

Supplementary Backward Equations for the Industrial Formulation IAPWS-IF97 of Water and Steam for Fast Calculations of Heat Cycles, Boilers, and Steam Turbines

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The paper gives an overview of the backward equations which were developed as a supplement to the "IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" (IAPWS-IF97). First, backward equations $p(h,s)$ for the liquid region 1 and vapor region 2 were developed and adopted as a Supplementary Release in 2001 (IAPWS-IF97-S01). An international survey revealed that backward equations in the critical and supercritical regions (region 3) were also required in process modeling. Thus, backward equations $T(p,h)$, $v(p,h)$, $T(p,s)$, and $v(p,s)$ for region 3 were developed and adopted by IAPWS as a Supplementary Release in 2003 (IAPWS-IF97-S03). An extended revision of this release will be adopted in 2004. Further backward equations $p(h,s)$ developed for region 3 have been evaluated successfully and will be adopted as a Supplementary Release in 2004. In addition, backward equations $v(p,T)$ for region 3 will be proposed in 2004. For steam-turbine calculations, a backward equation for the saturation temperature as a function of enthalpy and entropy in the important part of two-phase region 4 has been developed. In order to determine if a given state point is located in one of the single-phase regions 1, 2, 3 or in the two-phase region 4, iterations are necessary for the backward functions of the given properties (p,h) , (p,s) or (h,s) . For this reason, special boundary equations were developed. Using the IAPWS-IF97 equations, along with the supplementary backward and boundary equations here presented, all thermodynamic properties from given property pairs (p,T) , (p,h) , (p,s) , and (h,s) can be calculated without iterations over the entire range of validity including the determination of the region (except for high temperature region 5). Because the numerical consistency of the backward and boundary equations is sufficient for most heat-cycle, boiler, and steam-turbine calculations, they will significantly reduce the computing time of process modeling.

1. Introduction

In 1997, the International Association for the Properties of Water and Steam (IAPWS) adopted the "IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" (IAPWS-IF97) [1, 2]. The IAPWS-IF97 contains fundamental equations $g(p,T)$ for liquid region 1, vapor region 2 and high-temperature region 5, a fundamental equation $f(v,T)$ for the critical and supercritical regions (region 3) and for region 4 an equation pair for saturation pressure $p_{\text{sat}}(T)$ and for saturation temperature $T_{\text{sat}}(p)$. Fig. 1 shows the regions of the IAPWS-IF97. The IAPWS-IF97 equations are marked by the superscript "97".

Using the fundamental IAPWS-IF97 equations, all thermodynamic properties and derivatives can

be calculated from given pressure and temperature in regions 1, 2, 5, and from given specific volume or density and temperature in region 3.

In addition, the IAPWS-IF97 contains backward equations for the most commonly used implicit functions $T(p,h)$ and $T(p,s)$ in regions 1 and 2.

Further dependencies have to be calculated iteratively from the fundamental equations. This means that one-dimensional or two-dimensional iterations are necessary for determining thermodynamic properties in process modeling. For this purpose, the IAPWS working groups "Industrial Requirements and Solutions" (IRS) and "Thermophysical properties of Water and Steam" (TPWS) established the "Task Group on Supplementary Backward Equations for IAPWS-

IF97" and supplementary backward equations have been developed over the last 5 years.

The members of the task group are

- A. Dittmann
- K. Knobloch
- H.-J. Kretzschmar (chair)
- R. Mareš
- R. Span
- I. Stöcker
- W. Wagner.

Important contributions were made by

- J. R. Cooper
- D. G. Friend
- A. H. Harvey.

Besides these "developers" the members of the evaluation task group

- J. Gallagher
- K. Miyagawa (chair)
- N. Okita
- I. Weber

played a considerable part in the quality assurance of the developed equations.

The supplementary releases listed in Table 1 are the results of this work.

2. Structure of IAPWS-IF97 and Supplementary Backward Equations

Figure 1 shows, in addition to the IAPWS-IF97 equations, the supplementary backward equations for regions 1, 2, 3, and 4.

Besides the IAPWS-IF97 backward equations, $T_1^{97}(p, h)$, $T_1^{97}(p, s)$ for liquid region 1 and $T_2^{97}(p, h)$, $T_2^{97}(p, s)$ for vapor region 2, equations $p_1^{01}(h, s)$ and $p_2^{01}(h, s)$ were developed [4, 13]. They are included in of the supplementary release IAPWS-IF97-S01 [3].

For region 3, IAPWS-IF97 did not provide backward equations. Therefore, equations $T_3^{03}(p, h)$, $v_3^{03}(p, h)$, $T_3^{03}(p, s)$, $v_3^{03}(p, s)$ and $p_3^{04}(h, s)$ were developed [7, 9, 13] and adopted by IAPWS as the supplementary releases IAPWS-IF97-S03rev [6] and IAPWS-IF97-S04 [8].

In addition, IAPWS-IF97-S04 contains an equation $T_{sat}^{04}(h, s)$ for the part of wet-steam region 4 which is important for steam turbine calculations.

The equations developed for phase and region boundaries are not included in Fig. 1.

