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Edited by

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University of Waterloo

Poyilath V. Balakrishnan

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CALCULATION OF THERMODYNAMIC DERIVATIVES FOR WATER AND STEAM USING THE NEW INDUSTRIAL FORMULATION IAPWS-IF97

Hans-Joachim Kretzschmar, Ines Stöcker,
Department of Technical Thermodynamics, University of Applied Sciences of
Zittau and Görlitz, D-02754 Zittau, Germany

Jochen Klinger, and Achim Dittmann
Department of Technical Thermodynamics, Technical University of Dresden,
D-01062 Dresden, Germany

ABSTRACT: Thermodynamic derivatives of water and steam are required in the modelling of non-stationary processes of heat cycles and turbines. Using the new Industrial Formulation IAPWS-IF97, all differential quotients of first and second degree can be calculated with high accuracy. This is because the fundamental equations of the IAPWS-IF97 were fitted to the derivatives of the Scientific Formulation IAPWS-95.

In this paper, the formulas for setting up all differential quotients $\left(\frac{\partial z}{\partial x}\right)_y$ from the IAPWS-IF97 equations will be summarized. In each, the variables x, y, z can represent any of the thermodynamic properties: pressure p, temperature T, specific volume v, specific internal energy u, specific enthalpy h, specific entropy s, specific free enthalpy g, or specific free energy f. Tables using the dimensionless Gibbs free enthalpy equations $\gamma(\pi,\tau)$ of regions 1, 2 and 5 and the dimensionless Helmholtz free energy equation $\phi(\tau,\delta)$ of region 3 of IAPWS-IF97 (where π is dimensionless pressure, τ is dimensionless inverse temperature and δ is dimensionless density) will also be presented. These tables will prove useful as supplements to the Release of the IAPWS-IF97 Formulation.

In addition, the paper contains analogous tables using the Helmholtz free energy equation $\phi(\tau,\delta)$ of the Scientific Formulation IAPWS-95.

INTRODUCTION

The new Industrial Formulation IAPWS-IF97 for the thermodynamic properties of water and steam [1,2,3,4] in the following abbreviated as IF97 is being used in thermodynamic process modelling. Fig. 1 shows the range of validity of the IF97 and its subdivision into five calculation regions. The IF97 contains saturation pressure and temperature equations $p_s(T)$ and $T_s(p)$ and individual equations for the Gibbs free enthalpy $g(p,T)$ for regions 1, 2 and 5, for the Helmholtz free energy $f(T,v)$, originally formulated as $f(T,\rho)$, for region 3 and for the backward functions $T(p,h)$ and $T(p,s)$ for regions 1 and 2.

Using the fundamental equations $g(p,T)$ and their first and second derivatives

$$\left(\frac{\partial g}{\partial p}\right)_T , \left(\frac{\partial g}{\partial T}\right)_p , \left(\frac{\partial^2 g}{\partial p^2}\right)_T , \left(\frac{\partial^2 g}{\partial T^2}\right)_p , \left(\frac{\partial^2 g}{\partial p \partial T}\right) \text{ all thermodynamic properties:}$$

v, u, h, s, c_p, c_v, κ, w, etc. and any differential quotient $\left(\frac{\partial z}{\partial x}\right)_y$, where x, y, z represent

p, T, v, u, h, s, g, or f, can be calculated from given values of p and T for regions 1, 2 and 5.

For region 3, all thermodynamic properties and differential quotients can be formed using the fundamental equation $f(T,v)$ and their derivatives $\left(\frac{\partial f}{\partial T}\right)_v, \left(\frac{\partial f}{\partial v}\right)_T, \left(\frac{\partial^2 f}{\partial T^2}\right)_v, \left(\frac{\partial^2 f}{\partial v^2}\right)_T, \left(\frac{\partial^2 f}{\partial T \partial v}\right)$ as function of T and v.
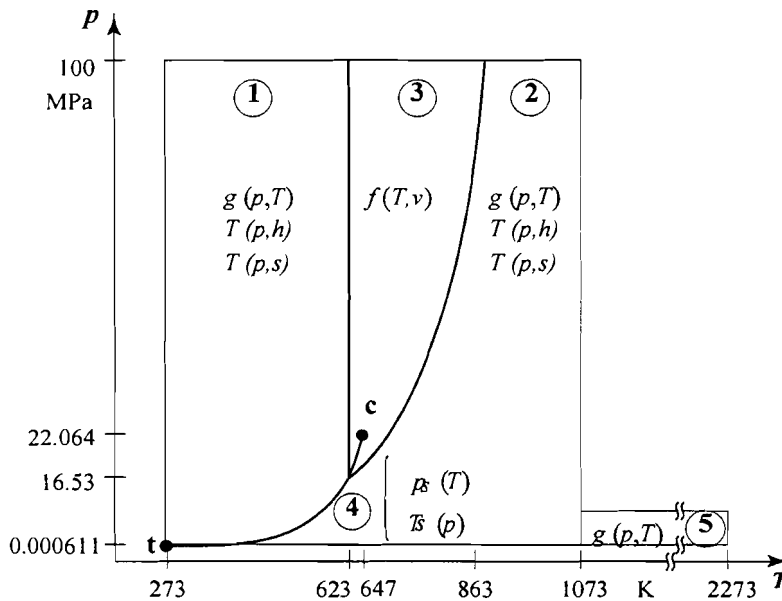

