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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

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This guideline has been authorized by the International Association for the Properties of Water and Steam (IAPWS) at its meeting in Vejle, Denmark, 24-29 August 2003, for issue by its Secretariat. The members of IAPWS are: Argentina and Brazil, Britain and Ireland, Canada, the Czech Republic, Denmark, France, Germany, Italy, Japan, Russia, the United States of America, and associate member Greece.

The Tabular Taylor Series Expansion (TTSE) method has been authorized by the International Association for the Properties of Water and Steam for issuance as a guideline. In the judgment of IAPWS, the method provides users with a means of rapid and accurate calculation of the thermodynamic properties of water and steam when used in conjunction with the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use (IAPWS-95).

The supporting document for this guideline is: 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, 707-712 (2001).

Further information about this guideline and other documents issued by IAPWS can be obtained from the Executive Secretary of IAPWS, or on the IAPWS Website at <http://www.iapws.org>.

1 Nomenclature

Thermodynamic properties and variables, units:

c_p	isobaric specific heat capacity, kJ/kg·K
c_v	isochoric specific heat capacity, kJ/kg·K
h	specific enthalpy, kJ/kg
κ	isentropic exponent
p	pressure, MPa
s	specific entropy, kJ/kg·K
T	absolute temperature, K
v	specific volume, m ³ /kg
w	speed of sound, m/s
x	independent variable
y	independent variable
z	dependent variable

Deviation:

Δ	deviation of properties from IAPWS-95
Max	maximum
RMS	root-mean square

Indices:

i	index for y -direction (specific enthalpy in the example)
j	index for x -direction (pressure in the example)

Subscript:

sat	saturation state
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2 Introduction

This guideline contains equations and additional information for using a method for rapid and accurate calculation of the properties of water and steam.

The method employs a two-dimensional six-term Taylor Series expansion around selected grid points on a suitable plane of independent variables. The calculations are fast because of the small number of numerical operations required in using a table of stored properties and their derivatives. The stored primitives and derivatives are precisely determined from a fundamental equation so that the accuracy of the TTSE method depends only on grid spacing of the storage tables.

This guideline contains a sample TTSE application based on a grid on the Mollier state plane. The fundamental equation used for this example is the Helmholtz equation of state for ordinary water substance, IAPWS-95. Like the IAPWS Industrial Formulation 1997 (IAPWS-IF97), this example well approximates the IAPWS-95 formulation; however, it is not intended to replace IAPWS-IF97 for contractual purposes and does not replace IAPWS-95 for general and scientific use.

3 Tabular Taylor Series Expansion (TTSE) Method

This IAPWS guideline presents a method of rapid and accurate calculation by using, as an example, a specific version [1] of the TTSE method which has enthalpy h and pressure p as the independent variables and is based on a Helmholtz function whose independent variables are temperature T and density ρ . Previously, the method has been demonstrated with pressure and temperature as independent variables for turbine stage-by-stage calculation [2]. It has also been used with the internal energy and density coordinates appropriate to the Denton three-dimensional time-marching method for the turbine flow field [3]. In these applications, the TTSE method achieves both high speed and high accuracy with modest requirements for computer memory.

The basic source of the thermodynamic data used in formulating this example version of the TTSE method is the wide-ranging Helmholtz equation included in the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use (IAPWS-95) [4, 5].

The range of states included in the example may be defined by their locations on the enthalpy-pressure plane. These cover enthalpies from 4.2563 to 4004.2563 kJ/kg and pressures from 0.0006128 to 105.81 MPa. Excluded are those metastable or unstable states located above an arbitrary boundary that is denoted as the upper limit of practical interest in the metastable liquid region and a boundary in the metastable vapor region which corresponds to approximately 5 % equilibrium liquid. The latter boundary may be considered the lowest possible location of the Wilson line and we denote it as the lower limit of practical interest. The definitions of these boundaries are given in detail in reference [1].