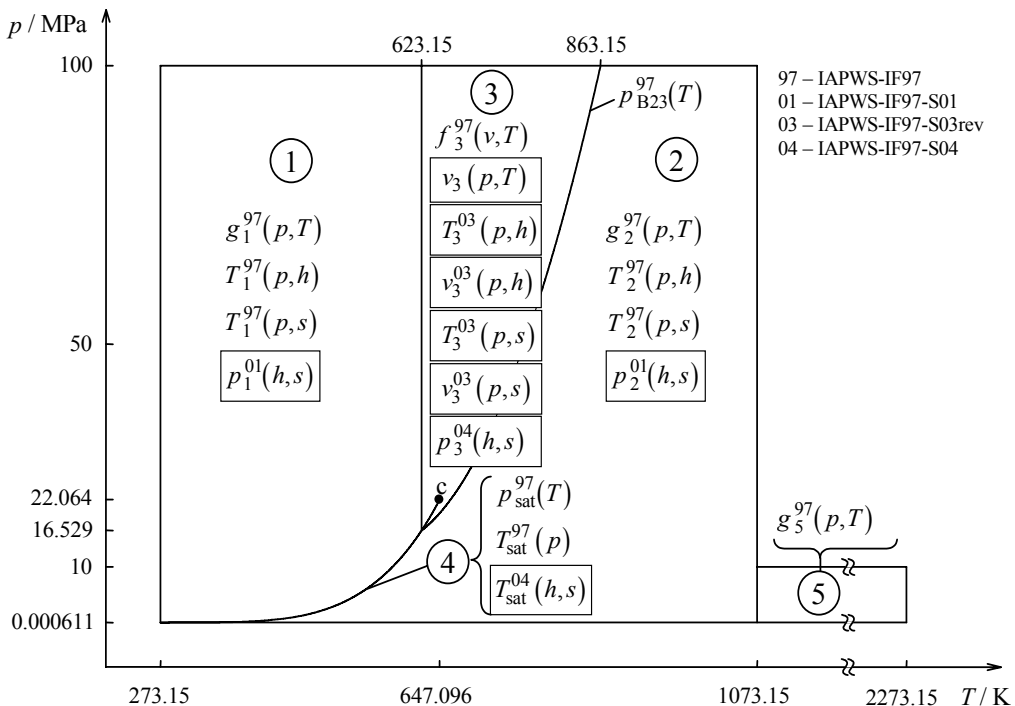


Fig. 1. p - T diagram with regions and equations of the IAPWS-IF97, and supplementary backward equations.

3. Backward and Boundary Equations for Functions of Pressure and Enthalpy (p, h)

3.1 Subregions and Backward Equations In process modeling, thermodynamic properties of water and steam are required for given properties (p, h).

Fig. 2 shows the range of validity of IAPWS-IF97 and the regions/subregions of the provided backward equations in a p - h diagram. In order to meet the extremely high numerical consistency requirements for the backward equations, region 2 was divided into three subregions, namely 2a, 2b, and 2c, and region 3 into subregions 3a and 3b.

The IAPWS-IF97 contains equations $T_1^{97}(p, h)$ in liquid region 1 and $T_{2a}^{97}(p, h)$, $T_{2b}^{97}(p, h)$, $T_{2c}^{97}(p, h)$ in vapor subregions 2a, 2b, and 2c. Using the temperature T calculated from these equations and given pressure, all thermodynamic properties can be calculated from the derivatives of the fundamental equations $g_1^{97}(p, T)$ or $g_2^{97}(p, T)$.

For region 3, equations $T_{3a}^{03}(p, h)$, $v_{3a}^{03}(p, h)$ and $T_{3b}^{03}(p, h)$, $v_{3b}^{03}(p, h)$ for subregions 3a and 3b are contents of IAPWS-IF97-S03rev. Using temperature T and specific volume v calculated from these equations, all other properties can be determined from the IAPWS-IF97 fundamental equation $f_3^{97}(v, T)$ of region 3.

The backward equations $T(p, h)$ and $v(p, h)$ have the following structures:

$$\frac{T(p, h)}{T^*} = \sum_{i=1}^N n_i \left(\frac{p}{p^*} + a \right)^{I_i} \left(\frac{h}{h^*} + b \right)^{J_i}, \quad (1)$$

$$\frac{v(p, h)}{v^*} = \sum_{i=1}^N n_i \left(\frac{p}{p^*} + a \right)^{I_i} \left(\frac{h}{h^*} + b \right)^{J_i}. \quad (2)$$

The numbers of coefficients N and non-linear parameters a and b of Eq. (1) and (2) are listed in Table 2. The coefficients n_i , exponents I_i , J_i , and reducing parameters T^* or v^* , p^* , and h^* can be taken from [1, 2] and [6, 7].

Table 1. Supplementary releases including backward equations for IAPWS-IF97.

Supplementary Release	Equations	Status	Ref.
IAPWS-IF97-S01: 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.	$p_1(h, s)$ $p_2(h, s)$	adopted in 2001	[3, 4]
IAPWS-IF97-S03: 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.	$T_3, v_3(p, h)$ $T_3, v_3(p, s)$	adopted in 2003	[5]
IAPWS-IF97-S03rev (Replacement for IAPWS-IF97-S03): 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.	$T_3, v_3(p, h)$ $T_3, v_3(p, s)$ $p_{3\text{sat}}(h)$ $p_{3\text{sat}}(s)$	adopted in 2004	[6, 7]
IAPWS-IF97-S04: 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.	$p_3(h, s)$ $T_{\text{sat}}(h, s)$ $h'(s)$, $h''(s)$ $h_{\text{B}13}(s)$ $T_{\text{B}23}(h, s)$	adopted in 2004	[8, 9]
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. (Draft)	$v_3(p, T)$	evaluated, to be adopted in 2005	[10, 11]

In the two-phase region 4, temperature can be directly calculated from given pressure p using the saturation temperature equation $T_{\text{sat}}^{97}(p)$.

The temperature has to be calculated iteratively from the IAPWS-IF97 fundamental equation $g_5^{97}(p, T)$ in high-temperature region 5.

Table 2. Numbers of Coefficients and non-linear parameters of the backward equations $T(p, h)$, Eq. (1), and $v(p, h)$, Eq. (2).

Equation	N	a	b
$T_1^{97}(p, h)$	20	0	1
$T_{2a}^{97}(p, h)$	34	0	-2.1
$T_{2b}^{97}(p, h)$	38	-2	-2.6
$T_{2c}^{97}(p, h)$	23	25	-1.8
$T_{3a}^{03}(p, h)$	31	0.24	-0.615
$T_{3b}^{03}(p, h)$	33	0.298	-0.720
$v_{3a}^{03}(p, h)$	32	0.128	-0.727
$v_{3b}^{03}(p, h)$	30	0.0661	-0.72

3.2 Boundary Equations Before calculating properties, the region/subregion has to be determined for given properties p and h . Fig. 2 shows the boundaries between regions or subregions to be calculated.

