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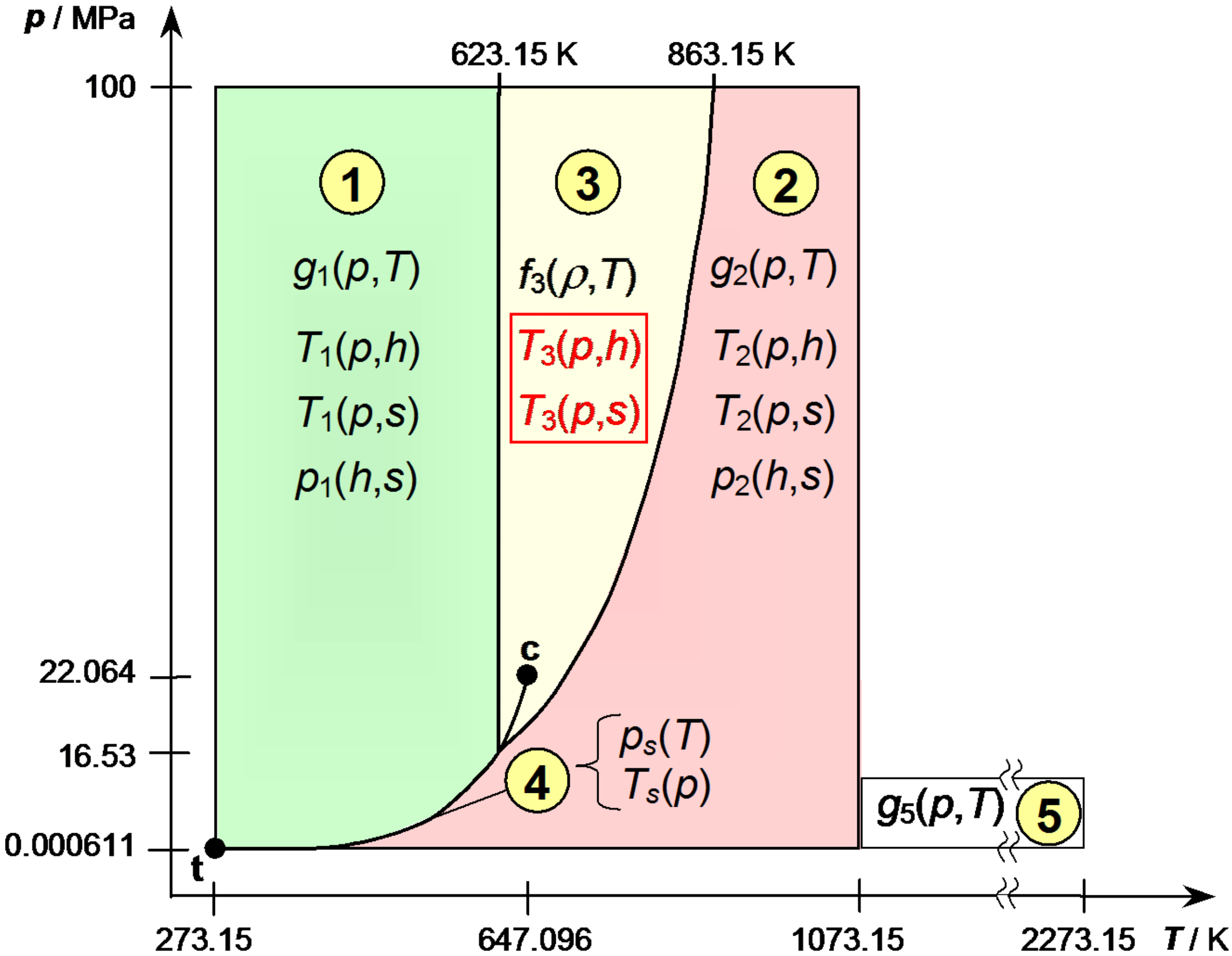
Development of Supplementary Backward Equations *T*(*p*,*h*) and *T*(*p*,*s*) for the Critical and Supercritical Regions of Water and Steam

Contents

IAPWS Meeting, Gaithersburg MD, 2001

The Industrial Formulation IAPWS-IF97

for the Thermodynamic Properties of Water and Steam



- International Survey: Backward equations $T_3(p,h)$ and $T_3(p,s)$ are required.
- IAPWS Task Group for developing those equations was established in Prague.

