Supplementary Backward Equations $v(p,T)$ for the Critical and Supercritical Regions (Region 3) of the Industrial Formulation IAPWS-IF97 for Water and Steam

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In addition to the "IAPWS Industrial Formulation 1997 for the thermodynamic properties of water and steam" (IAPWS-IF97), the paper presents supplementary backward equations to calculate the specific volume from given pressure and temperature $v(p,T)$ in the critical and supercritical regions (region 3). The presented equations together with the IAPWS-IF97 basic equation for the Helmholtz free energy $f(v,T)$ make it possible to determine all thermodynamic properties from pressure and temperature in region 3 without iteration. 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 presented backward equations $v(p,T)$. The range of validity of the equations is region 3 of IAPWS-IF97 except a small region very close to the critical point. To fulfill the high numerical consistency requirements, the range of validity was divided into 20 subregions. The deviations between the backward equations of the adjacent subregions are smaller than their numerical consistencies with the IAPWS-IF97 basic equation. Since the numerical consistency of the $v(p,T)$ equations with IAPWS-IF97 is sufficient for most applications in heat cycle and boiler calculations, the otherwise necessary iteration can be avoided. The calculation of specific volume from pressure and temperature using the presented equations are more than 17 times faster than the iteration from IAPWS-IF97.

1. Introduction

The IAPWS Industrial Formulation 1997 for the thermodynamic properties of water and steam (IAPWS-IF97) [1, 2] was adopted in 1997. After that, the IAPWS-IF97 was supplemented by three supplementary releases IAPWS-IF97-S01 [3, 4], IAPWS-IF97-S03 [5], IAPWS-IF97-S03rev [6, 7], and IAPWS-IF97-S04 [8, 9] which include further backward equations. The paper [13] gives an overview of all backward equations developed for IAPWS-IF97.

Fig. 1 shows that region 3 of IAPWS-IF97 is covered by a basic equation for the free energy $f_3(v,T)$. All thermodynamic properties can be derived from the basic equation as a function of specific volume v and temperature T. However, in modeling steam power cycles, thermodynamic properties as functions of the variables (p,T) are required in region 3. It is cumbersome to perform these calculations with IAPWS-IF97, because they require iterations using the function $p(v,T)$ derived from the basic equation $f_3(v,T)$.

In order to avoid such iterations, this paper provides backward equations $v_3(p,T)$; see Fig. 1. With specific volume calculated from the backward equations, the other properties in region 3 can be calculated using the IAPWS-IF97 basic equation $f_3(v,T)$.

2. Numerical Consistency Requirements

The permissible value for the numerical consistency of the equations for specific volume with the IAPWS-IF97 fundamental equation was determined based on the accuracy of the iteration otherwise used. The iteration accuracy depends on thermodynamic process calculations. To obtain specific enthalpy or entropy from pressure and temperature in region 3 with a maximum deviation of 0.001 % to the IAPWS-IF97, and isobaric heat capacity or speed of sound with a maximum deviation of 0.01 %, the relative iteration accuracy of $|\Delta v/v| = 0.001$ % is sufficient. Therefore, the permissible relative tolerance for the equations $v_3(p,T)$ was set to $|\Delta v/v|_{\mathrm{tol}} = 0.001$ %.

3. Structure of the Equation Set

The range of validity of the equations $v_3(p,T)$ is region 3 defined by:

$$623.15\ \mathrm{K} \le T \le 863.15\ \mathrm{K}\ \text{ for}$$

$$p_{\mathrm{B23}}^{97}(T) \le p \le 100\ \mathrm{MPa}.$$

The function $p_{\mathrm{B23}}^{97}(T)$ represents the B23-equation of IAPWS-IF97. Figs. 2 and 3 show the way in which the range of validity is divided into the subregions 3a to 3t.

