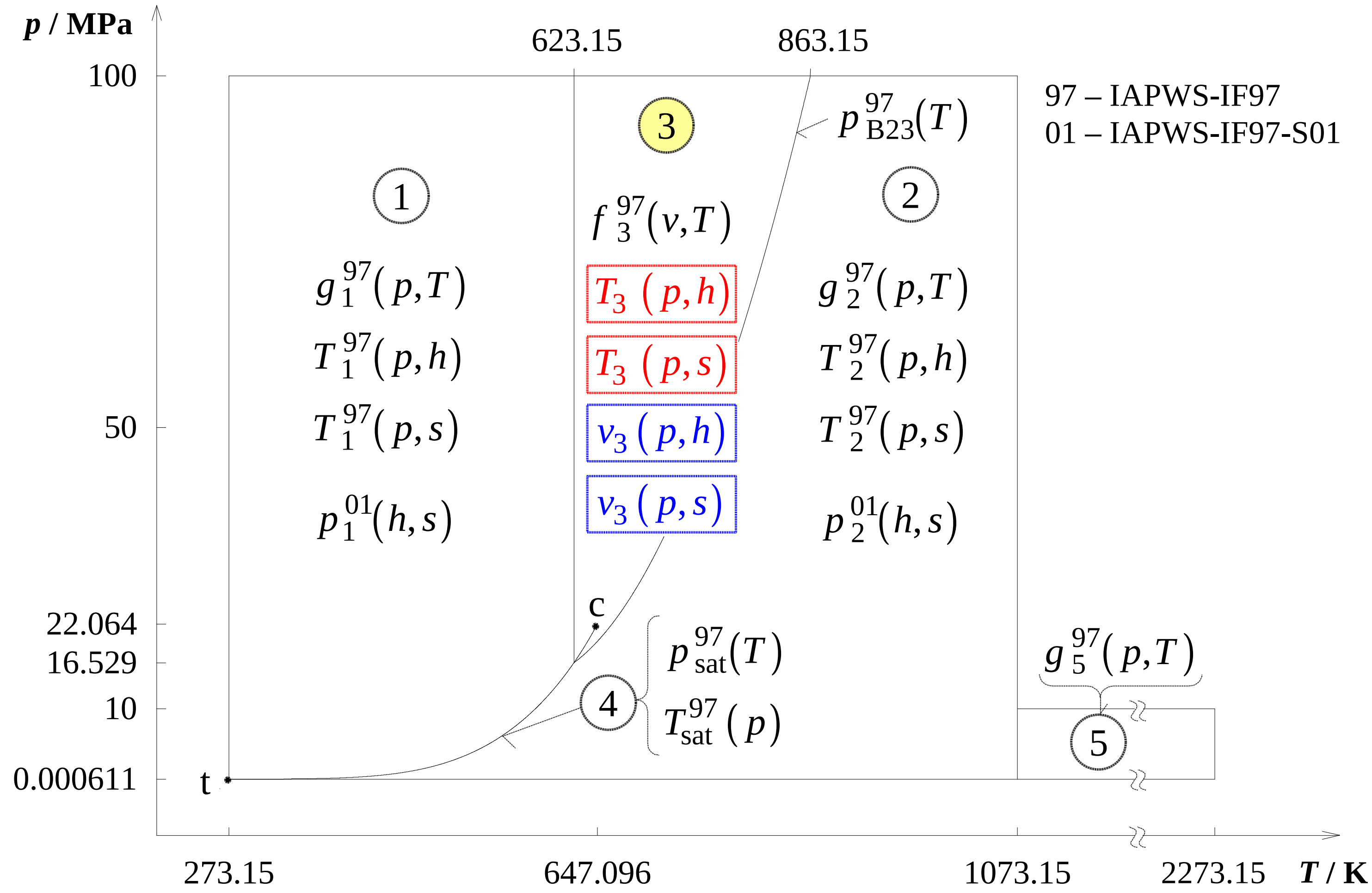
K. Knobloch, H.-J. Kretzschmar
University of Applied Sciences of Zittau and Görlitz, Germany
Department of Technical Thermodynamics
A. Dittmann
Technical University of Dresden, Germany
Department of Thermodynamics