Figure 1: Range of validity, calculation regions and equations of the IAPWS-IF97

The accuracy of the calculated properties and differential quotients is very high because the IF97 fundamental equations were fitted not only to the Helmholtz equation $f(T,v)$ of the Scientific Formulation IAPWS-95 [5,6] but also to its derivatives

$$\left(\frac{\partial f}{\partial T}\right)_v, \left(\frac{\partial f}{\partial v}\right)_T, \left(\frac{\partial^2 f}{\partial T^2}\right)_v, \left(\frac{\partial^2 f}{\partial v^2}\right)_T, \left(\frac{\partial^2 f}{\partial T \partial v}\right).$$

The ability of the IF97 fundamental equations to be accurate enough for calculating all thermodynamic properties and derivatives is one of the main advantages of the new Industrial Formulation. In comparison, the previous industrial standard IFC-67 [7,8,9] did not allow the user to calculate all properties and differential quotients in the entire range of validity. For example, the accuracy of the properties c_p, κ and w of steam at pressures greater than 12 MPa was less than the industrial requirements for these properties.

For the differential equations of non-stationary process modelling of heat cycles, turbines, nuclear reactors etc. a lot of different thermodynamic differential quotients have to be calculated. Therefore in this paper, the formulas for setting up differential quotients

$$\left(\frac{\partial z}{\partial x}\right)_y (p,T) \text{ for all IF97 regions and}$$

$$\left(\frac{\partial z}{\partial x}\right)_y (T,v) \text{ for IF97 region 3,}$$

where x, y, z can represent any of the thermodynamic properties: p, T, v, u, h, s, g, or f are summarized. The formulas are based on the dimensionless Gibbs free enthalpy equations

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$\gamma(\pi, \tau)$ of regions 1, 2 and 5 and the dimensionless Helmholtz free energy equation $\phi(\delta, \tau)$ of region 3 of IF97 (where π is dimensionless pressure, τ is dimensionless inverse temperature and δ is dimensionless density). In addition, analogous formulas for setting up any differential quotients for the Scientific Formulation IAPWS-IF95 based on its dimensionless Helmholtz equation $\phi(\delta, \tau)$ are presented.

DIFFERENTIAL QUOTIENTS $\left(\dfrac{\partial z}{\partial x}\right)_y$ (p, T) OF THE IAPWS-IF97

As *Fischer* [10] has shown, any differential quotient $\left(\dfrac{\partial z}{\partial x}\right)_y$ can be derived as function of pressure p and temperature T as follows:

The total differentials of the involved quantities z, x, and y as function of p and T are set up:

$$dz = \left(\frac{\partial z}{\partial p}\right)_T dp + \left(\frac{\partial z}{\partial T}\right)_p dT \tag{1}$$

$$dx = \left(\frac{\partial x}{\partial p}\right)_T dp + \left(\frac{\partial x}{\partial T}\right)_p dT \tag{2}$$

$$0 = dy = \left(\frac{\partial y}{\partial p}\right)_T dp + \left(\frac{\partial y}{\partial T}\right)_p dT . \tag{3}$$

The total differential of dy, Eq. (3) is equal to zero because y is constant in the differential quotient. Using Eqs. (1) and (2) the required differential quotient can be written under consideration of $y = $ const:

$$\left(\frac{\partial z}{\partial x}\right)_y \equiv \frac{dz_y}{dx_y} = \frac{\left(\dfrac{\partial z}{\partial p}\right)_T dp_y + \left(\dfrac{\partial z}{\partial T}\right)_p dT_y}{\left(\dfrac{\partial x}{\partial p}\right)_T dp_y + \left(\dfrac{\partial x}{\partial T}\right)_p dT_y} . \tag{4}$$

Now Eq. (3) is transposed into

$$dp_y = -\frac{\left(\dfrac{\partial y}{\partial T}\right)_p}{\left(\dfrac{\partial y}{\partial p}\right)_T} dT_y , \tag{5}$$

where the index y of dp_y and dT_y comes from $dy = 0$.

