Proposal

Supplementary Release on Backward Equations for Pressure as Function of Enthalpy and Entropy $p(h,s)$ to the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam

H.-J. Kretzschmar, I. Stöcker, K. Knobloch
University of Applied Sciences of Zittau and Görlitz

J. R. Cooper
Queen Mary and Westfield College, London

D. G. Friend
National Institute of Standards and Technology, Boulder

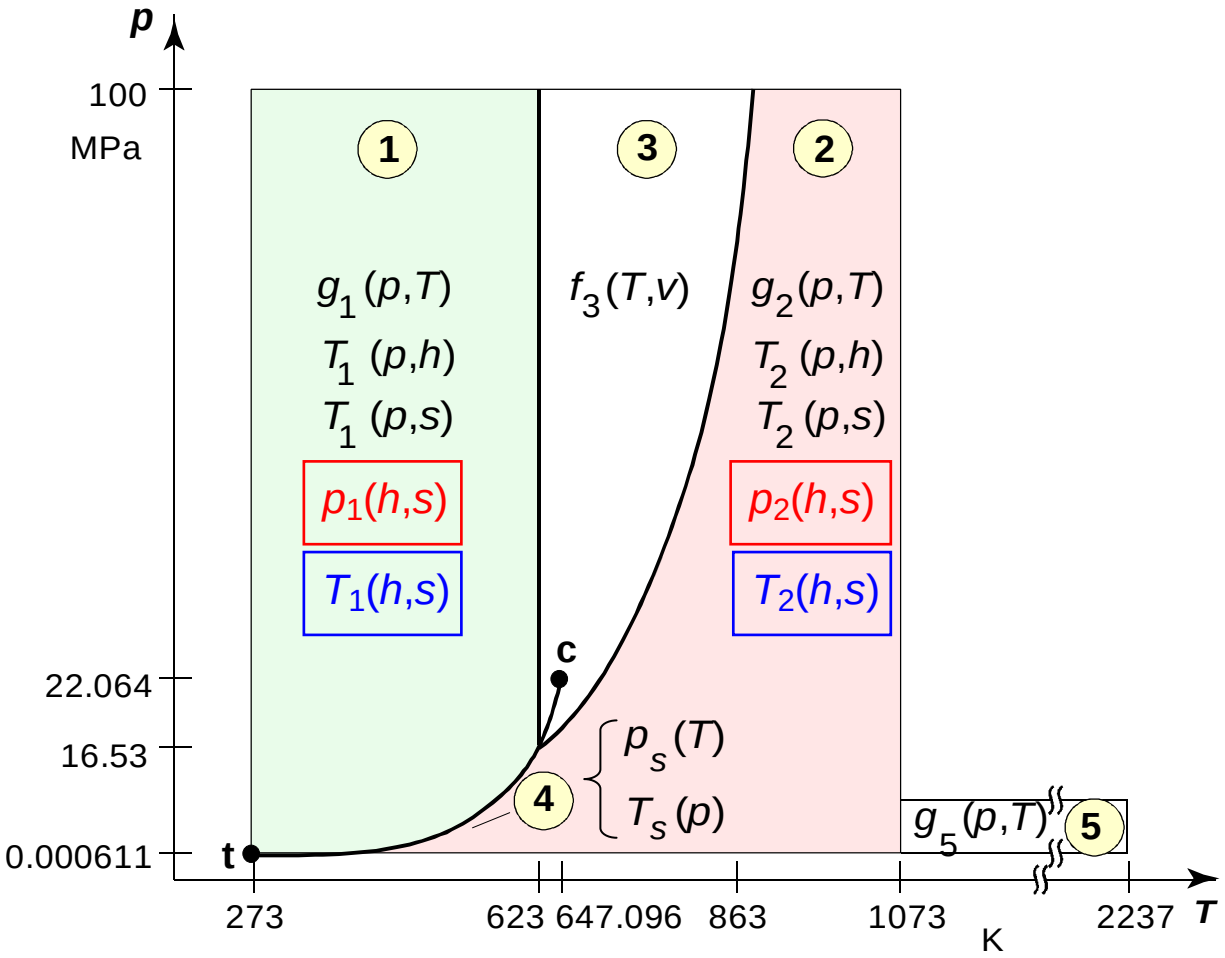
R. Mareš
University of West Bohemia, Plzeň

J. Trübenbach, Th. Willkommen, A. Dittmann
Technical University of Dresden

W. Wagner
Ruhr-University, Bochum

IAPWS Meeting, Prague 2000

The Industrial Formulation IAPWS-IF97
for the Thermodynamic Properties of Water and Steam



Why Equations $p_1(h,s)$ and $p_2(h,s)$?