Equations $T(p,h)$, $v(p,h)$ and $T(p,s)$, $v(p,s)$ for the Critical and Supercritical Regions of Water

Contents

15th Symposium on Thermophysical Properties, Boulder, 2003


p / MPa
100
50
22.064
16.529
10
0.000611
623.15
863.15
273.15
647.096
1073.15
2273.15
T / K
97 – IAPWS-IF97
01 – IAPWS-IF97-S01
1
2
3
4
5
$p_{B23}^{97}(T)$
$f_3^{97}(v,T)$
$T_3(p,h)$
$T_3(p,s)$
$v_3(p,h)$
$v_3(p,s)$
$g_1^{97}(p,T)$
$T_1^{97}(p,h)$
$T_1^{97}(p,s)$
$p_1^{01}(h,s)$
$g_2^{97}(p,T)$
$T_2^{97}(p,h)$
$T_2^{97}(p,s)$
$p_2^{01}(h,s)$
$p_{sat}^{97}(T)$
$T_{sat}^{97}(p)$
$g_5^{97}(p,T)$
c
t

Why Equations $T_3(p,h)$, $v_3(p,h)$ and $T_3(p,s)$, $v_3(p,s)$?

Functions of the variables (p,h) or (p,s)
in the critical and supercritical regions
are required in thermodynamic process modeling.

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Iterative Calculation Using the IAPWS-IF97 Basic Equation

Functions of (p,h)	Functions of (p,s)
Two-dimensional Iteration of v and T from:	Two-dimensional Iteration of v and T from:
$p = p_3^{97}(v,T)$ and $h = h_3^{97}(v,T)$ } Derivatives of $f_3^{97}(v,T)$	$p = p_3^{97}(v,T)$ and $s = s_3^{97}(v,T)$ } Derivatives of $f_3^{97}(v,T)$

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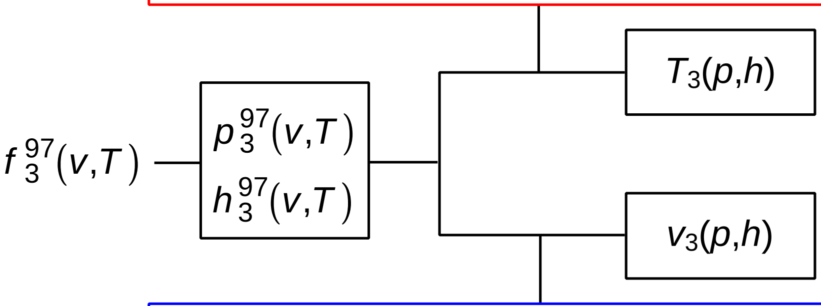
$T_3(p,h)$, $v_3(p,h)$ Backward equations $T_3(p,s)$, $v_3(p,s)$
are required to reduce computing time of process calculations.

Numerical Consistencies of *T*(*p*,*h*), *v*(*p*,*h*) and *T*(*p*,*s*), *v*(*p*,*s*)

Consistency Relations for Funktions *T*,*v*(*p*,*h*)

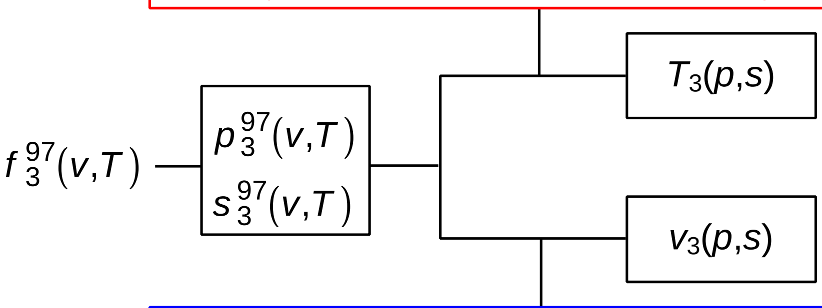
$$\left|\Delta T\right| = \left| T_3\left(p_3^{97}(v,T), h_3^{97}(v,T)\right) - T \right| \le \left|\Delta T\right|_{\mathrm{tol}}$$



$$\left|\frac{\Delta v}{v}\right| = \left| \frac{v_3\left(p_3^{97}(v,T), h_3^{97}(v,T)\right) - v}{v} \right| \le \left|\frac{\Delta v}{v}\right|_{\mathrm{tol}}$$