The insertion into Eq. (4) leads to:

$$\left(\frac{\partial z}{\partial x}\right)_y = \frac{\left(\frac{\partial z}{\partial p}\right)_T \cdot \left(\frac{\partial y}{\partial T}\right)_p - \left(\frac{\partial z}{\partial T}\right)_p \cdot \left(\frac{\partial y}{\partial p}\right)_T}{\left(\frac{\partial x}{\partial p}\right)_T \cdot \left(\frac{\partial y}{\partial T}\right)_p - \left(\frac{\partial x}{\partial T}\right)_p \cdot \left(\frac{\partial y}{\partial p}\right)_T} \quad . \tag{6}$$

Eq. (6) is the common expression for determining the differential quotient $\left(\frac{\partial z}{\partial x}\right)_y$ as function of p and T. In each, the variables x, y, z can stand for any of the thermodynamic properties: p, T, v, u, h, s, g, or f. Table 1 contains the derivatives used in Eq. (6) for these properties from p and T. As can be seen, besides the given parameters p and T the five quantities v, s, c_p $\left(\frac{\partial v}{\partial p}\right)_T$ and $\left(\frac{\partial v}{\partial T}\right)_p$ are required.

Table 1: Derivatives of x, y, z from p and T, where x, y, z can stand for p, T, v, u, h, s, g, or f

x y z	$\left(\frac{\partial}{\partial T}\right)_p$	$\left(\frac{\partial}{\partial p}\right)_T$
p	0	1
T	1	0
v	$\left(\frac{\partial v}{\partial T}\right)_p$	$\left(\frac{\partial v}{\partial p}\right)_T$
u	$c_p - p\left(\frac{\partial v}{\partial T}\right)_p$	$-T\left(\frac{\partial v}{\partial T}\right)_p - p\left(\frac{\partial v}{\partial p}\right)_T$
h	c_p	$v - T\left(\frac{\partial v}{\partial T}\right)_p$
s	$\frac{c_p}{T}$	$-\left(\frac{\partial v}{\partial T}\right)_p$
g	$-s$	v
f	$-p\left(\frac{\partial v}{\partial T}\right)_p - s$	$-p\left(\frac{\partial v}{\partial p}\right)_T$

The reason is that these quantities are the first and second derivatives of the free enthalpy g from p and T: $v = \left(\frac{\partial g}{\partial p}\right)_T$, $s = -\left(\frac{\partial g}{\partial T}\right)_p$, $\left(\frac{\partial v}{\partial p}\right)_T = \left(\frac{\partial^2 g}{\partial p^2}\right)_T$, $c_p = -T\left(\frac{\partial^2 g}{\partial T^2}\right)_p$, $\left(\frac{\partial v}{\partial T}\right)_p = \left(\frac{\partial^2 g}{\partial p \partial T}\right)$.

That means, with v, s, c_p, $\left(\frac{\partial v}{\partial p}\right)_T$ and $\left(\frac{\partial v}{\partial T}\right)_p$ any differential quotient $\left(\frac{\partial z}{\partial x}\right)_y$ can be calculated using Eq. (6) and Table 1.

In the following the expressions for calculating these five quantities using the dimensionless fundamental equations of the IF97 are summarized:

IF97 Region 1

The equations for the five quantities can be determined from the dimensionless Gibbs free enthalpy equation $\gamma(\pi,\tau)$ of IF97 region 1 (Figure 1). They read:

$$v = \frac{RT}{p}\pi\gamma_\pi \qquad\qquad \left(\frac{\partial v}{\partial T}\right)_p = \frac{R}{p}\pi\left(\gamma_\pi - \tau\gamma_{\pi\tau}\right)$$

$$s = R(\tau\gamma_\tau - \gamma) \qquad\qquad \left(\frac{\partial v}{\partial p}\right)_T = \frac{RT}{p^2}\pi^2\gamma_{\pi\pi} \qquad\qquad (7)$$

$$c_p = -R\tau^2\gamma_{\tau\tau} ,$$

where $\gamma = g/RT$, $\pi = p/p^*$, $\tau = T^*/T$ with the specific gas constant R and the reducing constants p^*, T^*. The constants, the equation $\gamma(\pi,\tau)$ and its derivatives

$$\gamma_\pi = \left(\frac{\partial\gamma}{\partial\pi}\right)_\tau , \gamma_\tau = \left(\frac{\partial\gamma}{\partial\tau}\right)_\pi , \gamma_{\pi\pi} = \left(\frac{\partial^2\gamma}{\partial\pi^2}\right)_\tau , \gamma_{\tau\tau} = \left(\frac{\partial^2\gamma}{\partial\tau^2}\right)_\pi \text{ and } \gamma_{\pi\tau} = \left(\frac{\partial^2\gamma}{\partial\pi\partial\tau}\right) \text{ are given in}$$

detail in the Release of the IF97 [1] or in the comprehensive paper [2].

IF97 Regions 2 and 5

The equations for the five quantities can be determined from the dimensionless Gibbs free enthalpy equation $\gamma(\pi,\tau) = \gamma^o(\pi,\tau) + \gamma^r(\pi,\tau)$ of IF97 regions 2 or 5 (Figure 1) as follows:

$$v = \frac{RT}{p}\left(1 + \pi\gamma_\pi^r\right) \qquad\qquad \left(\frac{\partial v}{\partial T}\right)_p = \frac{R}{p}\left(1 + \pi\gamma_\pi^r - \pi\tau\gamma_{\pi\tau}^r\right)$$

$$s = R\left(\tau\left(\gamma_\tau^o + \gamma_\tau^r\right) + \left(\gamma^o + \gamma^r\right)\right) \qquad \left(\frac{\partial v}{\partial p}\right)_T = \frac{RT}{p^2}\left(\pi^2\gamma_{\pi\pi}^r - 1\right) \qquad (8)$$

$$c_p = -R\tau^2\left(\gamma_{\tau\tau}^o + \gamma_{\tau\tau}^r\right),$$

where $\gamma = g/RT$, $\pi = p/p^*$, $\tau = T^*/T$ with the specific gas constant R and the reducing constants p^*, T^*. The constants, the equations $\gamma^o(\pi,\tau)$ and $\gamma^r(\pi,\tau)$ and their derivatives $\gamma_\tau^o, \gamma_{\tau\tau}^o$, $\gamma_\pi^r, \gamma_\tau^r, \gamma_{\pi\pi}^r, \gamma_{\tau\tau}^r$ and $\gamma_{\pi\tau}^r$ are given in [1,2].

IF97 Region 3

The equations for IF97 region 3 (Figure 1) can be determined from the dimensionless Helmholtz free energy equation $\phi(\tau,\delta)$ as follows:

Iteration of ρ using $p = \rho R T \delta \phi_\delta$

$$\left(\frac{\partial v}{\partial T}\right)_p = \frac{(\phi_\delta - \tau\phi_{\delta\tau})}{\rho T(2\phi_\delta + \delta\phi_{\delta\delta})}$$

$$s = R(\tau\phi_\tau - \phi)$$

$$\left(\frac{\partial v}{\partial p}\right)_T = -\frac{1}{\rho^2 R T\left(2\delta\phi_\delta + \delta^2\phi_{\delta\delta}\right)} \tag{9}$$

$$c_p = R\left(-\tau^2\phi_{\tau\tau} + \frac{(\delta\phi_\delta - \delta\tau\phi_{\delta\tau})^2}{2\delta\phi_\delta + \delta^2\phi_{\delta\delta}}\right),$$

where $\phi = f/RT$, $\tau = T^*/T$, $\delta = \rho/\rho^*$ with the specific gas constant R and the reducing constants T^*, ρ^*. The constants, the equation $\phi(\tau,\delta)$ and its derivatives

$$\phi_\tau = \left(\frac{\partial\phi}{\partial\tau}\right)_\delta, \phi_\delta = \left(\frac{\partial\phi}{\partial\delta}\right)_\tau, \phi_{\tau\tau} = \left(\frac{\partial^2\phi}{\partial\tau^2}\right)_\delta, \phi_{\delta\delta} = \left(\frac{\partial^2\phi}{\partial\delta^2}\right)_\tau, \text{ and } \phi_{\delta\tau} = \left(\frac{\partial^2\phi}{\partial\delta\,\partial\tau}\right) \text{ are given}$$

in [1,2]. First, the density ρ is iterated from the given values of p and T using the IF97 equation $p(T,\rho)$. Then the other quantities can be calculated from T and ρ or τ and δ respectively.

