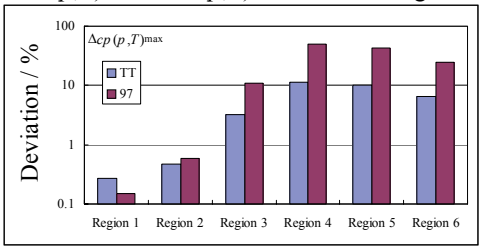

Figure 14-5. Maximum values of $\Delta c_p(p,T)_{TT}$ and $\Delta c_p(p,T)_{97}$ in each test region

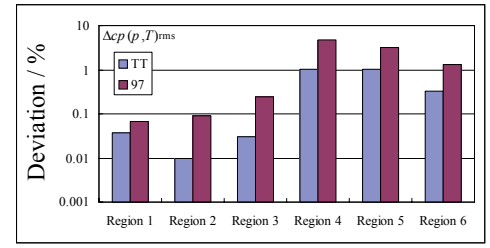

Figure 14-6. Root-mean-square of $\Delta c_p(p,T)_{TT}$ and $\Delta c_p(p,T)_{97}$ in each test region

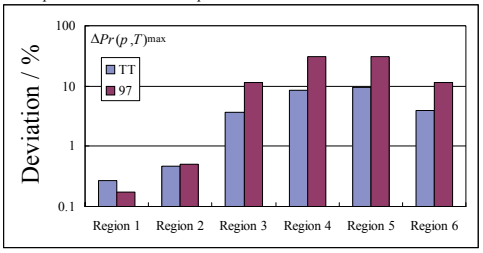

Figure 14-7. Maximum values of $\Delta Pr(p,T)_{TT}$ and $\Delta Pr(p,T)_{97}$ in each test region

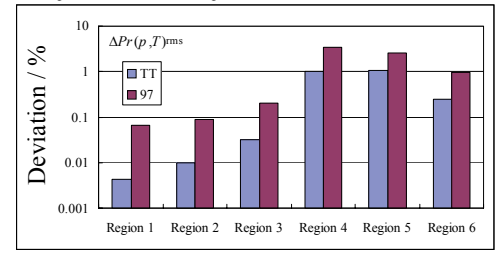

Figure 14-8. Root-mean-square of $\Delta Pr(p,T)_{TT}$ and $\Delta Pr(p,T)_{97}$ in each test region

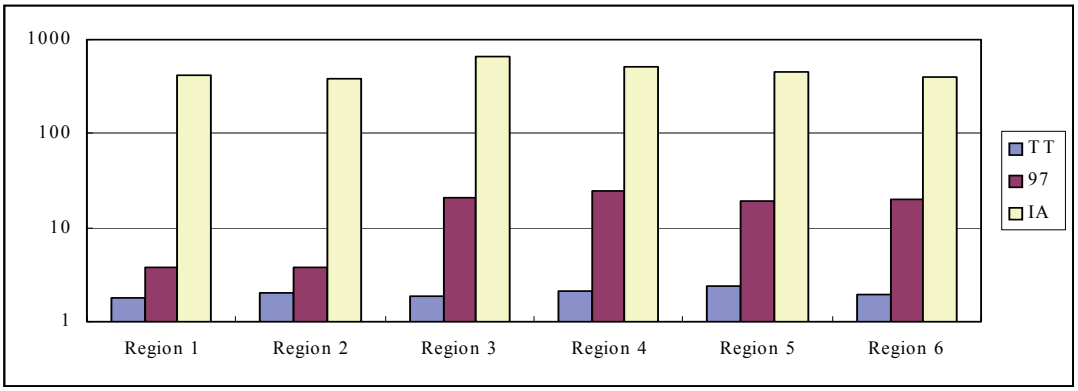

Figure 15. Computing time of $Pr(p,T)_{TT}$, $Pr(p,T)_{97}$, and $Pr(p,T)_{IA}$ in each test region (10^{-6}s/call)

expected discontinuity is twice the maximum deviation Δz_{TT}. If the increase of the discontinuity in the vicinity of the critical point is unfavorable for any application, the discontinuity can be reduced by extending the region of the basic equation shown with bold solid line in Figure 11 with sacrifice in computing time at the limited region.

Conclusions

A set of programs and data tables, TTSEtrans, has been developed for fast and accurate calculation of the transport properties of water and steam. TTSEtrans is based on the IAPWS equations.

The accuracy of TTSEtrans has been demonstrated by comparing against IAPWS equations at randomly selected test points. TTSEtrans represents the IAPWS equations comparably to or better than the common method in the industrial applications.

The computing time has been compared with that of the common method. For the calculation of Prandtl number $Pr(p,T)$ for the superheated-steam and compressed-water regions, the computing time of TTSEtrans calculation is about half of that of the common method. For the supercritical region, it is about one-tenth.

Acknowledgments

The development of TTSEtrans was initiated by suggestions of Ingo Weber and Axel Butterlin of Siemens. The author is grateful for their helpful advice on the development.

References

[1] Miyagawa, K., and Hill, P. G., *Rapid and Accurate Calculation of Water and Steam Properties using the Tabular Taylor Series Expansion Method, ASME J. Eng. Gas Turbines & Power*, **123**, pp. 707-712. Note: Information about downloading the software and related data for this application can be obtained at http://www.iapws.jp.

[2] International Association for the Properties of Water and Steam, *IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use*, *IAPWS Release*, IAPWS Secretariat.

[3] International Association for the Properties of Water and Steam, *Tabular Taylor Series Expansion (TTSE) Method for Calculation of Thermodynamic Properties of Water and Steam Applied to IAPWS-95 as an Example*, *IAPWS Guideline*, IAPWS Secretariat.

[4] Weber, I., et al., *Test Report of the Documentation and Software of TTSE Method applied to IAPWS-95 as an Example*, IAPWS Report, 2001. See note on [1].

[5] International Association for the Properties of Water and Steam, *The IAPS Formulation 1985 for the Viscosity of Ordinary Water Substance*, *IAPWS Release*, IAPWS Secretariat.

[6] International Association for the Properties of Water and Steam, IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam, *IAPWS Release*, IAPWS Secretariat.

[7] International Association for the Properties of Water and Steam, *The IAPS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance*, *IAPWS Release*, IAPWS Secretariat.