Because pressure is given, the boundary lines $x = 0$ between regions 4 and 1, $x = 1$ between region 4 and subregions 2a, 2b and 2c, the 350 °C isotherm and the 4 MPa isobare can be determined without iteration.

The equation $T_{B23}^{97}(p)$ is a converted polynomial of the second degree while $p_{2bc}^{97}(h)$ and $h_{3ab}^{03}(p)$ are polynomials of the second and third degree.

For calculating the saturated liquid line between two-phase region 4 and subregion 3a and the saturated vapor line between region 4 and subregion 3b using the IAPWS-IF97 fundamental equation $f_3^{97}(v, T)$ for given properties p and h , an iteration would be necessary. Therefore, IAPWS-IF97-S03rev provides an equation $p_{3\text{sat}}^{03}(h)$ which is described in [6, 7].

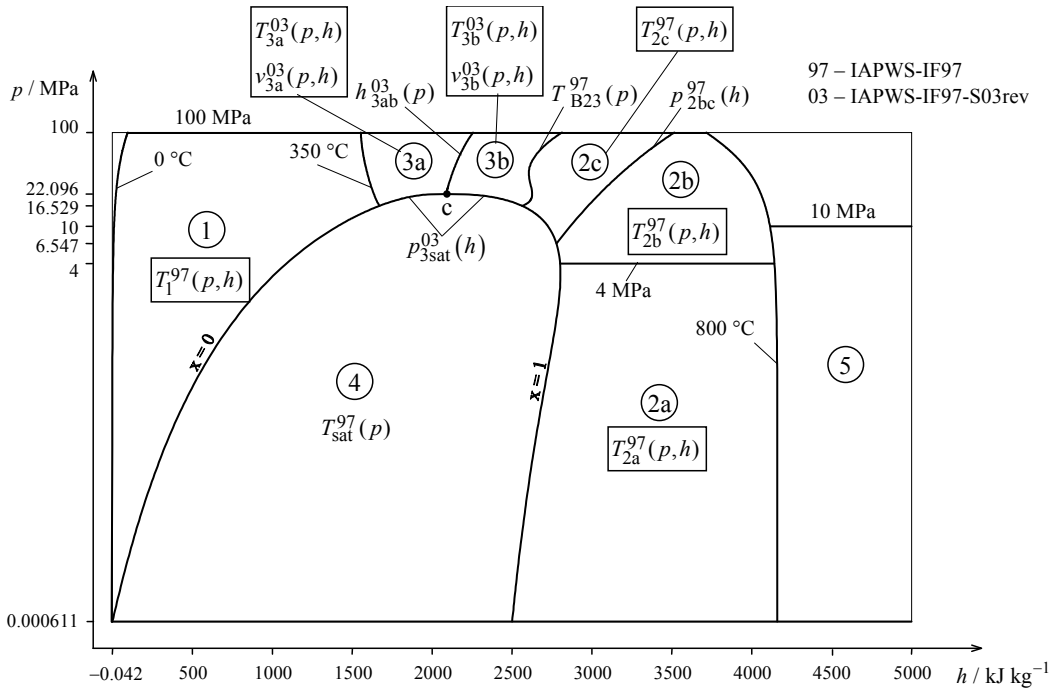


Fig. 2. p - h diagram with regions and subregions, backward equations and boundary equations for the function of (p, h) .

3.3 Numerical Consistency The numerical consistency of the backward equations $T(p, h)$ and $v(p, h)$ with the fundamental equations of IAPWS-IF97 results from process modeling requirements. Using results of an international survey [12], IAPWS has determined the permissible tolerances $|\Delta T|_{\text{tol}}$ for temperature, to be 25 mK for entropies less than or equal to $5.85 \text{ kJ kg}^{-1} \text{ K}^{-1}$ (region 1, subregions 3a, 3b, and 2c) and to be 10 mK for entropies greater than this value (subregions 2a and 2b). The permissible relative tolerance $|\Delta v/v|_{\text{tol}}$ for specific volume in subregions 3a and 3b was determined to be 0.01 %.

The numerical consistencies of the equations and the tolerated values are listed in Table 3. As can be seen, the maximum temperature differences $|\Delta T|_{\text{max}}$ and the maximum relative differences of specific volume $|\Delta v/v|_{\text{max}}$ are less than the permissible tolerances. In order to avoid numerical problems, the backward equations of subregions 3a and 3b represent the critical point exactly.

At the subregion boundaries $p = 4 \text{ MPa}$ and $p_{2bc}^{97}(h)$ of region 2, and at $h_{3ab}^{03}(p)$ of region 3 the differences between the backward equations of the adjacent subregions are smaller than their numerical consistencies with the IAPWS-IF97 fundamental equations. Therefore, numerical problems at subregion boundaries will be avoided.

Table 3. Numerical consistencies of the backward equations $T(p, h)$ and $v(p, h)$ with IAPWS-IF97.

Equation	$ \Delta T _{\text{tol}}$ mK	$ \Delta T _{\text{max}}$ mK
$T_1^{97}(p, h)$	25	23.6
$T_{2a}^{97}(p, h)$	10	9.3
$T_{2b}^{97}(p, h)$	10	9.6
$T_{2c}^{97}(p, h)$	25	23.7
$T_{3a}^{03}(p, h)$	25	23.6
$T_{3b}^{03}(p, h)$	25	19.6
Equation	$ \Delta v/v _{\text{tol}}$ %	$ \Delta v/v _{\text{max}}$ %
$v_{3a}^{03}(p, h)$	0.01	0.0080
$v_{3b}^{03}(p, h)$	0.01	0.0095

4. Backward and Boundary Equations for Functions of Pressure and Entropy (p, s)

4.1 Subregions and Backward Equations Figure 3 shows the range of validity of IAPWS-IF97 and the

regions/subregions of the provided backward equations as functions of (p, s) in a p - s diagram. As was done for the functions of (p, h), region 2 was also divided into three subregions, 2a, 2b, and 2c, and region 3 into subregions, 3a and 3b, in order to meet the numerical consistency requirements of process modeling.