For TTSE calculations of functions of two variables, $z(x,y)$, a grid is chosen composed of rectangular cells on the x - y plane. The nodes at which the information on a thermodynamic property z and its derivatives are stored is located at a point (x_j, y_i) , usually the center, of the cell. The Taylor series expansion may be expressed as:

$$z = z_{i,j} + (x-x_j) \left(\frac{\partial z}{\partial x} \right)_{i,j} + \frac{1}{2} (x-x_j)^2 \left(\frac{\partial^2 z}{\partial x^2} \right)_{i,j} + (y-y_i) \left(\frac{\partial z}{\partial y} \right)_{i,j} + \frac{1}{2} (y-y_i)^2 \left(\frac{\partial^2 z}{\partial y^2} \right)_{i,j} + (x-x_j)(y-y_i) \left(\frac{\partial^2 z}{\partial x \partial y} \right)_{i,j} \quad (1)$$

in which the subscripts i and j represent the locations of cells in the x - y plane. It has been found that truncating the Taylor Series expansion at the level of second derivatives (6 terms) provides high accuracy of property calculation with only modest memory capacity required for storage of the primitive and derivative quantities associated with each node location. The speed of the method is associated with only 6 coefficients for each property evaluation.

The variables x and y can be chosen so that they are the arguments of the functions most frequently computed. With enthalpy and pressure as independent variables, Eq. (1) can be used to calculate $T(p,h)$, $v(p,h)$, and $s(p,h)$ if the appropriate primitive and derivative values are tabulated for cell locations i and j . Table 1 shows how the appropriate first derivatives of these functions may be obtained directly from the Helmholtz function, which has density and temperature as independent variables.

The second and cross derivatives appearing in Eq. (1) could also have been obtained in closed form from the Helmholtz equation but it has been much easier to obtain them by a highly precise numerical differentiation. Since derivative quantities such as isobaric specific heat capacity c_p , isochoric specific heat capacity c_v , speed of sound w , and isentropic exponent κ are often of importance, it is useful to note that:

$$\left(\frac{\partial z}{\partial x} \right)_y = \left(\frac{\partial z}{\partial x} \right)_{i,j} + (x-x_j) \left(\frac{\partial^2 z}{\partial x^2} \right)_{i,j} + (y-y_i) \left(\frac{\partial^2 z}{\partial x \partial y} \right)_{i,j} \quad (2)$$

Table 2 shows how specific heat capacities, isentropic exponent and speed of sound can be evaluated using only the derivatives already stored for evaluation of T , v , and s .

Since Eq. (1) is quadratic, the inverse functions, in which p - T , p - s , and h - s are independent variables, can be solved directly. An important feature is that these inverse functions are fully consistent with the forward functions $z(p,h)$.

Table 1. Derivatives of T , v , and s

$\left(\frac{\partial T}{\partial h} \right)_p = \frac{1}{c_p}$	$\left(\frac{\partial T}{\partial p} \right)_h = \frac{1}{A} \left(\frac{\partial h}{\partial \rho} \right)_T$
$\left(\frac{\partial v}{\partial h} \right)_p = \frac{-1}{A \rho^2} \left(\frac{\partial p}{\partial T} \right)_p$	$\left(\frac{\partial v}{\partial p} \right)_h = \frac{1}{A \rho^2} \left(\frac{\partial h}{\partial T} \right)_p$
$\left(\frac{\partial s}{\partial h} \right)_p = \frac{1}{T}$	$\left(\frac{\partial s}{\partial p} \right)_h = \frac{-v}{T}$
where:	
$A = \left(\frac{\partial p}{\partial T} \right)_p \left(\frac{\partial h}{\partial \rho} \right)_T - \left(\frac{\partial p}{\partial \rho} \right)_T \left(\frac{\partial h}{\partial T} \right)_p$	

Table 2. Properties derived from the derivatives of basic TTSE functions

$c_p = 1 / \left(\frac{\partial T}{\partial h} \right)_p$ $c_v = \frac{-BT}{D}$	$w = \sqrt{\frac{v^2}{B} \left(\frac{\partial s}{\partial h} \right)_p}$ $\kappa = \frac{v}{B} \left(\frac{\partial s}{\partial h} \right)_p$
where:	
$B = \left(\frac{\partial v}{\partial h} \right)_p \left(\frac{\partial s}{\partial p} \right)_h - \left(\frac{\partial v}{\partial p} \right)_h \left(\frac{\partial s}{\partial h} \right)_p$ $D = \left(\frac{\partial T}{\partial h} \right)_p \left(\frac{\partial v}{\partial p} \right)_h - \left(\frac{\partial T}{\partial p} \right)_h \left(\frac{\partial v}{\partial h} \right)_p$	

4 Grid and Cell Structure

The grid of points (i,j) on the Mollier plane is of size 200×200 with uniform spacings of 20 kJ/kg in the enthalpy (i) direction where the enthalpy ranges from 4.2563 to 4004.2563 kJ/kg. In the pressure (j) direction the spacings are of equal pressure ratio of 1.06215 as the pressure ranges from 0.0006128 to 105.81 MPa. The critical point occupies the location (104,173) where the pressure is 22.064 MPa and the enthalpy is 2084.2563 kJ/kg.