Consistency Relations for Funktions *T*,*v*(*p*,*s*)

$$\left|\Delta T\right| = \left| T_3\left(p_3^{97}(v,T), s_3^{97}(v,T)\right) - T \right| \le \left|\Delta T\right|_{\mathrm{tol}}$$



$$\left|\frac{\Delta v}{v}\right| = \left| \frac{v_3\left(p_3^{97}(v,T), s_3^{97}(v,T)\right) - v}{v} \right| \le \left|\frac{\Delta v}{v}\right|_{\mathrm{tol}}$$

Numerical Consistencies of *T*(*p*,*h*), *v*(*p*,*h*) and *T*(*p*,*s*), *v*(*p*,*s*)

Determination of the permissible values ΔT_{tol} and Δv_{tol}

ΔT_{tol}: - IAPWS requirement for equation $T(p,h)$, $T(p,s)$ (Gaithersburg, 2001)

- At critical Point: The digits of the value T_c = 647.096 K should be met.

Δv_{tol}: - From the total Differentials

$$\Delta v_{tol} = \left(\frac{\partial v}{\partial T}\right)_h \Delta T_{tol} + \left(\frac{\partial v}{\partial h}\right)_T \Delta h_{tol} \quad \text{for } v(p,h)$$

$$\Delta v_{tol} = \left(\frac{\partial v}{\partial T}\right)_s \Delta T_{tol} + \left(\frac{\partial v}{\partial s}\right)_T \Delta s_{tol} \quad \text{for } v(p,s)$$

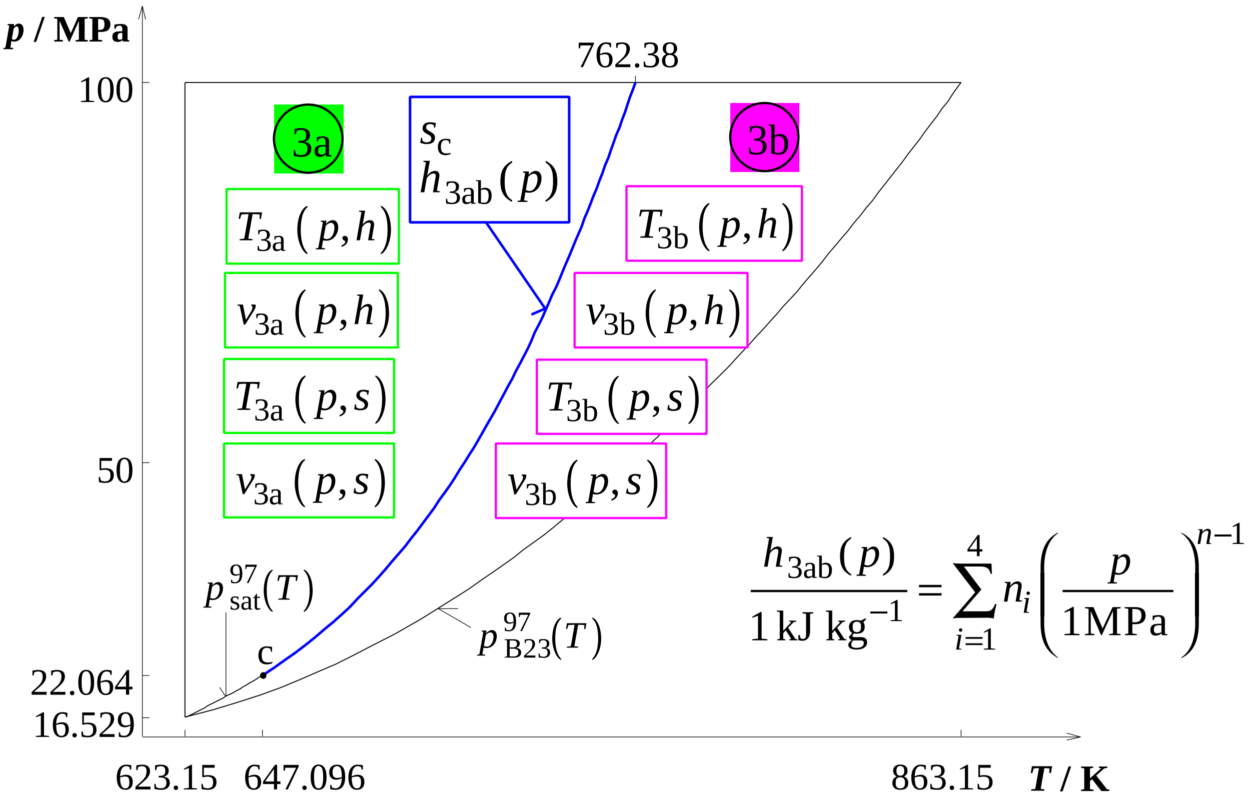
- Calculation of $\left(\frac{\partial v}{\partial T}\right)_h$, $\left(\frac{\partial v}{\partial h}\right)_T$, $\left(\frac{\partial v}{\partial T}\right)_s$ and $\left(\frac{\partial v}{\partial s}\right)_T$ using the IAPWS-IF97 equations
- Δh_{tol}, Δs_{tol} of adjacent region 1 and subregion 2c from survey of IAPWS