The subregion boundary equations, except $T_{3\mathrm{ab}}(p)$, $T_{3\mathrm{ef}}(p)$, and $T_{3\mathrm{op}}(p)$, have the following dimensionless form:

$$\frac{T(p)}{T^*} = \theta(\pi) = \sum_{i=1}^{N} n_i\, \pi^{I_i} \qquad (1)$$

where $\theta = T/T^*$, $\pi = p/p^*$ with $T^* = 1$ K and $p^* = 1$ MPa. The boundary equations $T_{3\mathrm{ab}}(p)$ and $T_{3\mathrm{op}}(p)$ have the form:

$$\frac{T(p)}{T^*} = \theta(\pi) = \sum_{i=1}^{N} n_i\, (\ln \pi)^{I_i}\ . \qquad (2)$$

The subregion boundary equation $T_{3\mathrm{ef}}(p)$ is a straight line from 22.064 MPa up to 40 MPa having the slope of the saturation-temperature curve of IAPWS-IF97 at the critical point. The coefficients n_i and the exponents I_i of the subregion boundary equations are listed in [10-12].

Table 1 summarizes pressures ranges and corresponding subregion boundary equations for determining the correct subregion (SR) 3a to 3t; see Figs. 2 and 3.

Investigations in the process of developing the equations $v_3(p,T)$ have shown, that the high numerical consistency requirement of 0.001 % can not be achieved by using simple functional forms in the region

$$T_{3\mathrm{q}}(p) < T < T_{3\mathrm{r}}(p)\ \text{ for}$$

$$p_{\mathrm{sat}}^{97}(643.15\ \mathrm{K}) < p < 22.5\ \mathrm{MPa};\ \text{see Figs. 2 and 3.}$$

The explanation for this limit is the complicated structure of the specific volume in the p-T plane, including an infinite slope at the critical point. For completing, [10-12] contain auxiliary equations for this small region very close to the critical point.

4. Backward Equations $v(p,T)$ for the Subregions 3a to 3t

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

$$\omega(\pi,\theta) = \left[\sum_{i=1}^{N} n_i \left[(\pi - a)^c\right]^{I_i} \left[(\theta - b)^d\right]^{J_i}\right]^e , \qquad (3)$$

and the backward equation $v(p,T)$ for the subregion 3n has the following dimensionless form:

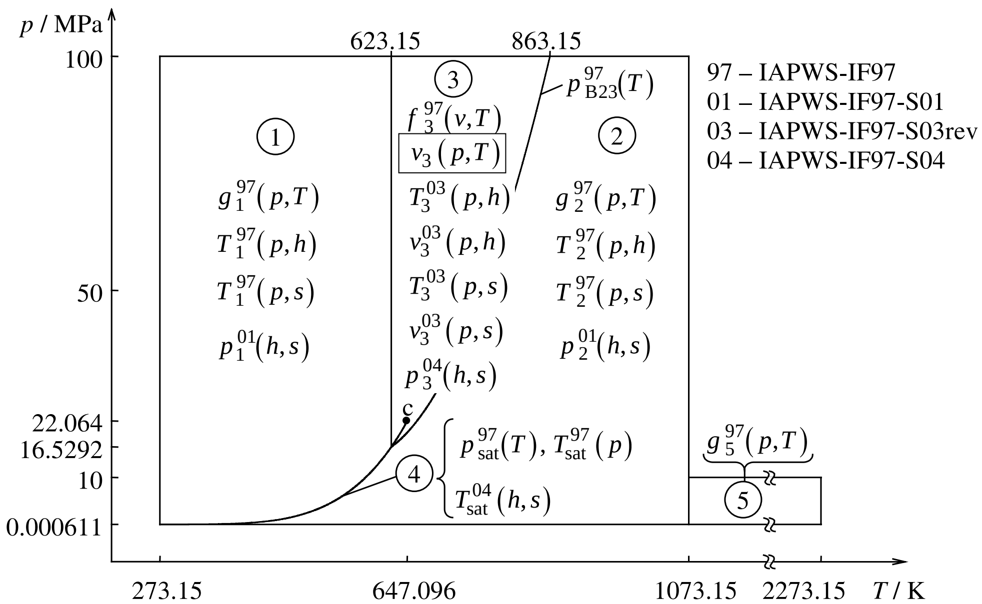

Fig. 1. Regions and equations of the IAPWS-IF97, supplementary backward equations, and equations $v_3(p,T)$ of this paper

$$\omega_{3n}(\pi,\theta) = \exp\left[\sum_{i=1}^{N} n_i\,(\pi - a)^{I_i}\,(\theta - b)^{J_i}\right], \qquad (4)$$

with $\omega = v/v^*$, $\pi = p/p^*$, and $\theta = T/T^*$. The reducing quantities v^*, p^*, and T^*, the non-linear parameters a and b, the powers c, d, and e, and the number of coefficients N are listed in Table 2 for the equations of the subregions 3a to 3t. The coefficients n_i and exponents I_i and J_i of the equations for the subregions 3a to 3t are listed in [10-12].