The IAPWS-IF97 contains equations $T_1^{97}(p, s)$ in liquid region 1 and $T_{2a}^{97}(p, s)$, $T_{2b}^{97}(p, s)$, $T_{2c}^{97}(p, s)$ in vapor subregions 2a, 2b, and 2c. Using the temperature T calculated from these equations and given pressure, all thermodynamic properties can be calculated from the fundamental equations $g_1^{97}(p, T)$ or $g_2^{97}(p, T)$.

In region 3, equations $T_{3a}^{03}(p, s)$, $v_{3a}^{03}(p, s)$ and $T_{3b}^{03}(p, s)$, $v_{3b}^{03}(p, s)$ for subregions 3a and 3b are provided by IAPWS-IF97-S03rev. Using T and v calculated from these equations, all other properties can be determined from the fundamental equation $f_3^{97}(v, T)$.

The backward equations $T(p, s)$ and $v(p, s)$ have the following structures:

$$\frac{T(p, s)}{T^*} = \sum_{i=1}^N n_i \left(\frac{p}{p^*} + a \right)^{I_i} \left(\frac{s}{s^*} + b \right)^{J_i}, \quad (3)$$

$$\frac{v(p, s)}{v^*} = \sum_{i=1}^N n_i \left(\frac{p}{p^*} + a \right)^{I_i} \left(\frac{s}{s^*} + b \right)^{J_i}. \quad (4)$$

The numbers of coefficients N and non-linear parameters a and b are listed in Table 4. The coefficients n_i , exponents I_i , J_i , and reducing parameters T^* or v^* , p^* , and s^* can be taken from [1, 2] and [6, 7].

In the two-phase region 4, temperature can be directly calculated from given pressure p using the saturation temperature equation $T_{\text{sat}}^{97}(p)$.

In high-temperature region 5, on the other hand, temperature must be calculated iteratively using the IAPWS-IF97 fundamental equation $g_5^{97}(p, T)$.

4.2 Boundary Equations Before calculating properties, the region/subregion has to be determined for given properties p and s . Figure 3 shows the boundaries between regions or subregions to be calculated.

Because pressure and entropy are given, the boundary lines $x = 0$ between regions 4 and 1, $x = 1$ between region 4 and subregions 2a, 2b and 2c, the $350 \text{ }^\circ\text{C}$ isotherm, isentropic lines s_c and $s = 5.85 \text{ kJ kg}^{-1} \text{ K}^{-1}$, and the 4 MPa isobare can be calculated without iteration.

The equation $T_{B23}^{97}(p)$ is a converted polynomial of the second degree.

For calculating the saturated liquid line between two-phase region 4 and subregion 3a and the saturated vapor line between region 4 and subregion 3b from IAPWS-IF97 fundamental

Table 4. Numbers of coefficients and nonlinear parameters of the backward equations $T(p,s)$, Eq. (3), and $v(p,s)$, Eq. (4).

Equation	N	a	b
$T_1^{97}(p,s)$	20	0	2
$T_{2a}^{97}(p,s)$	46	0	-2
$T_{2b}^{97}(p,s)$	44	0	10
$T_{2c}^{97}(p,s)$	30	0	2
$T_{3a}^{03}(p,s)$	33	0.24	-0.703
$T_{3b}^{03}(p,s)$	28	0.76	-0.818
$v_{3a}^{03}(p,s)$	28	0.187	-0.755
$v_{3b}^{03}(p,s)$	31	0.298	-0.816

equation $f_3^{97}(v,T)$ for given properties p and s , an iteration would be necessary. Therefore, IAPWS-IF97-S03rev, described in [6, 7], provides the boundary equation $p_{3sat}^{03}(s)$.

4.3 Numerical Consistency For the numerical consistencies of the backward equations $T(p,s)$ and $v(p,s)$ with the fundamental equations of IAPWS-IF97, IAPWS has determined the permissible tolerance $|\Delta T|_{tol} = 25$ mK for entropies less than or equal to $5.85 \text{ kJ kg}^{-1} \text{ K}^{-1}$ (region 1, subregions 3a, 3b, and 2c) and 10 mK for entropies greater than this value (subregions 2a and 2b). The permissible relative tolerance for specific volume in subregions 3a and 3b was determined as $|\Delta v/v|_{tol} = 0.01\%$.

Table 5 shows the numerical consistencies of the backward equations in comparison with the tolerated values. As can be seen, the maximum temperature differences $|\Delta T|_{max}$ and maximum relative differences of specific volume $|\Delta v/v|_{max}$ are less than the permissible tolerances.