- At critical Point: The digits of the value $v_c = \frac{1}{322}$ m^3 kg^{-1} should be met.

	$\lvert\Delta T_{tol}\rvert$	$\lvert\Delta h_{tol}\rvert$	$\lvert\Delta s_{tol}\rvert$	$\lvert\Delta v / v\rvert_{tol}$
Region 3	25 mK	80 J kg^{-1}	0.10 J kg^{-1} K^{-1}	0.01 %
Critical Point	0.49 mK	-	-	0.0001 %

mean value for functions $v(p,h)$ and $v(p,s)$ (refers to 0.01 %)

Structure of the Equation Set



Backward Equations *T*(*p*,*h*) for Region 3

Subregion 3a

$$\frac{T_{3a}(p,h)}{760\,\mathrm{K}} = \sum_{i=1}^{31} n_i \cdot \left(\frac{p}{100\,\mathrm{MPa}} + 0.240\right)^{I_i} \cdot \left(\frac{h}{2300\,\mathrm{kJ\cdot kg^{-1}}} - 0.615\right)^{J_i}$$

$$I_i = -12 \ldots 0 \ldots +12 \quad , \quad J_i = 0 \ldots +22$$

Subregion 3b

$$\frac{T_{3b}(p,h)}{860\,\mathrm{K}} = \sum_{i=1}^{33} n_i \cdot \left(\frac{p}{100\,\mathrm{MPa}} + 0.298\right)^{I_i} \cdot \left(\frac{h}{2800\,\mathrm{kJ\cdot kg^{-1}}} - 0.720\right)^{J_i}$$

$$I_i = -12 \ldots 0 \ldots +8 \quad , \quad J_i = 0 \ldots +16$$

Backward Equations *v*(*p*,*h*) for Region 3

Subregion 3a

$$\frac{v_{3a}(p,h)}{0.0028\,\mathrm{m^3\cdot kg^{-1}}} = \sum_{i=1}^{32} n_i \cdot \left(\frac{p}{100\,\mathrm{MPa}} + 0.128\right)^{I_i} \cdot \left(\frac{h}{2100\,\mathrm{kJ\cdot kg^{-1}}} - 0.727\right)^{J_i}$$