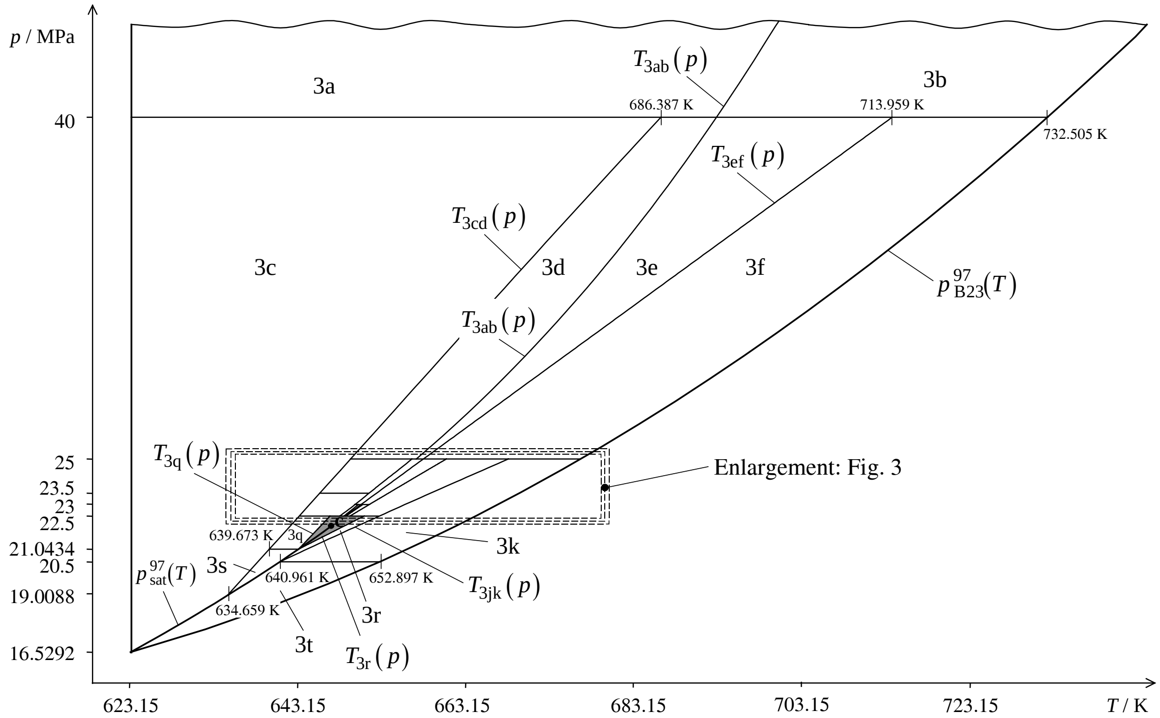

Fig. 2. Division of region 3 into subregions for the backward equations $v_3(p,T)$