Example

For example, the Joule-Thomson coefficient $\left(\frac{\partial T}{\partial p}\right)_h$ is to be calculated as function of p and T for the superheated steam region 2 (Figure 1). The comparison to the common differential quotient $\left(\frac{\tilde{z}}{\tilde{x}}\right)_y$ leads to $z = T$, $x = p$ and $y = h$. Considering these relations, Eq. (6) reads formally:

$$\left(\frac{\partial T}{\partial p}\right)_h = \frac{\left(\frac{\partial T}{\partial p}\right)_T \cdot \left(\frac{\partial h}{\partial T}\right)_p - \left(\frac{\partial T}{\partial T}\right)_p \cdot \left(\frac{\partial h}{\partial p}\right)_T}{\left(\frac{\partial p}{\partial p}\right)_T \cdot \left(\frac{\partial h}{\partial T}\right)_p - \left(\frac{\partial p}{\partial T}\right)_p \cdot \left(\frac{\partial h}{\partial p}\right)_T} \ . \tag{I}$$

According to Table 1 the derivatives are:

$$\left(\frac{\partial T}{\partial p}\right)_T = 0 \qquad \left(\frac{\partial h}{\partial T}\right)_p = c_p$$

$$\left(\frac{\partial T}{\partial T}\right)_p = 1 \qquad \left(\frac{\partial h}{\partial p}\right)_T = v - T\left(\frac{\partial v}{\partial T}\right)_p \tag{II}$$

$$\left(\frac{\partial p}{\partial p}\right)_T = 1 \qquad \left(\frac{\partial p}{\partial T}\right)_p = 0 \ .$$

The insertion into Eq. (I) leads to

$$\left(\frac{\partial T}{\partial p}\right)_h = \frac{T\left(\frac{\partial v}{\partial T}\right)_p - v}{c_p} \ . \tag{III}$$

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Finally v, $\left(\frac{\partial v}{\partial T}\right)_p$ and c_p can be calculated using the IF97 equations $\gamma^o(\pi,\tau)$, $\gamma^r(\pi,\tau)$ and their derivatives using Eq. (8).

DIFFERENTIAL QUOTIENTS $\left(\frac{\partial z}{\partial x}\right)_y$ (T, v) OF THE IAPWS-IF97

The differential quotient $\left(\frac{\partial z}{\partial x}\right)_y$ can be derived as a function of T and v in the analogous way as showed in the previous section. The result is the common equation

$$\left(\frac{\partial z}{\partial x}\right)_y = \frac{\left(\frac{\partial z}{\partial v}\right)_T \cdot \left(\frac{\partial y}{\partial T}\right)_v - \left(\frac{\partial z}{\partial T}\right)_v \cdot \left(\frac{\partial y}{\partial v}\right)_T}{\left(\frac{\partial x}{\partial v}\right)_T \cdot \left(\frac{\partial y}{\partial T}\right)_v - \left(\frac{\partial x}{\partial T}\right)_v \cdot \left(\frac{\partial y}{\partial v}\right)_T} .$$

(10)

Again the variables x, y, z can represent any of the thermodynamic properties: p, T, v, u, h, s, g, or f. Table 2 contains the derivatives of the these eight properties from T and v.

Table 2: Derivatives of x, y, z from T and v, where x, y, z can stand for p, T, v, u, h, s, g, or f

$x\,y\,z$	$\left(\frac{\partial}{\partial T}\right)_v$	$\left(\frac{\partial}{\partial v}\right)_T$
p	$\left(\frac{\partial p}{\partial T}\right)_v$	$\left(\frac{\partial p}{\partial v}\right)_T$
T	1	0
v	0	1
u	c_v	$T\left(\frac{\partial p}{\partial T}\right)_v - p$
h	$c_v + v\left(\frac{\partial p}{\partial T}\right)_v$	$T\left(\frac{\partial p}{\partial T}\right)_v + v\left(\frac{\partial p}{\partial v}\right)_T$
s	$\dfrac{c_v}{T}$	$\left(\frac{\partial p}{\partial T}\right)_v$
g	$v\left(\frac{\partial p}{\partial T}\right)_v - s$	$v\left(\frac{\partial p}{\partial v}\right)_T$
f	$-s$	$-p$