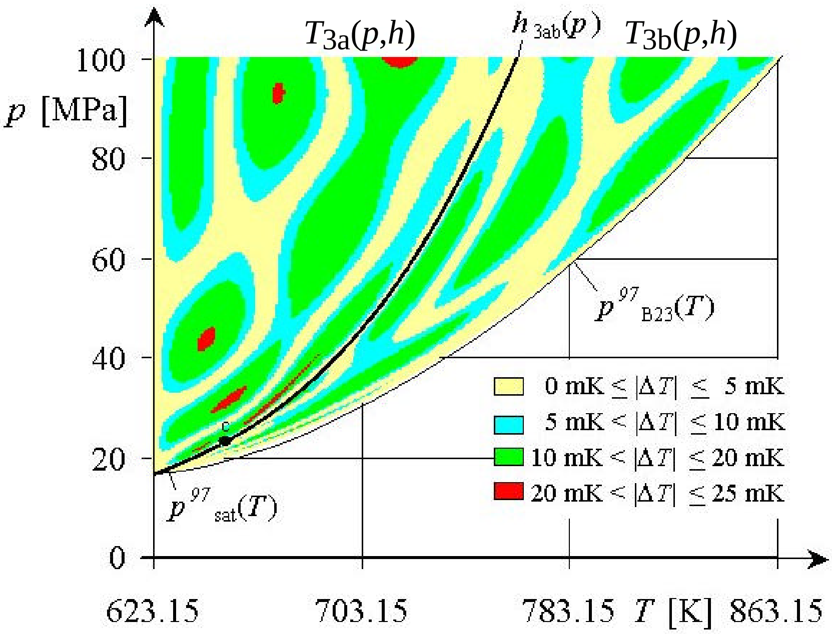
$$I_i = -12 \ldots 0 \ldots +8 \quad , \quad J_i = 0 \ldots +22$$

Subregion 3b

$$\frac{v_{3b}(p,h)}{0.0088\,\mathrm{m^3\cdot kg^{-1}}} = \sum_{i=1}^{30} n_i \cdot \left(\frac{p}{100\,\mathrm{MPa}} + 0.0661\right)^{I_i} \cdot \left(\frac{h}{2800\,\mathrm{kJ\cdot kg^{-1}}} - 0.720\right)^{J_i}$$