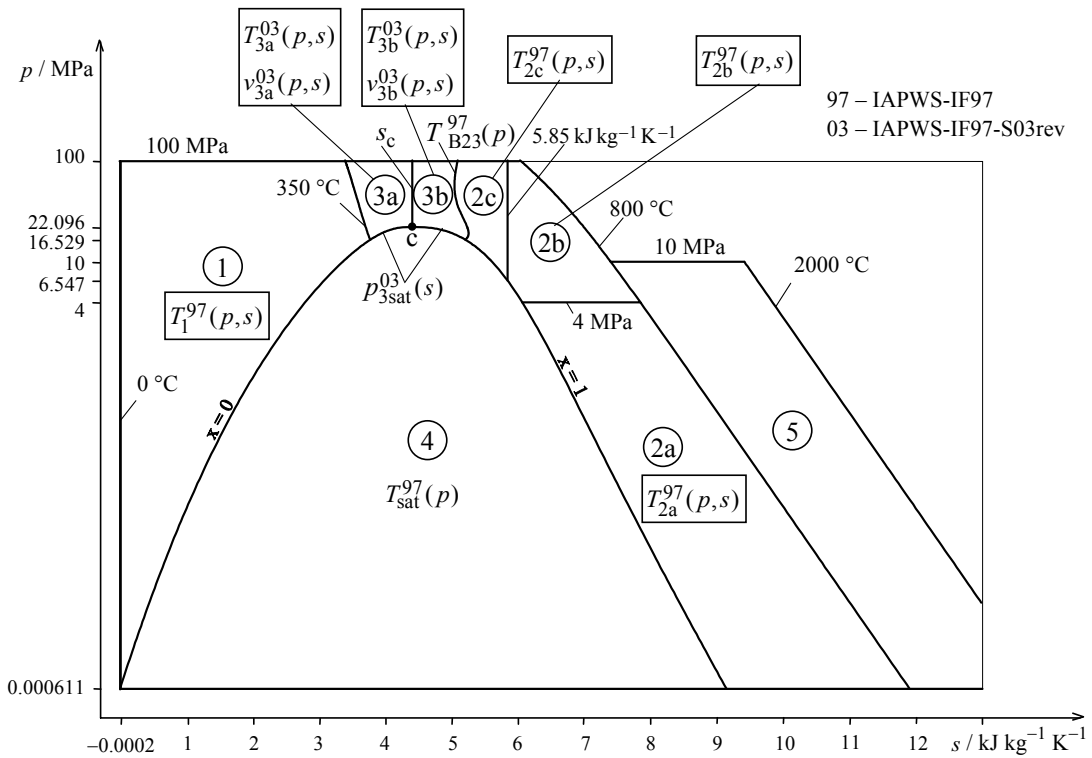


Fig. 3. p - s diagram with regions and subregions, backward equations and boundary equations for the function of (p,s) .

Table 5. Numerical consistencies of the backward equations $T(p,s)$ and $v(p,s)$ with IAPWS-IF97.

Equation	$ \Delta T _{\text{tol}}$ mK	$ \Delta T _{\text{max}}$ mK
$T_1^{97}(p,s)$	25	21.8
$T_{2a}^{97}(p,s)$	10	8.8
$T_{2b}^{97}(p,s)$	10	6.5
$T_{2c}^{97}(p,s)$	25	19.0
$T_{3a}^{03}(p,s)$	25	24.8
$T_{3b}^{03}(p,s)$	25	22.1
Equation	$ \Delta v/v _{\text{tol}}$ %	$ \Delta v/v _{\text{max}}$ %
$v_{3a}^{03}(p,s)$	0.01	0.0096
$v_{3b}^{03}(p,s)$	0.01	0.0077

In order to avoid numerical problems, the backward equations of subregions 3a and 3b again represent the critical point exactly.

At the subregion boundaries $p = 4 \text{ MPa}$ and $s = 5.85 \text{ kJ kg}^{-1} \text{ K}^{-1}$ of region 2, and s_c of region 3, the differences between the backward

equations of the adjacent subregions are smaller than their numerical consistencies with the IAPWS-IF97 fundamental equations. This avoids numerical problems at subregion boundaries.

5. Backward and Boundary Equations for Functions of Enthalpy and Entropy (h,s)

5.1 Subregions and Backward Equations The h - s diagram in Fig. 4 shows the range of validity of IAPWS-IF97 and the regions/subregions of the backward equations as functions of (h,s) presented here.

As with the other backward functions, region 2 has also been divided into subregions 2a, 2b, and 2c and region 3 into subregions 3a and 3b to meet the numerical consistency requirements of process modeling.

The supplementary release IAPWS-IF97-S01 contains equations $p_1^{01}(h,s)$ in liquid region 1 and $p_{2a}^{01}(h,s)$, $p_{2b}^{01}(h,s)$, $p_{2c}^{01}(h,s)$ in vapor subregions 2a, 2b, and 2c. Using pressure p calculated from these equations, temperature T can be calculated by using the equations $T_1^{97}(p,h)$ in liquid region and $T_{2a}^{97}(p,h)$, $T_{2b}^{97}(p,h)$, $T_{2c}^{97}(p,h)$ in vapor subregions.

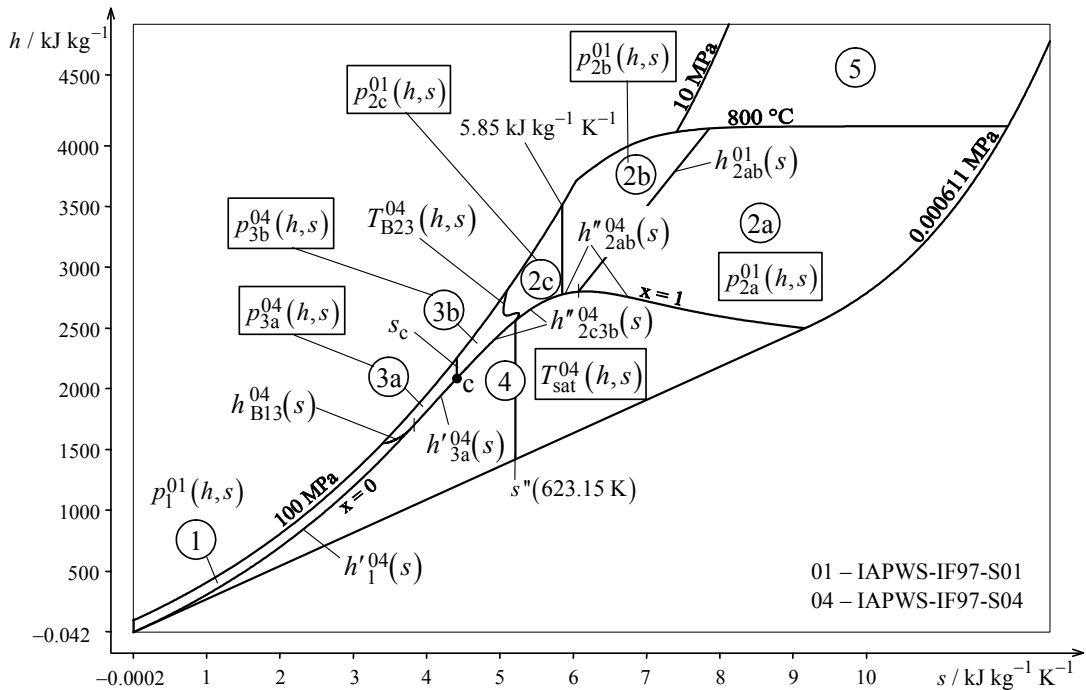


Fig. 4. h - s diagram with regions and subregions, backward equations and boundary equations for the function of (h,s).