Frequencies of call of functions of h and s in process modelling

- Worldwide survey of IAPWS

Function of:	**(*h*,*s*)**	**(*p*,*h*)**	**(*p*,*s*)**
Liquid region	2.5 %	23.4 %	4.3 %
Vapor region	2.8 %	34.4 %	14.4 %

- 2.0 % - Program KRAWAL of Siemens, Power Generation Group

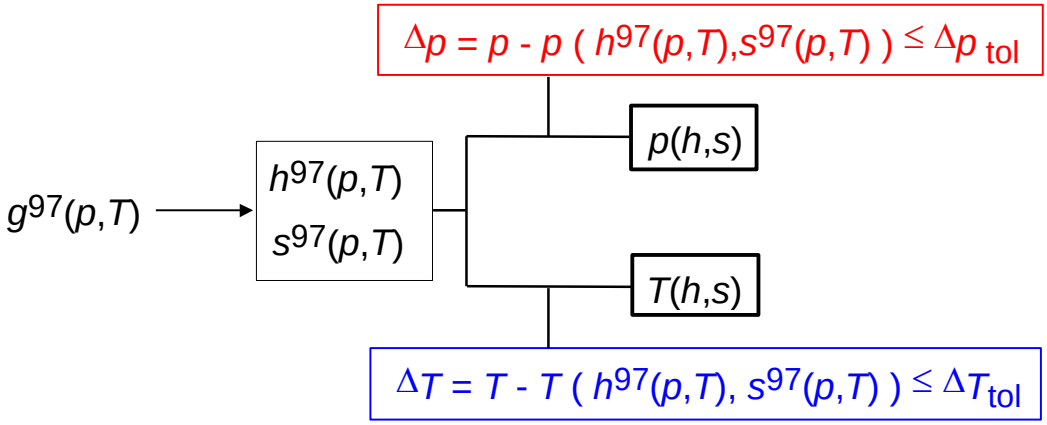
Functions $p(h,s)$ and $T(h,s)$ demand 75 % of the computing time of all property functions

Reason: two-dimensional iterative calculations

Backward equations $p(h,s)$ and $T(h,s)$ are required to reduce computing time of process calculations