The primitives of the temperature T , specific volume v , entropy s , and its derivatives have been evaluated at a node point in each cell. As a general rule, the node point has been located at the center of the cell, as long as the Helmholtz equation is valid there. At the column $j=173$, and when the center is out of the valid region, the node point is set on the saturation line. In addition, at cells where $j=172$ and which include the liquid saturation line, the node point is set on the saturation line. The exceptions are required if the center is in an invalid region or outside the defined region of practical interest.

The evaluated values are used as TTSE coefficients after being stored in double precision and in binary form. Three 6×200×200 arrays include all coefficients needed for the calculation of the properties T , v , and s . The size of the binary file is about 1.92 megabytes for each property.

For the saturation function $T_{\text{sat}}(p)$, a truncated Taylor expansion is applied. With a single dependent variable, only 3 coefficients are required for the primitive and first and second derivatives of temperature with respect to pressure; these have been determined from a subroutine of IAPWS-95. The same pressure scale as for $z(p,h)$ has been used.

The time to find the indices of the cell in which the values of the input variables $h-p$, $p-T$, $p-s$, or $h-s$ are located is significant and fast cell location strategies have been developed [1].

5 Accuracy

To indicate the accuracy of the method (relative to the underlying Helmholtz function) in determining the functions $T(p,h)$, $v(p,h)$, and $s(p,h)$, tests of the method have been performed over 6 regions (see Figs. 1 and 2) 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 near critical point 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

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

Deviations from the basic equation were calculated using random inputs with uniform distribution in p and T . The number of test points was 10,000,000 for regions 1 to 3 and 300,000 for regions 4 to 6. The maximum and root-mean-square of deviations are listed in Table 3.

Corresponding results of random access tests for the functions $c_p(p,h)$, $c_v(p,h)$, and $w(p,h)$, *i.e.*, functions requiring second derivatives, for regions 1 to 3 are given in Table 4. In the vicinity of the critical point, this example does not accurately simulate these properties.

Reference [1] provides additional information on accuracy tests of this example, as well as for the saturation function $T_{\text{sat}}(p)$. In general it may be said that this example represents IAPWS-95 much better than the accuracy specification of IAPWS-IF97 [6] or at least (for specific heat capacities and speed of sound) satisfies the IAPWS-IF97 specification.