$$I_i = -12 \ldots 0 \ldots +2 \quad , \quad J_i = 0 \ldots +10$$

Results for Numerical Consistencies with IAPWS-IF97 Basic Equation

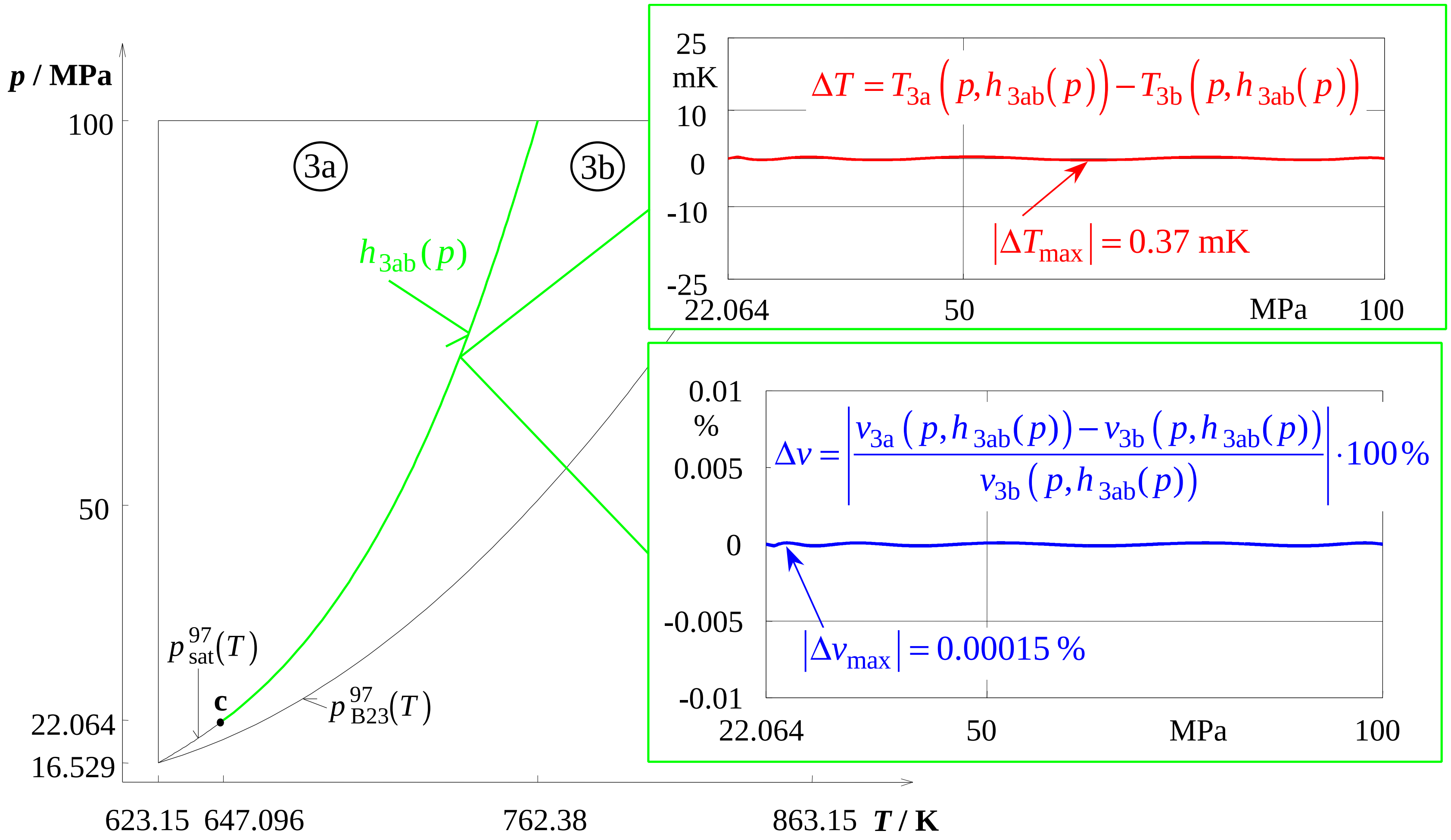


Equation	$\|\Delta T_{tol}\|$	$\|\Delta T_{max}\|$	ΔT_{RMS}
$T_{3a}(p,h)$	25 mK	23.6 mK	10.5 mK
$T_{3b}(p,h)$	25 mK	19.6 mK	9.6 mK

Equation	$\|\Delta v_{tol} / v\|$	$\|\Delta v_{max} / v\|$	$\|\Delta v_{RMS} / v\|$
$v_{3a}(p,h)$	0.01 %	0.0080 %	0.0032 %
$v_{3b}(p,h)$	0.01 %	0.0095 %	0.0042 %

The critical Temperature and the critical specific volume are met exactly by the equations $T(p,h)$ and $v(p,h)$.

Numerical Consistency Between Backward Equations at Subregion Boundary $h_{3ab}(p)$



Backward Equations $T(p,s)$ for Region 3

Subregion 3a

$$\frac{T_{3a}(p,s)}{760\ \mathrm{K}} = \sum_{i=1}^{33} n_i \cdot \left(\frac{p}{100\ \mathrm{MPa}} + 0.240\right)^{I_i} \cdot \left(\frac{s}{4.4\ \mathrm{kJ\cdot kg^{-1}\cdot K^{-1}}} - 0.703\right)^{J_i}$$

$$I_i = -12 \ldots 0 \ldots +10 \quad , \quad J_i = 0 \ldots +36$$

Subregion 3b

$$\frac{T_{3b}(p,s)}{860\ \mathrm{K}} = \sum_{i=1}^{28} n_i \cdot \left(\frac{p}{100\ \mathrm{MPa}} + 0.760\right)^{I_i} \cdot \left(\frac{s}{5.3\ \mathrm{kJ\cdot kg^{-1}\cdot K^{-1}}} - 0.818\right)^{J_i}$$

$$I_i = -12 \ldots 0 \ldots +14 \quad , \quad J_i = 0 \ldots +24$$

Backward Equations $v(p,s)$ for Region 3

Subregion 3a

$$\frac{v_{3a}(p,s)}{0.0028\,\mathrm{m^3\cdot kg^{-1}}} = \sum_{i=1}^{28} n_i \cdot \left(\frac{p}{100\ \mathrm{MPa}} + 0.187\right)^{I_i} \cdot \left(\frac{s}{4.4\ \mathrm{kJ\cdot kg^{-1}\cdot K^{-1}}} - 0.755\right)^{J_i}$$