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

Consistency Relations



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

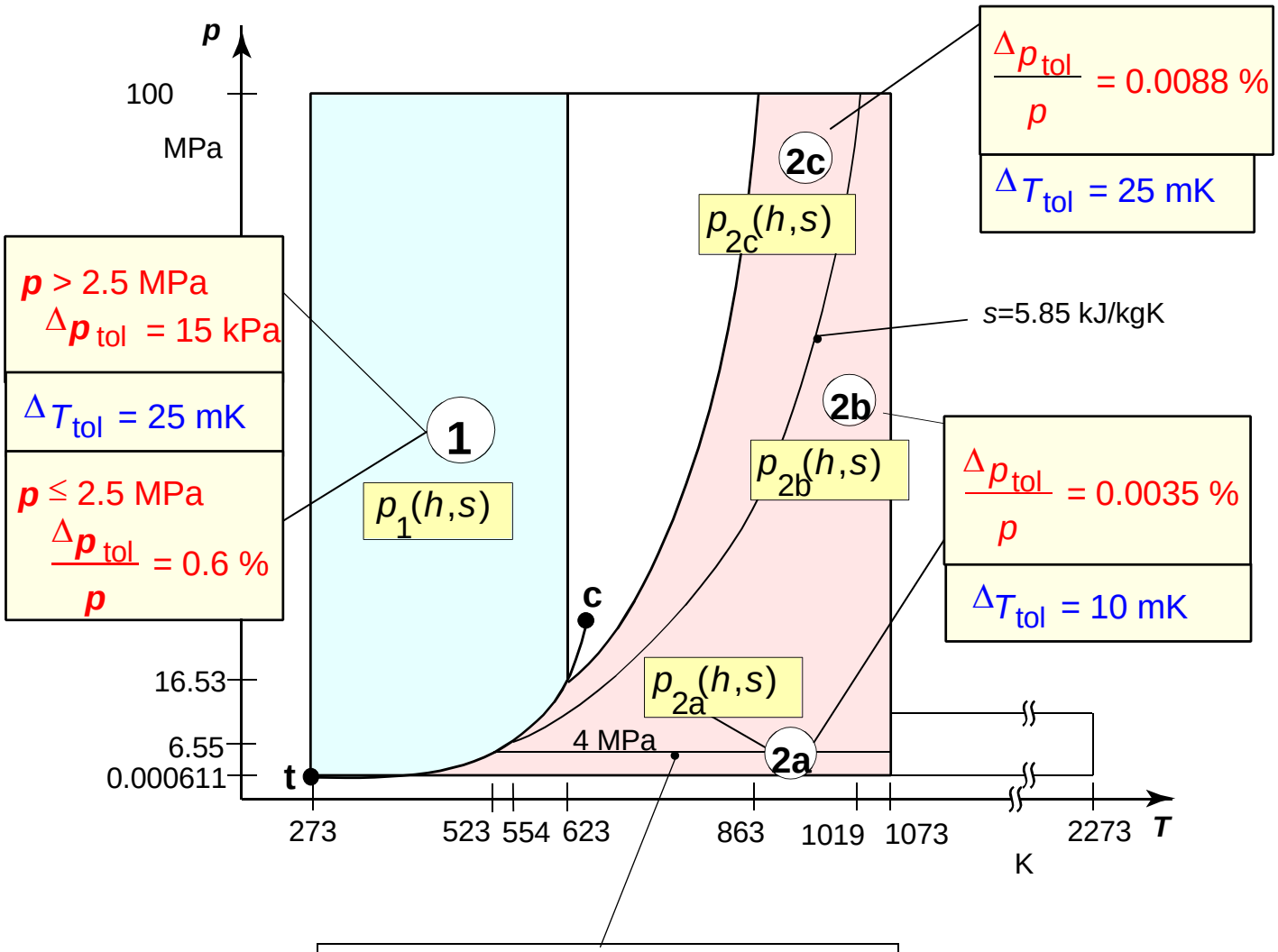
$$\Delta p_{tol} = \left(\frac{\partial p}{\partial h}\right)_s \Delta h_{tol} + \left(\frac{\partial p}{\partial s}\right)_h \Delta s_{tol}$$

- Calculation of $\left(\frac{\partial p}{\partial h}\right)_s$ and $\left(\frac{\partial p}{\partial s}\right)_h$ using the IF97 equations
- Δh_{tol}, Δs_{tol} - from survey of IAPWS

ΔT_{tol} - IAPWS requirements for IF97 equations $T(p,h)$ and $T(p,s)$

IF97 Region		Δh_{tol}	Δs_{tol}	Δp_{tol}	ΔT_{tol}
1		80 J kg^{-1}	0.1 J kg^{-1} K^{-1}	$p \le 2.5$ MPa: 0.6%	25 mK
				$p > 2.5$ MPa: 15 kPa	
2	$s < 5.85$ kJ kg^{-1}K^{-1}	80 J kg^{-1}	0.10 J kg^{-1} K^{-1}	0.0088 %	25 mK
	$s \ge 5.85$ kJ kg^{-1}K^{-1}	32 J kg^{-1}	0.04 J kg^{-1} K^{-1}	0.0035 %	10 mK

Subregions



$$\frac{h_{2ab}(s)}{1\,\mathrm{kJ\,kg^{-1}}} = \sum_{i=1}^{4} n_i \cdot \left(\frac{s}{1\,\mathrm{kJ\,kg^{-1}K^{-1}}} \right)^{i-1}$$