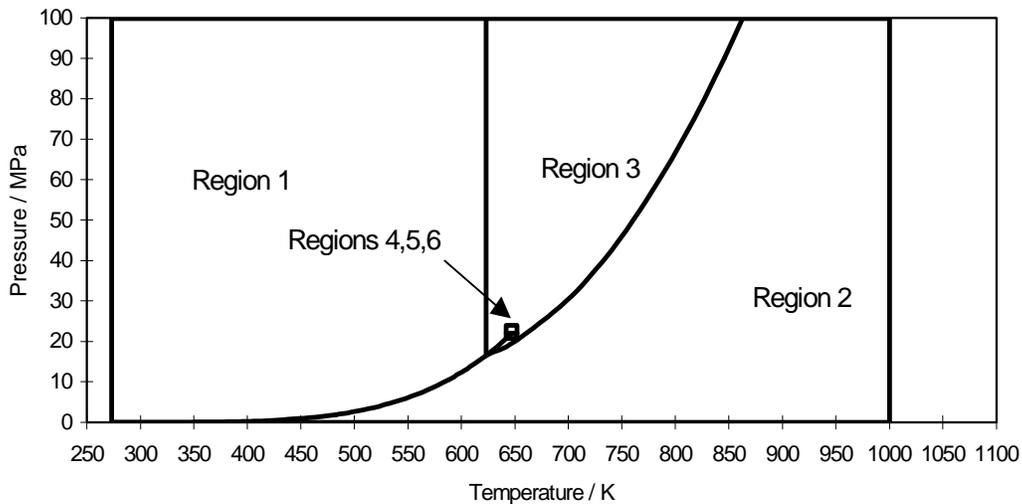


Figure 1. Definition of test regions

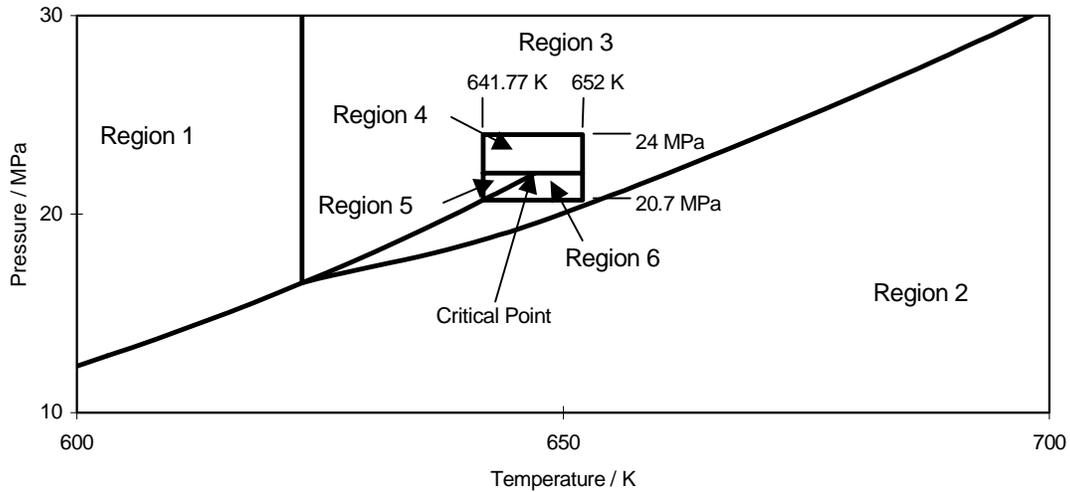


Figure 2. Definition of test regions (detail of regions 4, 5 and 6)

Table 3. Deviation of TTSE functions $T(p,h)$, $v(p,h)$, and $s(p,h)$ from IAPWS-95

	$\Delta T / \text{mK}$		$\Delta v / \%$		$\Delta s / \text{J}/(\text{kg}\cdot\text{K})$	
	Max.	RMS	Max.	RMS	Max.	RMS
Region 1	1.78	0.03	0.00208	0.00003	0.0030	0.0002
Region 2	9.21	0.25	0.00413	0.00103	0.0055	0.0014
Region 3	9.29	0.38	0.03826	0.00057	0.0044	0.0005
Region 4	16.21	1.31	0.08945	0.00557	0.0051	0.0006
Region 5	37.02	3.59	0.11248	0.01027	0.0053	0.0006
Region 6	0.88	0.21	0.00466	0.00132	0.0044	0.0011

Table 4. Deviation of TTSE functions $c_p(p,h)$, $c_v(p,h)$, and $w(p,h)$ from IAPWS-95

	$\Delta c_p / \%$		$\Delta c_v / \%$		$\Delta w / \%$	
	Max.	RMS	Max.	RMS	Max.	RMS
Region 1	0.32	0.004	0.22	0.004	0.51	0.013
Region 2	0.52	0.010	0.61	0.029	0.26	0.072
Region 3	8.33	0.032	5.32	0.043	2.95	0.076

6 Computing Time

The details of calculation speed tests of this example relative to IAPWS-IF97 are given in reference [1]. This example and IAPWS-IF97 are comparable in computing speed; both of them are 100 to 200 times faster than IAPWS-95 for the functions in this example.

7 Further Information about this Example

This example was examined by a evaluation task group established in IAPWS. Detailed information about accuracy, computing time, and applicability is seen in the test report of the task group [7].

8 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, 707-712 (2001). NOTE: Information about downloading the software and related data for this application can be obtained at <http://www.iapws.jp>.
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- [7] Weber, I., Kodl, I., Kretzschmar, H.-J., and Knobloch, K., Test Report of the Documentation and Software of TTSE Method applied to IAPWS-95 as an Example, IAPWS Report, 2001. See note on [1].