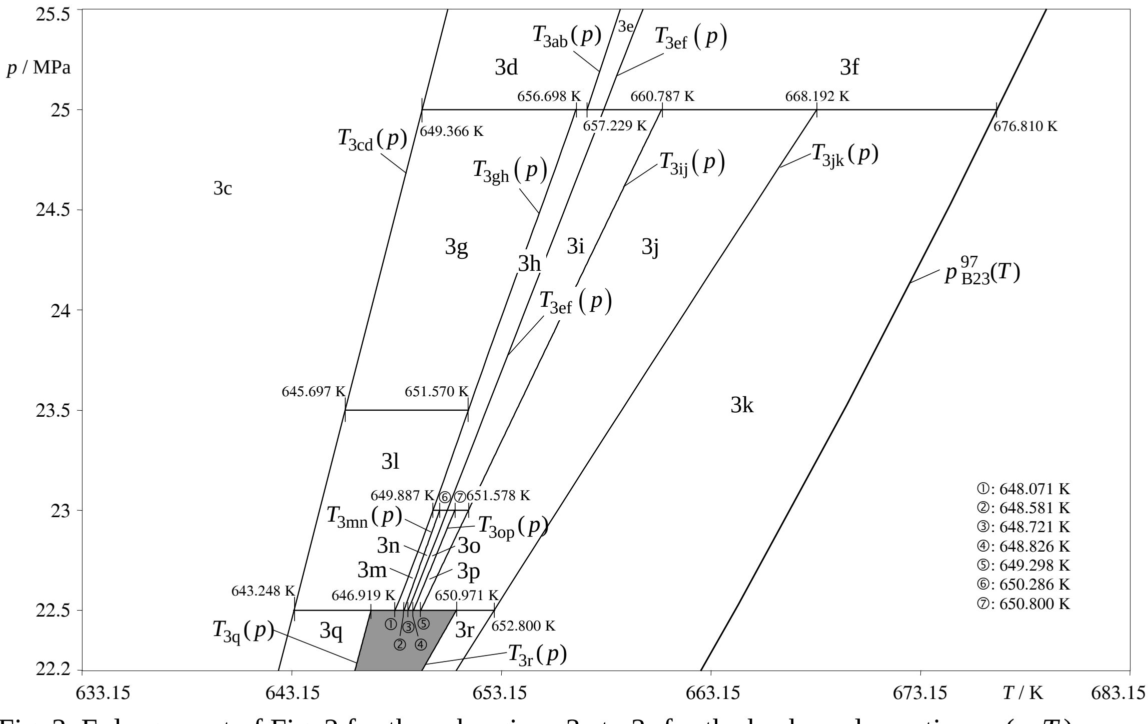

Fig. 3. Enlargement of Fig. 2 for the subregions 3c to 3r for the backward equations $v(p,T)$

Table 1. Pressure ranges and corresponding subregion boundary equations for determining the correct subregion, 3a to 3t, for the backward equations $v_3(p,T)$

Pressure Range in MPa	SR[1)]	For
$40 < p \le 100$	3a	$T \le T_{3ab}(p)$
	3b	$T > T_{3ab}(p)$
$25 < p \le 40$	3c	$T \le T_{3cd}(p)$
	3d	$T_{3cd}(p) < T \le T_{3ab}(p)$
	3e	$T_{3ab}(p) < T \le T_{3ef}(p)$
	3f	$T > T_{3ef}(p)$
$23.5 < p \le 25$	3c	$T \le T_{3cd}(p)$
	3g	$T_{3cd}(p) < T \le T_{3gh}(p)$
	3h	$T_{3gh}(p) < T \le T_{3ef}(p)$
	3i	$T_{3ef}(p) < T \le T_{3ij}(p)$
	3j	$T_{3ij}(p) < T \le T_{3jk}(p)$
	3k	$T > T_{3jk}(p)$
$23 < p \le 23.5$	3c	$T \le T_{3cd}(p)$
	3l	$T_{3cd}(p) < T \le T_{3gh}(p)$
	3h	$T_{3gh}(p) < T \le T_{3ef}(p)$
	3i	$T_{3ef}(p) < T \le T_{3ij}(p)$
	3j	$T_{3ij}(p) < T \le T_{3jk}(p)$
	3k	$T > T_{3jk}(p)$
$22.5 < p \le 23$	3c	$T \le T_{3cd}(p)$
	3l	$T_{3cd}(p) < T \le T_{3gh}(p)$
	3m	$T_{3gh}(p) < T \le T_{3mn}(p)$
	3n	$T_{3mn}(p) < T \le T_{3ef}(p)$
	3o	$T_{3ef}(p) < T \le T_{3op}(p)$
	3p	$T_{3op}(p) < T \le T_{3ij}(p)$
	3j	$T_{3ij}(p) < T \le T_{3jk}(p)$
	3k	$T > T_{3jk}(p)$
$p_{sat}^{97}(643.15\ \mathrm{K}) < p \le 22.5$	3c	$T \le T_{3cd}(p)$
	3q	$T_{3cd}(p) < T \le T_{3q}(p)$
	3r	$T_{3r}(p) \le T \le T_{3jk}(p)$
	3k	$T > T_{3jk}(p)$
$20.5 < p \le p_{sat}^{97}(643.15\ \mathrm{K})$	3c	$T \le T_{3cd}(p)$
	3s	$T_{3cd}(p) < T \le T_{sat}^{97}(p)$
	3r	$T_{sat}^{97}(p) \le T \le T_{3jk}(p)$
	3k	$T > T_{3jk}(p)$
$19.0088 < p \le 20.5$	3c	$T \le T_{3cd}(p)$
	3s	$T_{3cd}(p) < T \le T_{sat}^{97}(p)$
	3t	$T \ge T_{sat}^{97}(p)$
$p_{sat}^{97}(623.15\ \mathrm{K}) \le p \le 19.0088$	3c	$T \le T_{sat}^{97}(p)$
	3t	$T \ge T_{sat}^{97}(p)$