Backward Equations $p(h,s)$

Liquid - Region 1

$$\frac{p_1(h,s)}{100\ \text{MPa}} = \sum_{i=1}^{19} n_i \cdot \left(\frac{h}{3400\ \text{kJ}\cdot\text{kg}^{-1}} + 0.05 \right)^{I_i} \cdot \left(\frac{s}{7.6\ \text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}} + 0.05 \right)^{J_i}$$

$$I_i = 0 \ldots +5,\ J_i = 0 \ldots +10$$

Vapor - Region 2

Subregion 2a

$$\frac{p_{2a}(h,s)}{4\ \text{MPa}} = \left[\sum_{i=1}^{29} n_i \cdot \left(\frac{h}{4200\ \text{kJ}\cdot\text{kg}^{-1}} - 0.5 \right)^{I_i} \cdot \left(\frac{s}{12\ \text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}} - 1.2 \right)^{J_i} \right]^4$$

$$I_i = 0 \ldots +7,\ J_i = 0 \ldots +22$$

Subregion 2b

$$\frac{p_{2b}(h,s)}{100\ \text{MPa}} = \left[\sum_{i=1}^{33} n_i \cdot \left(\frac{h}{4100\ \text{kJ}\cdot\text{kg}^{-1}} - 0.6 \right)^{I_i} \cdot \left(\frac{s}{7.9\ \text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}} - 1.01 \right)^{J_i} \right]^4$$

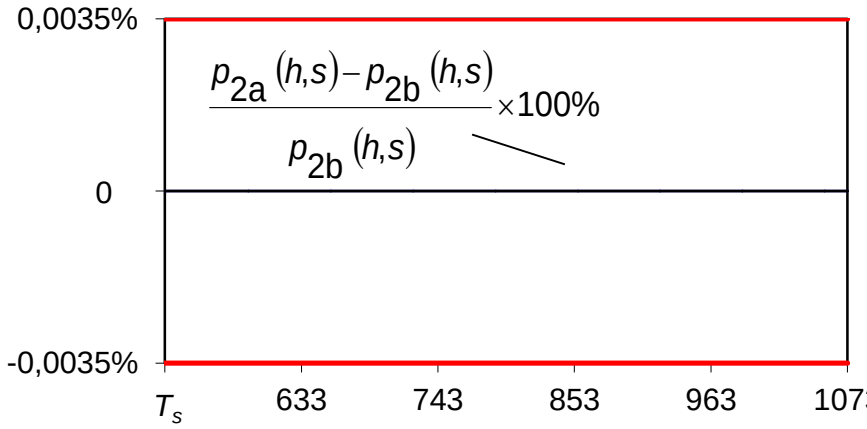
$$I_i = 0 \ldots +14,\ J_i = 0 \ldots +18$$

Subregion 2c

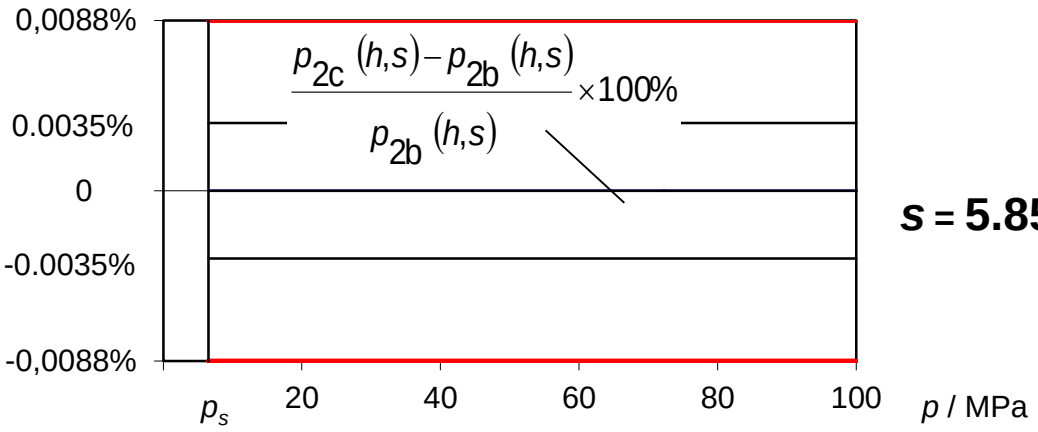
$$\frac{p_{2c}(h,s)}{100\ \text{MPa}} = \left[\sum_{i=1}^{31} n_i \cdot \left(\frac{h}{3500\ \text{kJ}\cdot\text{kg}^{-1}} - 0.7 \right)^{I_i} \cdot \left(\frac{s}{5.9\ \text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}} - 1.1 \right)^{J_i} \right]^4$$