Presentation of first results.

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

Iterative Calculation of $T(p,h)$ Using IAPWS-IF97 Basic Equation

Two-dimensional Iteration of T and ρ from:

$$\left.\begin{array}{c} p = p_3^{97}(\rho,T) \\ \text{and} \\ h = h_3^{97}(\rho,T) \end{array}\right\} \text{Derivatives of } f_3^{97}(\rho,T)$$

Iterative Calculation of $T(p,s)$ Using IAPWS-IF97 Basic Equation

Two-dimensional Iteration of T and ρ from:

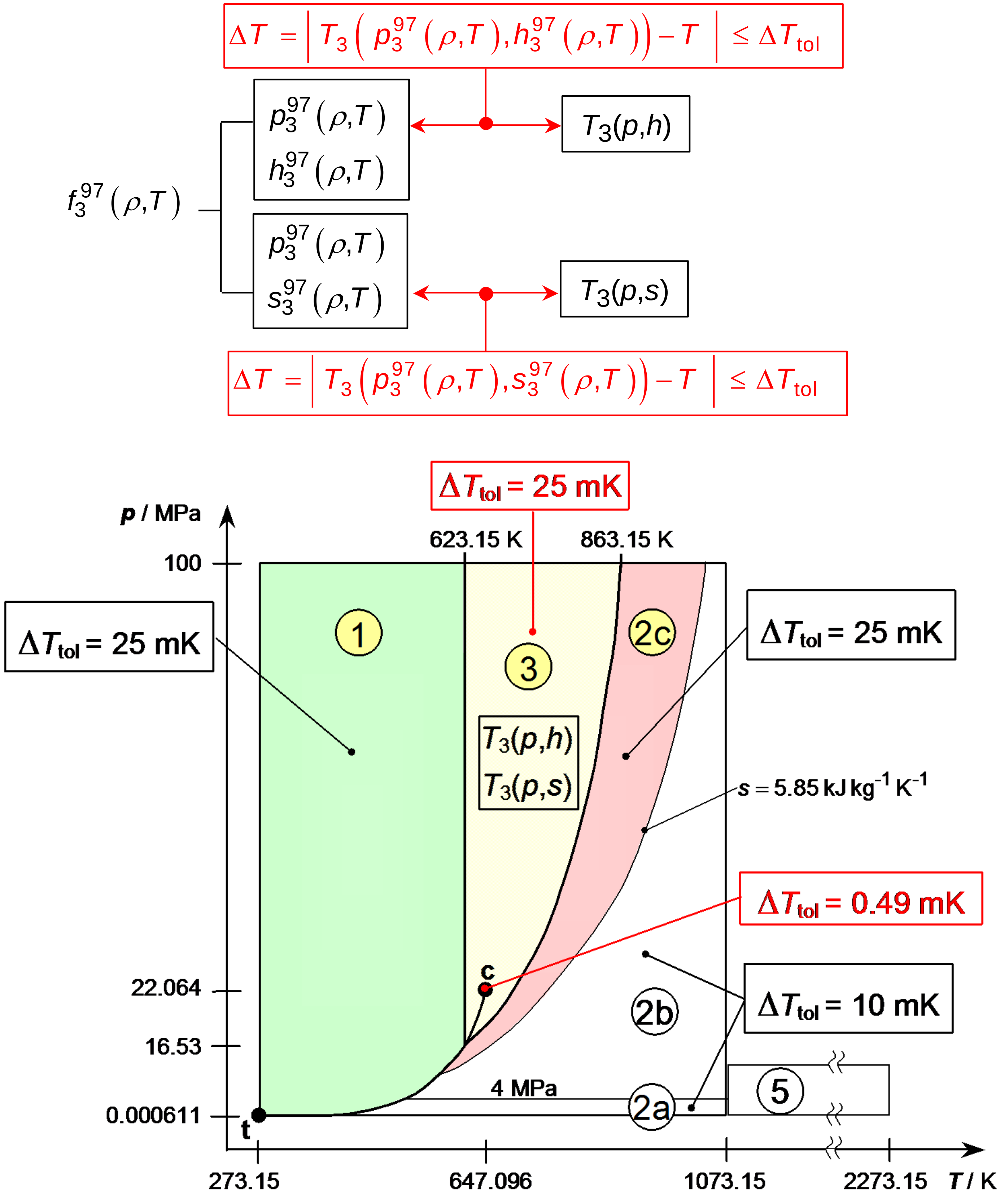
$$\left.\begin{array}{c} p = p_3^{97}(\rho,T) \\ \text{and} \\ s = s_3^{97}(\rho,T) \end{array}\right\} \text{Derivatives of } f_3^{97}(\rho,T)$$