All thermodynamic properties can then be calculated from the derivatives of the fundamental equations $g_1^{97}(p, T)$ or $g_2^{97}(p, T)$.

For region 3, equations $p_{3a}^{04}(h, s)$ and $p_{3b}^{04}(h, s)$ in subregions 3a and 3b are provided by IAPWS-IF97-S04. Using pressure p calculated from these equations, temperature T and specific volume can be determined by using the equations $T_{3a}^{03}(p, h)$, $T_{3b}^{03}(p, h)$ and $v_{3a}^{03}(p, s)$, $v_{3b}^{03}(p, s)$ of IAPWS-IF97-S03. Now, all other thermodynamic properties can be calculated from the IAPWS-IF97 fundamental equation $f_3^{97}(v, T)$.

The backward equations $p(h, s)$ have the following structure:

$$\frac{p(h, s)}{p^*} = \left[\sum_{i=1}^N n_i \left(\frac{h}{h^*} + a \right)^{I_i} \left(\frac{s}{s^*} + b \right)^{J_i} \right]^c. \quad (5)$$

The numbers of coefficients N , and non-linear parameters a , b , and c are listed in Table 6. The coefficients n_i , exponents I_i , J_i and reducing parameters p^* , h^* , and s^* can be taken from [3, 4] and [8, 9].

In the part of the two-phase region 4 which is important for steam-turbine calculations, IAPWS-IF97-S04 provides an equation $T_{\text{sat}}^{04}(h, s)$; see Fig. 4. The equation is valid for entropies $s \geq s^*(350^\circ\text{C}) = 5.21 \text{ kJ kg}^{-1} \text{ K}^{-1}$. Using saturation temperature T_{sat} , saturation pressure p_{sat} can be calculated from IAPWS-IF97 equation $p_{\text{sat}}^{97}(T_{\text{sat}})$ and vapor fraction x from $x = (h - h') / (h'' - h')$, where $h' = h_1^{97}(p_{\text{sat}}, T_{\text{sat}})$ and $h'' = h_2^{97}(p_{\text{sat}}, T_{\text{sat}})$.

Table 6. Numbers of coefficients and nonlinear parameters of the backward equations $p(h, s)$, Eq. (5).

Equation	N	a	b	c
$p_1^{01}(h, s)$	19	0.05	0.05	1
$p_{2a}^{01}(h, s)$	29	-0.5	-1.2	4
$p_{2b}^{01}(h, s)$	33	-0.6	-1.01	4
$p_{2c}^{01}(h, s)$	31	-0.7	-1.1	4
$p_{3a}^{04}(h, s)$	33	-1.01	-0.75	1
$p_{3b}^{04}(h, s)$	35	-0.681	-0.7921	1

All other thermodynamic properties in the two-phase region can then be determined from the fundamental equations $g_1^{97}(p, T)$ and $g_2^{97}(p, T)$.

The backward equation $T_{\text{sat}}^{04}(h, s)$ has the following structure:

$$\frac{T_{\text{sat}}(h, s)}{T^*} = \sum_{i=1}^{36} n_i \left(\frac{h}{h^*} - 0.119 \right)^{I_i} \left(\frac{s}{s^*} - 1.07 \right)^{J_i}. \quad (6)$$

The coefficients n_i , exponents I_i , J_i and reducing parameters p^* , h^* and s^* can be taken from [8, 9].

In the other part of the two-phase region 4, saturation temperature, saturation pressure and vapor fraction have to be calculated iteratively from the IAPWS-IF97 saturation pressure equation in combination with the fundamental equations.

In high-temperature region 5, temperature and pressure must be calculated using the IAPWS-IF97 fundamental equation $g_5^{97}(p, T)$ via two-dimensional iteration.

5.2 Boundary Equations Before calculating properties, the region/subregion has to be determined for given properties h and s . Figure 4 shows the boundaries between regions or subregions to be considered.

Because enthalpy and entropy are given, all region boundaries would have to be determined iteratively by using IAPWS-IF97 fundamental equations except the subregion boundary lines s_c , $s = 5.85 \text{ kJ kg}^{-1} \text{ K}^{-1}$, and $h_{2ab}^{01}(s)$. Therefore, IAPWS-IF97-S04 provides the following boundary equations:

- $h_1^{04}(s)$ for saturated liquid line $x = 0$ between region 4 and region 1
- $h_{3a}^{04}(s)$ for saturated liquid line $x = 0$ between region 4 and subregion 3a
- $h_{2c3b}^{04}(s)$ for saturated vapor line $x = 1$ between region 4 and subregions 2c and 3b
- $h_{2ab}^{04}(s)$ for saturated vapor line $x = 1$ between region 4 and subregions 2a and 2b
- $h_{B13}^{04}(s)$ for the isotherm $T = 350^\circ\text{C}$ between regions 1 and 3
- $T_{B23}^{04}(h, s)$ in addition to $p_{2c}^{01}(h, s)$ for the $p_{B23}^{97}(T)$ line of IAPWS-IF97 between regions 2 and 3.

The equations and the determination of the subregions are described comprehensively in [8, 9].