$$I_i = 0 \ldots +16,\ J_i = 0 \ldots +18$$

Consistency of $p_2(h,s)$ at Subregion Boundaries



$h_{2ab}(s)$



$s = 5.85\ \mathrm{kJ\ kg^{-1}K^{-1}}$

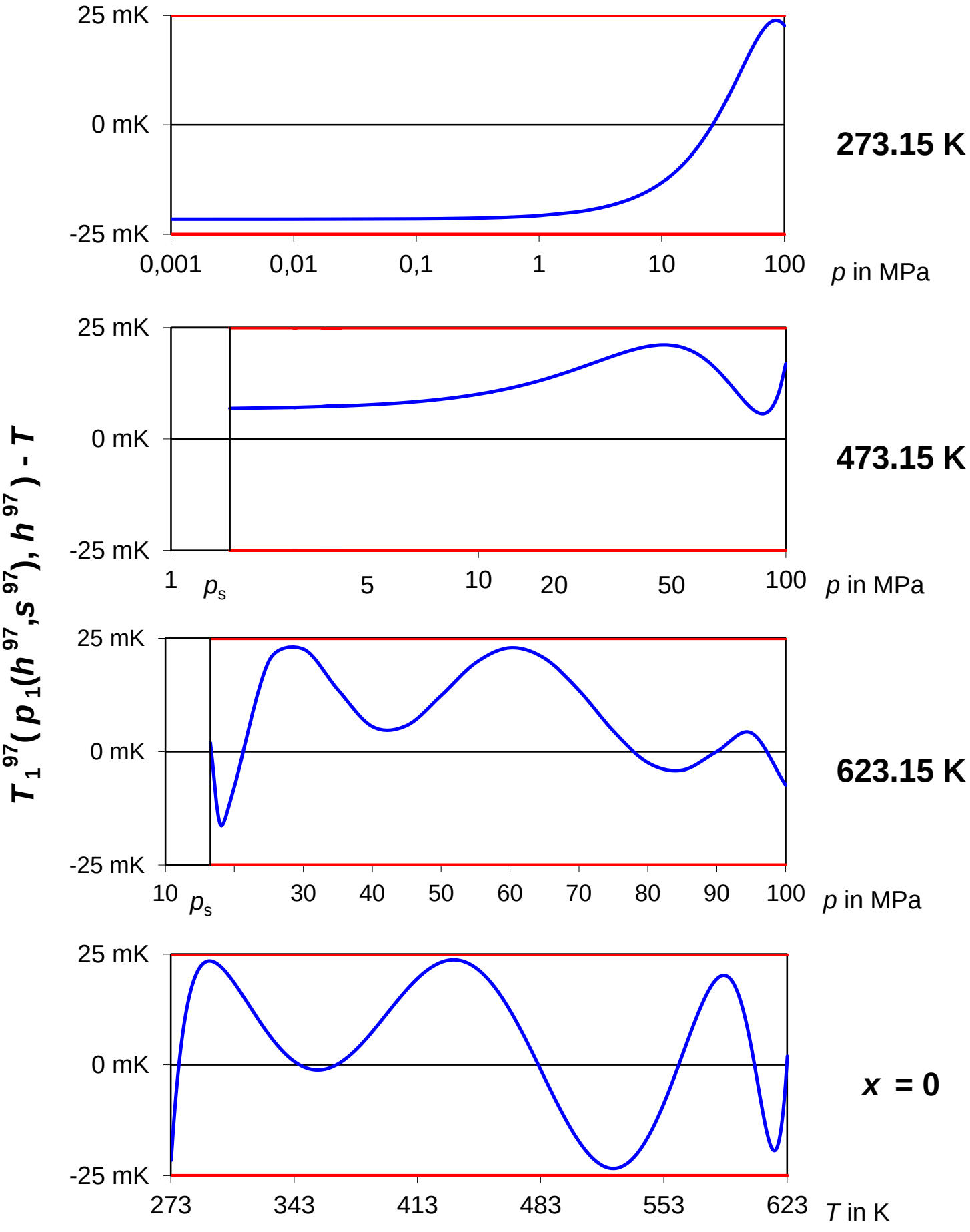