⇩

Backward equations $T_3(p,h)$ and $T_3(p,s)$ are required

to reduce computing time of process calculations.

Numerical Consistency Requirements



Approximation Method

Algorithm of *Trübenbach*, *Willkommen, Dittmann* and *Kretzschmar*

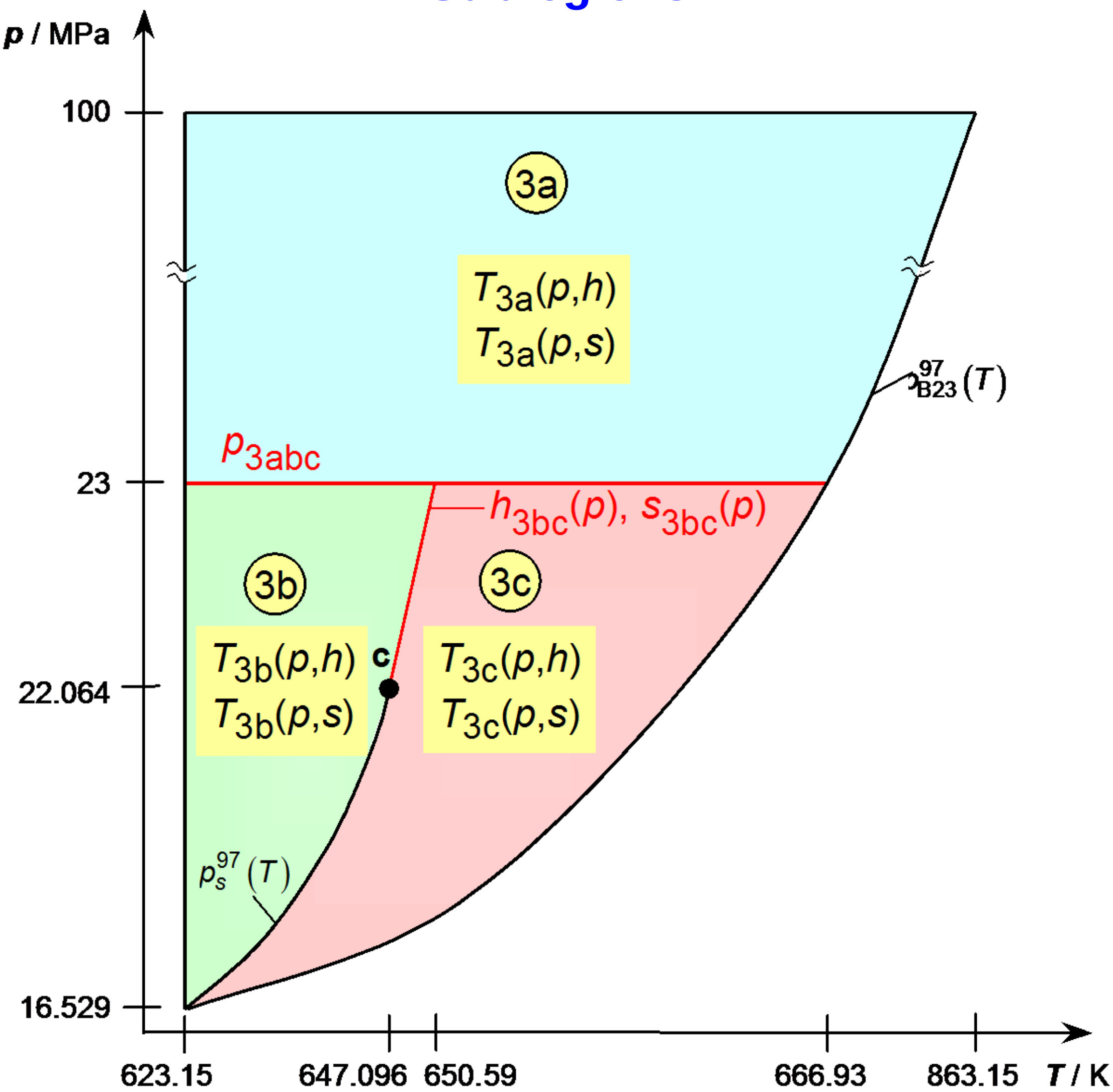
Basis: Regressions Analysis of *Wagner*

Modifications:

- Automatic generation and optimization of the bank of terms
- Optimization of the non-linear parameters
- Automatic weighting of the data points for minimizing the maximum deviation of the equation to the data
- Considering the application computing time in the process of optimizing the equation structure

Data Basis: IAPWS-IF97

Subregions



$$\frac{h_{3bc}(p)}{1\,\mathrm{kJkg^{-1}}} = \mathrm{a} \cdot \frac{p}{1\,\mathrm{MPa}} + \mathrm{b}$$

$$\frac{s_{3bc}(p)}{1\,\mathrm{kJkg^{-1}K^{-1}}} = \mathrm{c} \cdot \frac{p}{1\,\mathrm{MPa}} + \mathrm{d}$$

Approximated functions between the critical point and isobaric line p_{3abc}

at $T = T_c + \left.\frac{\partial T_s}{\partial p_s}\right|_c \cdot (p_{3abc} - p_c)$

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