[1)] SR = Subregion

Table 2. Reducing quantities v^*, p^*, and T^*, nonlinear parameters a and b, powers c, d, and e, and number of coefficients N for the equations $v(p,T)$ of the subregions 3a to 3t

SR[1)]	v^* m³ kg^{-1}	p^* MPa	T^* K	a	b	c	d	e	N
3a	0.0024	100	760	0.085	0.817	1	1	1	30
3b	0.0041	100	860	0.280	0.779	1	1	1	32
3c	0.0022	40	690	0.259	0.903	1	1	1	35
3d	0.0029	40	690	0.559	0.939	1	1	4	38
3e	0.0032	40	710	0.587	0.918	1	1	1	29
3f	0.0064	40	730	0.587	0.891	0.5	1	4	42
3g	0.0027	25	660	0.872	0.971	1	1	4	38
3h	0.0032	25	660	0.898	0.983	1	1	4	29
3i	0.0041	25	660	0.910	0.984	0.5	1	4	42
3j	0.0054	25	670	0.875	0.964	0.5	1	4	29
3k	0.0077	25	680	0.802	0.935	1	1	1	34
3l	0.0026	24	650	0.908	0.989	1	1	4	43
3m	0.0028	23	650	1.00	0.997	1	1/4	1	40
3n	0.0031	23	650	0.976	0.997	-	-	-	39
3o	0.0034	23	650	0.974	0.996	0.5	1	1	24
3p	0.0041	23	650	0.972	0.997	0.5	1	1	27
3q	0.0022	23	650	0.848	0.983	1	1	4	24
3r	0.0054	23	650	0.874	0.982	1	1	1	27
3s	0.0022	21	640	0.886	0.990	1	1	4	29
3t	0.0088	20	650	0.803	1.02	1	1	1	33

5. Calculation of Thermodynamic Properties by using the $v_3(p,T)$ Backward Equations

The $v_3(p,T)$ equations described in Section 4 together with IAPWS-IF97 basic equation $f_3(v,T)$ make it possible to determine all thermodynamic properties, *e.g.* enthalpy, entropy, isobaric heat capacity, speed of sound, in region 3 from pressure p and temperature T without iteration.
The following steps should be made:

- Identify the subregion (3a to 3t) for given pressure p and temperature T following the instructions of Table 2 in conjunction with Figs. 2 and 3. Then, calculate the specific volume v for the subregion using the corresponding equation $v(p,T)$.
- Calculate the desired thermodynamic property from the previously calculated specific volume v and the given temperature T using the derivatives of the IAPWS-IF97 basic equation $f(v,T)$ of region 3; see Table 31 in [1].

6. Numerical Consistency

6.1 Numerical Consistency with the Basic Equation of IAPWS-IF97 The maximum relative deviations of specific volume, calculated from the backward equations $v(p,T)$ for subregions 3a to 3t, to the IAPWS-IF97 basic equation $f(v,T)$ of region 3 are listed in Table 3.

In addition, Table 3 contains the maximum relative deviations of enthalpy, entropy, isobaric heat capacity and speed of sound, calculated as described in Section 5.

Table 3 shows that the deviations of the specific volume, enthalpy, and entropy to the IAPWS-IF97 basic equation are less than 0.001 % and the deviations of isobaric heat capacity and speed of sound are less than 0.01 %. That means, 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 $v_3(p,T)$. In absolute terms, the maximum deviations are less than 5.4 J kg^{-1} for enthalpy and less than 0.01 J kg^{-1} K^{-1} for entropy.