$$I_i = -12 \ldots 0 \ldots +6 \quad , \quad J_i = 0 \ldots +28$$

Subregion 3b

$$\frac{v_{3b}(p,s)}{0.0088\,\mathrm{m^3\cdot kg^{-1}}} = \sum_{i=1}^{31} n_i \cdot \left(\frac{p}{100\ \mathrm{MPa}} + 0.298\right)^{I_i} \cdot \left(\frac{s}{5.3\ \mathrm{kJ\cdot kg^{-1}\cdot K^{-1}}} - 0.816\right)^{J_i}$$

$$I_i = -12 \ldots 0 \ldots +2 \quad , \quad J_i = 0 \ldots +12$$

Results for Numerical Consistency

Numerical Consistency with IAPWS-IF97 Basic Equation

Equation	$\lvert \Delta T_{tol} \rvert$	$\lvert \Delta T_{max} \rvert$	ΔT_{RMS}
$T_{3a}(p,s)$	25 mK	24.8 mK	11.2 mK
$T_{3b}(p,s)$	25 mK	22.1 mK	10.1 mK

Equation	$\lvert \Delta v_{tol} / v \rvert$	$\lvert \Delta v_{max} / v \rvert$	$\lvert \Delta v_{RMS} / v \rvert$
$v_{3a}(p,s)$	0.01 %	0.0096 %	0.0052 %
$v_{3b}(p,s)$	0.01 %	0.0077 %	0.0037 %

Numerical Consistency Between Backward Equations at Subregion Boundary s_c

Relation	$\lvert \Delta T_{tol} \rvert$	$\lvert \Delta T_{max} \rvert$
$T_{3a}(p,s_c) - T_{3b}(p,s_c)$	25 mK	0.093 mK

Relation	$\lvert \Delta v_{tol} / v \rvert$	$\lvert \Delta v_{max} / v \rvert$
$[v_{3a}(p,s_c) - v_{3b}(p,s_c)] / v_{3b}(p,s_c)$	0.01 %	0.00046 %

Computing Time in Relation to IAPWS-IF97

Measurement of the Computing Time

Basis: IAPWS benchmark program NIFBENCH

Computing Time Ratio (*CTR* Value)

$$CTR = \frac{\text{Computing time using IAPWS} - \text{IF97 equations only}}{\text{Computing time using the new equations}}$$

Iteration Method

- 2-dimensional Newton-Method
- Convergence Criteria: $|\Delta T_{\text{it}}| = 25\,\text{mK}$ and $|\Delta v / v|_{\text{it}} = 0.01\%$

Measured Computing Times and Resulting CTR Values

	Calculation of *T* and *v* from *p* and *h* using: Backward Equations	Calculation of *T* and *v* from *p* and *h* using: Two-dimensional Iteration	
Subregion	**Computing Time**	**Computing Time**	**CTR**
3a	0.47 μs/call	7.65 μs/call	**16**
3b	0.45 μs/call	7.82 μs/call	**17**

	Calculation of *T* and *v* from *p* and *s* using: Backward Equations	Calculation of *T* and *v* from *p* and *s* using: Two-dimensional Iteration	
Subregion	**Computing Time**	**Computing Time**	**CTR**
3a	0.46 μs/call	8.31 μs/call	**18**
3b	0.43 μs/call	8.51 μs/call	**19**

Summary

Backward equations $T(p,h)$, $v(p,h)$ and $T(p,s)$, $v(p,s)$
for region 3 of IAPWS-IF97 were presented.

Numerical Consistency is sufficient for process modelling

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2-dimensional Iterations can be avoided

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The calculation of $T,v(p,h)$ is 16 times faster than IAPWS-IF97.
The calculation of $T,v(p,s)$ is 18 times faster than IAPWS-IF97.

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Evaluation of the
Equations $T(p,h)$, $v(p,h)$ and $T(p,s)$, $v(p,s)$
by IAPWS since IAPWS-Meeting 2002

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Supplementary Release
to the IAPWS-IF97
in 2003