5.3 Numerical Consistency Table 7 shows the numerical consistencies of the backward equations $p(h, s)$ and of the related backward functions $T(h, s)$ and $v(h, s)$ in comparison with the tolerated values. As can be seen, the maximum relative pressure differences $|\Delta p/p|_{\text{max}}$, the maximum temperature differences $|\Delta T|_{\text{max}}$ and

the maximum relative differences of specific volume $|\Delta v/v|_{\max}$ in all regions and subregions are less than the permissible tolerances. This is also true for saturation pressure, saturation temperature, and vapor fraction in two-phase region 4.

6. Backward Equations for Functions of Pressure and Temperature (p, T) in Region 3

6.1 Subregions and Backward Equations Because an iteration is necessary to calculate properties in region 3 from the IAPWS-IF97 fundamental equation $f_3^{97}(v, T)$ for given properties p and T , the backward equations $v_3(p, T)$ are provided for region 3 [10, 13]. The p - T diagrams in Figs. 2 and 3 of the paper [11] show the subregions (3a to 3t) into which region 3 is divided. All in all, 20 subregions were necessary in order to meet the extremely high process modeling numerical consistency requirements. Once we have the specific volume v , calculated from the backward equations, all other thermodynamic properties can be determined using the IAPWS-IF97 fundamental equation $f_3^{97}(v, T)$.

For a small area very near the critical point, it was not possible to meet the numerical consistency requirements fully. This near-critical

region is covered with reasonable consistency by six subregions with auxiliary equations.

The backward equations $v(p, T)$ for subregions 3a to 3t, except 3n, have the following structure:

$$\frac{v(p, T)}{v^*} = \left[\sum_{i=1}^N n_i \left[\left(\frac{p}{p^*} - a \right)^c \right]^{I_i} \left[\left(\frac{T}{T^*} - b \right)^d \right]^{J_i} \right]^e \quad (7)$$

and for subregion 3n:

$$\frac{v_{3n}(p, T)}{v^*} = \exp \left[\sum_{i=1}^N n_i \left(\frac{p}{p^*} - a \right)^{I_i} \left(\frac{T}{T^*} - b \right)^{J_i} \right] \quad (8)$$

Coefficients n_i , exponents I_i , J_i , reducing parameters v^* , p^* , and T^* , and non-linear parameters a , b , c , d , and e can be taken from [10, 13].

6.2 Subregion-Boundary Equations Before calculating the correct $v(p, T)$ equation, the subregion has to be determined for given properties p and T . The subregion-boundary equations are described in the paper [11]. The coefficients are listed in [10, 13].

Table 7. Numerical consistencies of the backward equations $p(h, s)$, of the related backward functions $T(h, s)$ and $v(h, s)$, and of $T_{\text{sat}}(h, s)$ with IAPWS-IF97.

Equation	$ \Delta p/p _{\text{tol}}$ %	$ \Delta p/p _{\text{max}}$ %	$ \Delta T _{\text{tol}}$ mK	$ \Delta T _{\text{max}}$ mK	$ \Delta v/v _{\text{tol}}$ %	$ \Delta v/v _{\text{max}}$ %
$p_1^{01}(h, s)$ $p \leq 2.5 \text{ MPa}$	0.60	0.55	25	24.0		
$p_1^{01}(h, s)$ $p > 2.5 \text{ MPa}$	15 kPa	14 kPa				
$p_{2a}^{01}(h, s)$	0.0035	0.0029	10	9.7		
$p_{2b}^{01}(h, s)$	0.0035	0.0034	10	9.8		
$p_{2c}^{01}(h, s)$	0.0088	0.0063	25	24.9		
$p_{3a}^{04}(h, s)$	0.01	0.0070	25	23.7	0.01	0.0097
$p_{3b}^{04}(h, s)$	0.01	0.0084	25	22.4	0.01	0.0095
Equation	$ \Delta T _{\text{tol}}$ mK	$ \Delta T _{\text{max}}$ mK	$ \Delta p/p _{\text{tol}}$ %	$ \Delta p/p _{\text{max}}$ %	$ \Delta x _{\text{tol}}$ -	$ \Delta x _{\text{max}}$ -
$T_{\text{sat}}^{04}(h, s)$ $s \leq 5.85 \text{ kJ kg}^{-1} \text{ K}^{-1}$	25	0.86	0.0088	0.0034	4.4×10^{-6}	0.57×10^{-6}
$T_{\text{sat}}^{04}(h, s)$ $s > 5.85 \text{ kJ kg}^{-1} \text{ K}^{-1}$	10	0.67	0.0035	0.0029	0.64×10^{-6}	0.25×10^{-6}

6.3 Numerical Consistency The maximum relative deviations of specific volume, enthalpy, entropy, isobaric heat capacity and the speed of sound calculated from the backward equations $v(p,T)$ to the IAPWS-IF97 fundamental equation $f_3^{97}(v,T)$ of region 3 are listed in Table 3 of [11].

As can be seen, the deviations of the specific volume, enthalpy, and entropy calculated from the presented $v(p,T)$ equations to the IAPWS-IF97 fundamental equation are less than 0.001 % and the deviations of isobaric heat capacity and speed of sound are less than 0.01 %. This means that the values of specific volume, enthalpy and, entropy of IAPWS-IF97 are represented with 5 significant figures, and the values of isobaric heat capacity and speed of sound with 4 significant figures by using the backward equations $v(p,T)$.

At subregion boundaries, the differences between the calculated properties are smaller than their numerical consistencies with the fundamental equation mentioned before. Therefore, numerical problems at subregion boundaries will be avoided.