As can be seen besides the given parameters T and v the five quantities p, s, c_v, $\left(\dfrac{\partial p}{\partial T}\right)_v$ and

$\left(\dfrac{\partial p}{\partial v}\right)_T$ are required. These quantities are the first and second derivatives of the Helmholtz free energy f from T and v:

$$p = -\left(\frac{\partial f}{\partial v}\right)_T \; , \quad s = -\left(\frac{\partial f}{\partial T}\right)_v \; , \quad \left(\frac{\partial p}{\partial v}\right)_T = -\left(\frac{\partial^2 f}{\partial v^2}\right)_T \; , \quad c_v = -T\left(\frac{\partial^2 f}{\partial T^2}\right)_v \; , \quad \left(\frac{\partial p}{\partial T}\right)_v = -\left(\frac{\partial^2 f}{\partial T\,\partial v}\right) . \quad \text{That}$$

means, when having p, s, c_v, $\left(\dfrac{\partial p}{\partial v}\right)_T$ and $\left(\dfrac{\partial p}{\partial T}\right)_v$ any differential quotient $\left(\dfrac{\partial z}{\partial x}\right)_y$ can be calculated using Eq. (10) and Table 2.

IF97 Region 3

The expressions for calculating p, s, c_v, $\left(\dfrac{\partial p}{\partial v}\right)_T$ and $\left(\dfrac{\partial p}{\partial T}\right)_v$ using the dimensionless Helmholtz free energy equation $\phi(\tau,\delta)$ of IF97 region 3 (Figure 1) read:

$$p = \rho R T \delta \phi_\delta$$

$$\left(\frac{\partial p}{\partial T}\right)_v = \rho R \delta \left(\phi_\delta - \tau \phi_{\delta\tau}\right)$$

$$s = R\left(\tau \phi_\tau - \phi\right)$$

$$\left(\frac{\partial p}{\partial v}\right)_T = -\rho^2 R T \left(2\delta\phi_\delta + \delta^2 \phi_{\delta\delta}\right) \tag{11}$$

$$c_v = -R\tau^2 \phi_{\tau\tau} \; ,$$

where ϕ, τ, δ are as given in Eq. (9). The constants, equation $\phi(\tau,\delta)$ and its derivatives ϕ_τ, ϕ_δ, $\phi_{\tau\tau}$, $\phi_{\delta\delta}$, $\phi_{\delta\tau}$ are described in [1,2].

DIFFERENTIAL QUOTIENTS OF THE SCIENTIFIC STANDARD IAPWS-95

For extremely high accuracy demands, especially near the critical point, the differential quotients can be calculated using the Scientific Formulation IAPWS-95 [5,6]. In the following, the formulas for setting up any differential quotients are summarized.

Differential Quotients $\left(\dfrac{\partial z}{\partial x}\right)_y$ (p, T) of the IAPWS-95

Any differential quotient $\left(\dfrac{\partial z}{\partial x}\right)_y$ can be calculated as a function of p and T using Eq. (6) and Table 1. In each, the variables x, y, z can stand for any of the thermodynamic properties: p, T, v, u, h, s, g, or f.

The quantities v, s, c_p, $\left(\frac{\partial v}{\partial p}\right)_T$ and $\left(\frac{\partial v}{\partial T}\right)_p$ required in Table 1 can be calculated from the dimensionless Helmholtz free energy equation $\phi(\tau,\delta) = \phi^o(\tau,\delta)+\phi^r(\tau,\delta)$ of the IAPWS-95 as follows:

Iteration of ρ using $p = \rho RT\left(1 + \delta\phi_\delta^r\right)$

$$\left(\frac{\partial v}{\partial T}\right)_p = \frac{-\rho\left(1+\delta\phi_\delta^r - \tau\,\delta\phi_{\tau\delta}^r\right)}{T\left(-2\rho^2\delta\phi_\delta^r - \rho^2\delta^2\phi_{\delta\delta}^r - \rho^2\right)}$$

$$s = R\left[\tau\left(\phi_\tau^o + \phi_\tau^r\right) - \phi^o - \phi^r\right]$$