Backward Function $T(h,s)$

Equations of the Supplementary Release: $p(h,s)$

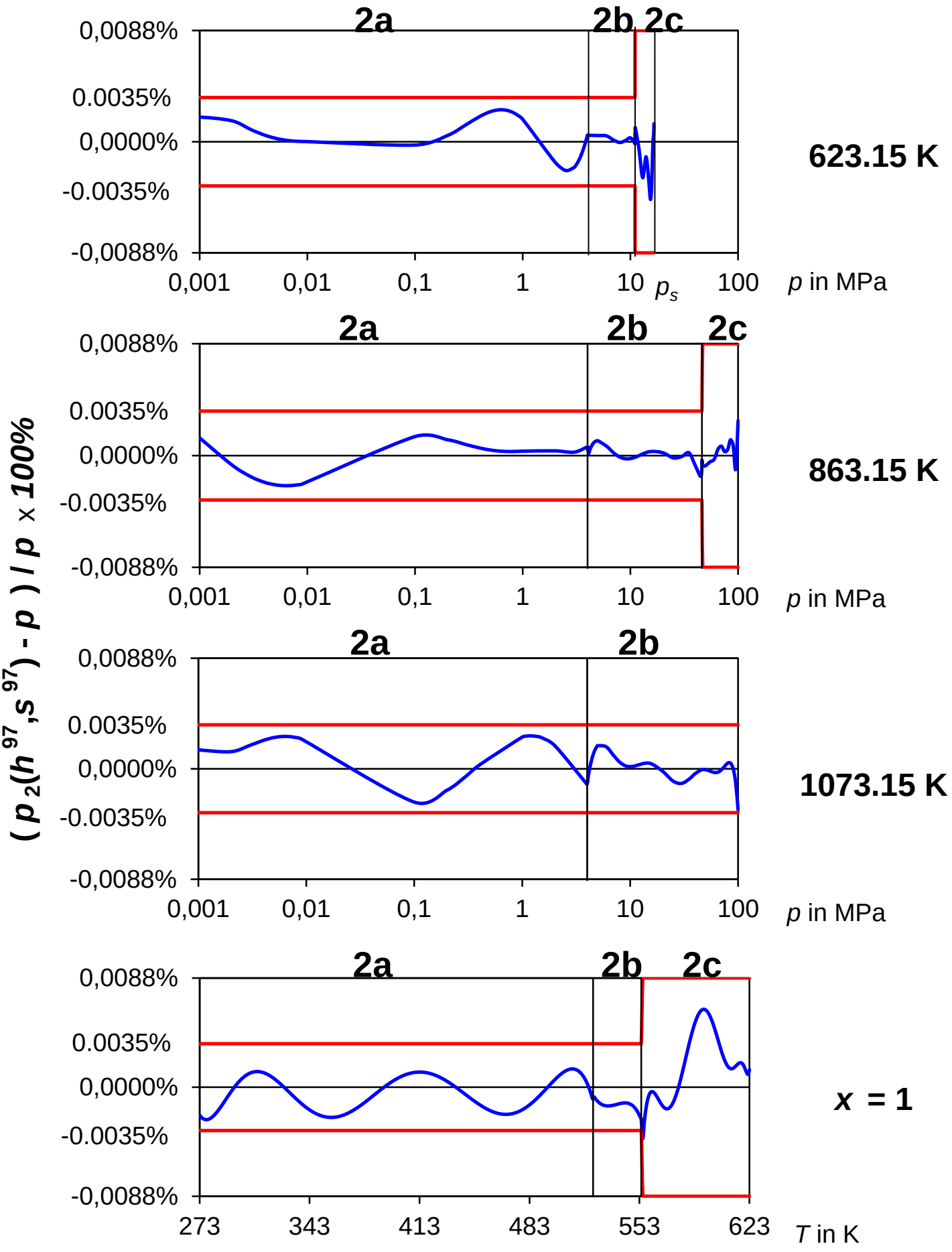
IF97 backward equations: $T^{97}(p,h)$ ⇨ $T(h,s)$ calculable