7. Computing Times in Comparison with IAPWS-IF97 Fundamental Equations

A very important motivation for the development of the backward equations was reducing the computing time needed to obtain thermodynamic properties. Using IAPWS-IF97 fundamental equations, time-consuming iterations such as the two-dimensional Newton method are required for backward functions. Table 8 shows the resulting computing time ratios (*CTR*), defined by

$$CTR = \frac{\text{Computing time of fundamental eq.}}{\text{Computing time of backward eq.}} \quad (9)$$

The calculations of the functions of given properties (p,h) by using the backward equations are between 14 times faster in region 2 and 43 times faster in region 1 than the corresponding iterations using the IAPWS-IF97 fundamental equations [15].

The calculations of functions of (p,s) by using the backward equations are between 17 times faster in region 2 and 70 times faster in region 1 than the corresponding iterations [15].

The calculations of functions of (h,s) by using the backward equations are between 10 times faster in region 3 and 38 times faster in region 2.

The calculations of functions of (p,T) in region 3 by using the backward equations are

17 times faster than the corresponding iterations using the IAPWS-IF97 fundamental equation [16]. Table 8. Computing time ratios between backward equations and iterations from IAPWS-IF97 fundamental equations.

Function	Reg.	Backward Equation(s)	CTR
(p,h)	1	$T_1^{97}(p,h)$	43
	2	$T_2^{97}(p,h)$	14
	3	$T_3^{03}(p,h)$ & $v_3^{03}(p,h)$	16
(p,s)	1	$T_1^{97}(p,s)$	70
	2	$T_2^{97}(p,s)$	17
	3	$T_3^{03}(p,s)$ & $v_3^{03}(p,s)$	18
(h,s)	1	$p_1^{01}(h,s)$ & $T_1^{97}(p,h)$	23
	2	$p_2^{01}(h,s)$ & $T_2^{97}(p,h)$	38
	3	$p_3^{04}(h,s)$ & $T_3^{03}(p,h)$ & $v_3^{03}(p,s)$	10
	4	$T_{\text{sat}}^{04}(h,s)$ & $p_{\text{sat}}^{97}(T)$ & $x = \frac{h-h'}{h''-h'}$	11
(p,T)	3	$v_3(p,T)$	17

An additional motivation for the development of the equations for region boundaries was reducing the computing time needed to determine the region for a given state point. By using boundary equations, users can determine the region without time-consuming iterations of IAPWS-IF97 fundamental equations. Table 9 shows the resulting *CTR* values.

The calculations of the phase boundary between two-phase region 4 and region 3 for given properties (p,h) or (p,s) by using the boundary equations are more than 9 times faster than the corresponding iterations using the IAPWS-IF97 fundamental equations.

The calculations of the phase boundaries and the boundaries between regions 1 and 2 or between regions 2 and 3 for given properties (h,s) by using the boundary equations are between 20 and 90 times faster than the corresponding iterations.

In conclusion, these factors show that the calculations of backward functions, including determination of the region using the backward equations and boundary equations, are between 5 and 20 times faster than the iteration of IAPWS-IF97 fundamental equations.

Taking in consideration the frequency of use for the various backward equations in process modeling, the calculations of heat-cycles, boilers, and particularly of steam turbines can be expected to be 2 to 3 times faster when using the supplementary backward and boundary equations.

Table 9. Computing time ratios between boundary equations and iterations from IAPWS-IF97 fundamental equations.

Funct.	Bound.	Reg.-Reg.	Bound. Eq.	CTR
(p,h)	$x = 0$	3 - 4	$p_{3sat}^{03}(h)$	12
	$x = 1$			
(p,s)	$x = 0$	3 - 4	$p_{3sat}^{03}(s)$	9
	$x = 1$			
(h,s)	$x = 0$	1 - 4	$h_1^{04}(s)$	24
		3 - 4	$h_{3a}^{04}(s)$	90
	$x = 1$	2 - 4	$h_{2ab}^{*04}(s)$,	20
			$h_{2c3b}^{*04}(s)$	
		3 - 4	$h_{2c3b}^{*04}(s)$	60
	623.15 K	1 - 3	$h_{B13}^{04}(s)$	37
$p_{B23}^{97}(T)$	2 - 3		$T_{B23}^{04}(h,s)$,	20
			$p_{2c}^{01}(h,s)$	

8. Application of the Backward and Boundary Equations

The numerical consistency of the backward equations and boundary equations described in Sections 3 to 6 with the IAPWS-IF97 fundamental equations is sufficient for most applications in heat cycle, boiler, and steam turbine calculations. For users not satisfied with the numerical consistency of the backward equations or boundary equations, they are still recommended for generating good starting points for an iterative process. It will significantly reduce the time required to meet the convergence criteria of the iteration.

The equations presented can only be used within their ranges of validity. They should not be used to determine any thermodynamic derivatives. The determination of thermodynamic derivatives from IAPWS-IF97 fundamental equations is described in [14].

The backward and boundary equations should also not be used together with the fundamental equations in iterative calculations of other backward functions. Iterations of backward

functions can only be performed using the fundamental equations.

In any case, depending on the application, a conscious decision is required whether to use the backward or boundary equations or to calculate the corresponding values by iteration from the IAPWS-IF97 fundamental equations.

9. Conclusions

The paper has presented backward equations and equations for region boundaries for calculating the functions of (p,h) , (p,s) , (h,s) and (p,T) in process modeling. The equations can be used as supplement to the Industrial Formulation IAPWS-IF97 for water and steam.

The numerical consistencies of the backward and boundary equations with the IAPWS-IF97 fundamental equations are sufficient for most applications in heat-cycle, boiler, and steam-turbine calculations.

Therefore, by using the backward and boundary equations, the properties as functions of (p,T) , (p,h) , (p,s) , and (h,s) , including determination of the region, can be calculated without iterations.

As a result, process calculations will be between 2 and 3 times faster when using the supplementary backward and boundary equations.

For applications where the demands on numerical consistency are extremely high, iterations using the IAPWS-IF97 fundamental equations may still be necessary. In these cases, the backward or boundary equations presented here can be used for calculating very accurate starting values.

Users who are interested in the equations here presented can receive the source code upon request; see <http://thermodynamics.hs-zigr.de>.

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