$$\left(\frac{\partial v}{\partial p}\right)_T = \frac{1}{RT\left(-2\rho^2\delta\phi_\delta^r - \rho^2\delta^2\phi_{\delta\delta}^r - \rho^2\right)}$$

$$c_p = R\left[-\tau^2\left(\phi_{\tau\tau}^o + \phi_{\tau\tau}^r\right) + \frac{\left(1 + \delta\phi_\delta^r - \delta\tau\phi_{\delta\tau}^r\right)^2}{1 + 2\delta\phi_\delta^r + \delta^2\phi_{\delta\delta}^r}\right] \quad , \tag{12}$$

where ϕ, τ and δ are as given in Eq. (9). The constants, the equations $\phi^o(\tau,\delta)$ and $\phi^r(\tau,\delta)$ and their derivatives $\phi_\tau^o, \phi_{\tau\tau}^o, \phi_\tau^r, \phi_\delta^r, \phi_{\tau\tau}^r, \phi_{\delta\delta}^r, \phi_{\delta\tau}^r$ are given in detail in the Release of the IAPWS-95 [5] or in the comprehensive paper [6].

First, the density ρ has to be iterated from the given values of p and T using the IAPWS-95 equation $p(T,\rho)$. Then the other quantities can be calculated from T and ρ or τ and δ respectively.

Differential Quotients $\left(\frac{\partial z}{\partial x}\right)_y$ (T,v) of the IAPWS-95

Any differential quotient $\left(\frac{\partial z}{\partial x}\right)_y$ can be calculated as function of T and v using Eq. (10) and Table 2. The quantities p, s, c_v, $\left(\frac{\partial p}{\partial T}\right)_v$, and $\left(\frac{\partial p}{\partial v}\right)_T$ needed in Table 2 can be calculated from the dimensionless Helmholtz free energy equation $\phi(\tau,\delta) = \phi^o(\tau,\delta)+\phi^r(\tau,\delta)$ of the IAPWS-95 as follows:

$$p = \rho RT\left(1 + \delta\phi_\delta^r\right)$$

$$\left(\frac{\partial p}{\partial T}\right)_v = \rho R\left[1 + \delta\phi_\delta^r - \tau\delta\phi_{\delta\tau}^r\right]$$

$$s = R\left[\tau\left(\phi_\tau^o + \phi_\tau^r\right) - \phi^o - \phi^r\right]$$

$$\left(\frac{\partial p}{\partial v}\right)_T = RT\left(-\rho^2 - 2\rho^2\delta\phi_\delta^r - \rho^2\delta^2\phi_{\delta\delta}^r\right) \tag{13}$$

$$c_v = -R\tau^2\left(\phi_{\tau\tau}^o + \phi_{\tau\tau}^r\right),$$

where ϕ, τ and δ are as given in Eq. (9). The constants, the equations $\phi^o(\tau,\delta)$ and $\phi^r(\tau,\delta)$ and their derivatives $\phi_\tau^o, \phi_{\tau\tau}^o, \phi_\tau^r, \phi_\delta^r, \phi_{\tau\tau}^r, \phi_{\delta\delta}^r, \phi_{\delta\tau}^r$ are given in [5,6].

SUMMARY

The paper has presented a common procedure for calculating any thermodynamic differential quotients of the properties p, T, v, u, h, s, g, or f using the fundamental equations of the new

Industrial Formulation IAPWS-IF97. The formulas can be formally applied by the user without knowledge of the thermodynamic differential equations.

In addition, the corresponding algorithm for calculating any differential quotients using the new Scientific Formulation IAPWS-95 is shown. The formulas will prove useful as supplements to the Releases of the IAPWS-IF97 and IAPWS-95 Formulations.

In order to make it possible to calculate any differential quotient it is highly recommended that steam tables contain values for the differential quotients $\left(\frac{\partial v}{\partial p}\right)_T$ and $\left(\frac{\partial v}{\partial T}\right)_p$ as well as values for the properties v, h, s, c_p. Steam property program packages should also offer functions for these differential quotients.

Users who are interested in the programs for calculating the derivatives of the IF97 equations can receive the source code upon request.

Furthermore, the authors offer software packages for calculating the properties of water and steam using the new industrial standard IAPWS-IF97 including all differential quotients. The programs can be used as Dynamic Link Library in Mathcad® or other Windows applications. An Add-In allows the user to use property functions in the DLL from within Microsoft Excel® and to represent the calculated values in thermodynamic charts.

ACKNOWLEDGMENT

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