($T^{97}(p,h)$ fits better than $T^{97}(p,s)$)

Numerical Consistency of the Temperature Calculated by $T_1^{97}(p_1(h,s), h)$



Numerical Consistency of the Equations $p_2(h,s)$



Results for Numerical Consistencies

Subregion	$p(h,s)$		$T^{97}(p(h,s),h)$	
	$\lvert\Delta p\rvert_{max}$	Δp_{tol}	$\lvert\Delta T\rvert_{max}$	ΔT_{tol}
1	$p \leq$ 2,5 MPa: 0.55 % $p >$ 2,5 MPa: 14 kPa	0.60 % 15 kPa	24.0 mK	25 mK
2a	0.0029 %	0.0035 %	9.7 mK	10 mK
2b	0.0034 %	0.0035 %	9.8 mK	10 mK
2c	0.0063 %	0.0088 %	24.9 mK	25 mK

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Numerical Consistency is sufficient for process modelling

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Iterations can be avoided

Computing Time Investigations

- Theoretical estimation
- Comparison with an iteration algorithm
- Comparison with commercial program packages

⇒ Conclusions and final wording of the Supplementary Release

Measurement of the Computing Times

- IAPWS benchmark program NIFBENCH
- Compaq Visual Fortran 6.1 compiler
- PC: Intel Pentium III 733 MHz processor, 133 MHz bus

Computing Time Ratio (CTR Value)

$$\mathrm{CTR} = \frac{\text{Computing time using IF97 equations only}}{\text{Computing time using the new } p(h,s) \text{ equations}}$$

Iterative Calculation of $p,T(h,s)$ Using IF97 Equations Only

Iteration Variants

a) Two-dimensional
Iteration of p and T
from: $s = s^{97}(p,T)$
$h = h^{97}(p,T)$

b) One-dimensional
Iteration of p
from: $s = s^{97}(p,T)$
$\uparrow$
$T^{97}(p,h$
)

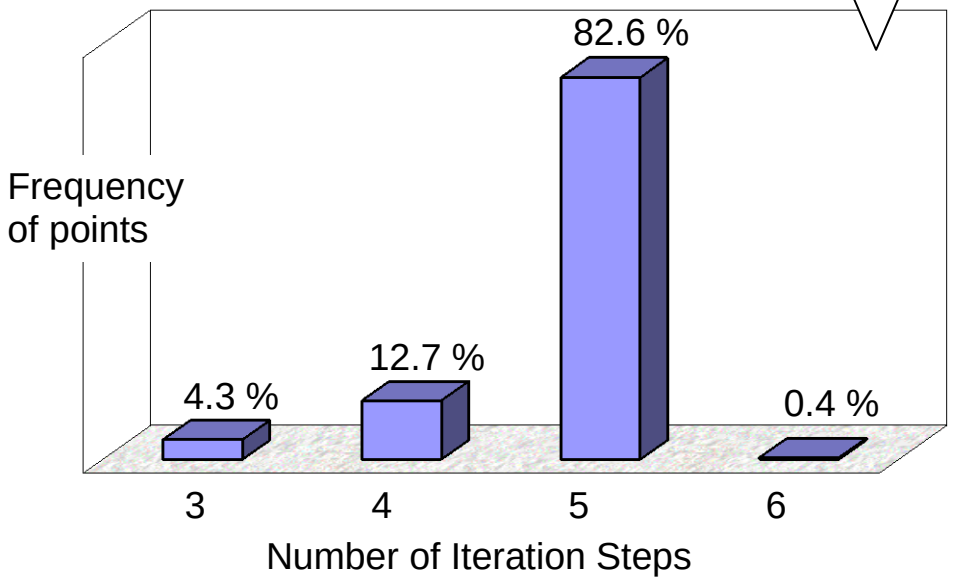
c) One-dimensional
Iteration of p
from: $h = h^{97}(p,T)$
$\uparrow$
$T^{97}(p,s$
)