6.2 Consistency at Subregion Boundaries The relative specific volume differences between the backward equations $v(p,T)$ of the adjacent subregions and the maximum relative deviations of enthalpy and entropy along the subregion boundary equations and along pressure subregion boundaries are smaller than 0.001 %.

Furthermore, the maximum relative deviations of isobaric heat capacity and speed of sound along the subregion boundaries are smaller than 0.01 %.

Numerical problems will be avoided since the differences between the calculated properties are smaller than their numerical consistencies with the IAPWS-IF97 basic equation $f(v,T)$ of region 3 at subregion boundaries.

7. Computing Time in Relation to IAPWS-IF97

A very important motivation for the development of the backward equations $v(p,T)$ for region 3 was reducing the computing time to obtain thermodynamic properties from given variables (p,T). In IAPWS-IF97, a time-consuming iteration is required. Using the $v_3(p,T)$ equations, the calculation speed is about 17 times faster than the iteration of v from p and T from IAPWS-IF97 fundamental equation [14].

8. Application of the $v_3(p,T)$ Equations

The numerical consistency of specific volume v obtained in the described way is sufficient for most heat-cycle and boiler calculations.

For users not satisfied with the numerical consistency of the backward equations, the equations are still recommended for generating good starting points for an iterative process. It will significantly reduce the time to meet the convergence criteria of the iteration.

The backward equations $v_3(p,T)$ can be used only in their ranges of validity described in Section 3. They should not be used for determining any thermodynamic derivatives.

In any case, depending on the application, a conscious decision is required whether to use the backward equations $v_3(p,T)$ or to calculate the corresponding values by iterations from the basic equation of IAPWS-IF97.

Table 3. Maximum relative deviations of the specific volume, calculated from the equations for subregions 3a to 3t, and maximum relative deviations of the enthalpy, of the entropy, of isobaric heat capacity, and speed of sound, calculated as described in Section 5, to the IAPWS-IF97 basic equation $f(v,T)$ of region 3

Sub-region	$\lvert\Delta v/v\rvert$ max %	$\lvert\Delta h/h\rvert$ max %	$\lvert\Delta s/s\rvert$ max %	$\lvert\Delta c_p/c_p\rvert$ max %	$\lvert\Delta w/w\rvert$ max %
3a	0.00061	0.00018	0.00026	0.0016	0.0015
3b	0.00064	0.00017	0.00016	0.0012	0.0008
3c	0.00080	0.00026	0.00025	0.0059	0.0023
3d	0.00059	0.00018	0.00014	0.0035	0.0012
3e	0.00072	0.00018	0.00014	0.0017	0.0006
3f	0.00068	0.00018	0.00013	0.0015	0.0002
3g	0.00047	0.00014	0.00011	0.0032	0.0010
3h	0.00085	0.00022	0.00017	0.0066	0.0006
3i	0.00067	0.00018	0.00013	0.0019	0.0002
3j	0.00034	0.00009	0.00007	0.0020	0.0002
3k	0.00034	0.00008	0.00007	0.0018	0.0002
3l	0.00033	0.00010	0.00008	0.0035	0.0008
3m	0.00057	0.00015	0.00011	0.0062	0.0006
3n	0.00064	0.00017	0.00012	0.0050	0.0002
3o	0.00031	0.00008	0.00006	0.0007	0.0001
3p	0.00044	0.00012	0.00009	0.0026	0.0002
3q	0.00036	0.00012	0.00009	0.0040	0.0010
3r	0.00037	0.00010	0.00008	0.0030	0.0002
3s	0.00030	0.00010	0.00007	0.0033	0.0009
3t	0.00095	0.00022	0.00018	0.0046	0.0004

9. Conclusions

The paper presents backward equations to calculate the specific volume from given pressure and temperature $v(p,T)$ in the critical and supercritical regions (region 3).

The presented equations $v_3(p,T)$ together with the IAPWS-IF97 basic equation $f_3(v,T)$ make it possible to determine all thermodynamic properties from pressure and temperature in region 3 without iteration.

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 $v_3(p,T)$.

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

Since the numerical consistency of the $v_3(p,T)$ equations with IAPWS-IF97 is sufficient for most applications in heat cycle and boilers calculations, the otherwise necessary iteration can be avoided. Therefore, calculation of specific volume from pressure and temperature using the presented equations are more than 17 times faster than the iteration from IAPWS-IF97.

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