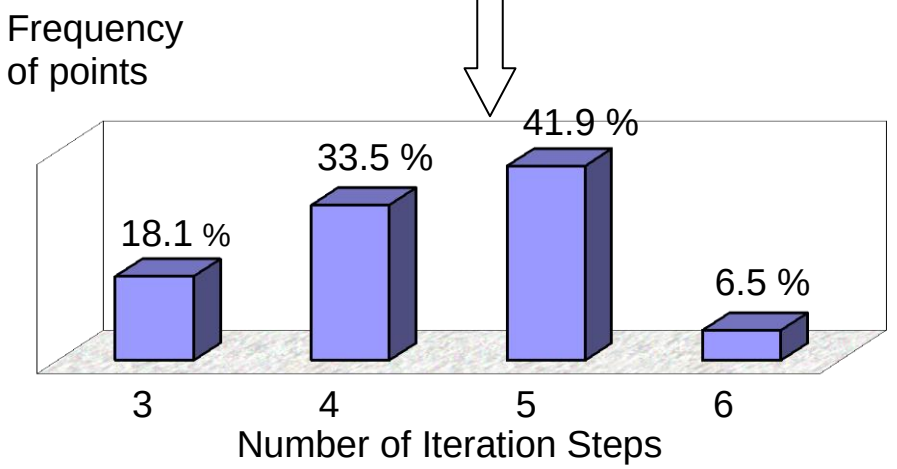
Calculation of $p,T(h,s)$ Using the New $p(h,s)$ Equations

$p = p\ (h,s)$
$\downarrow$
$T = T^{97}(p,h)$

Comparison with Theoretical Estimation and an Iteration Algorithm

CTR-Values				
Calculation of $p,T(h,s)$ using the new $p(h,s)$ equations in comparison with:	Liquid Region 1		Vapor Region 2	
	Theoretical (5 steps)	Iteration Algorithm	Theoretical (5 steps)	Iteration Algorithm
a) Two-dimensional iteration from $h^{97}(p,T)$ and $s^{97}(p,T)$	29.6	51.0	21.8	30.4
b) One-dimensional iteration from $s^{97}(p,T)$ and $T^{97}(p,h)$	11.5	14.2	9.4	11.3
c) One-dimensional iteration from $h^{97}(p,T)$ and $T^{97}(p,s)$	7.8	11.0	7.3	9.1





Comparison with Commercial Program Packages

ASME Steam Properties for Industrial Use based on IAPWS-IF97

CTR Values	
Liquid Region 1	Vapor Region 2
44.6	32.6

JSME Steam Tables 1999 based on IAPWS-IF97

CTR Value
Vapor Subregions 2a and 2b
841.8

Conclusions and Final Wording of the Supplementary Release

The calculations using the new backward equations $p(h,s)$ are

11 times faster for liquid region 1

and

9 times faster for vapor region 2

than the iterative calculations using the IAPWS-IF97 equations only.

Depending on the iteration variant, the mathematical iteration method and the starting values for p and T the factors can slightly differ.

In case, two-dimensional iterations from IF97 equations $h^{97}(p,T)$ and $s^{97}(p,T)$ were used before, the calculations using the new $p(h,s)$ equations even will be 51 times faster for liquid region 1 and 30 times faster for vapor region 2.

Summary

Equations $p(h,s)$ are ready for evaluation by IAPWS

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Supplementary Release

to the IAPWS-IF97

Computing Times

Function, Package	Computing Time [μs]	
	Region 1	Region 2
p (h,s)	0.195	0.453
p,T (h,s)	0.369	0.754
$h^{97}(p,T)$	0.411	0.558
$s^{97}(p,T)$	0.681	1.090
$T^{97}(p,h)$	0.165	0.326
$T^{97}(p,s)$	0.163	0.541
Iteration Algorithm		
p,T from $h^{97}(p,T)$, $s^{97}(p,T)$	18.815	22.900
p,T from $s^{97}(p,T)$, $T^{97}(p,h)$	5.227	8.535
p,T from $h^{97}(p,T)$, $T^{97}(p,s)$	4.054	6.882
ASME		
p,T (h,s)	16.432	24.794
JSME		
p,T (h,s)	-	634.683 (Subregions 2a and 2b)

IAPWS Benchmark Program NIFBENCH
Compaq Visual Fortran 6.1 Compiler
Pentium III 733 MHz Processor on 133 MHz Board