Subregion 3a

$$\frac{T_{3a}(p,h)}{860\,\mathrm{K}} = \sum_{i=1}^{37} n_i \cdot \left(\frac{p}{100\,\mathrm{MPa}} + 0.253\right)^{I_i} \cdot \left(\frac{h}{2800\,\mathrm{kJ\cdot kg^{-1}}} - 0.544\right)^{J_i}$$

$$I_i = -12 \ldots 0 \ldots +4 \quad , \qquad J_i = 0 \ldots +32$$

Subregion 3b

$$\frac{T_{3b}(p,h)}{650\,\mathrm{K}} = \sum_{i=1}^{13} n_i \cdot \left(\frac{p}{23\,\mathrm{MPa}} - 0.536\right)^{I_i} \cdot \left(\frac{h}{2600\,\mathrm{kJ\cdot kg^{-1}}} - 0.556\right)^{J_i}$$

$$I_i = 0 \ldots +7 \quad , \qquad J_i = 0 \ldots +18$$

Subregion 3c

$$\frac{T_{3c}(p,h)}{670\,\mathrm{K}} = \sum_{i=1}^{12} n_i \cdot \left(\frac{p}{23\,\mathrm{MPa}} - 0.634\right)^{I_i} \cdot \left(\frac{h}{3300\,\mathrm{kJ\cdot kg^{-1}}} - 0.456\right)^{J_i}$$

$$I_i = 0 \ldots +3 \quad , \qquad J_i = 0 \ldots +6$$

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

Subregion 3a

$$\frac{T_{3a}(p,s)}{860\,\mathrm{K}} = \sum_{i=1}^{39} n_i \cdot \left(\frac{p}{100\,\mathrm{MPa}} + 0.092\right)^{I_i} \cdot \left(\frac{s}{5.2\,\mathrm{kJ\cdot kg^{-1}\cdot K^{-1}}} - 0.649\right)^{J_i}$$

$$I_i = -12 \ldots 0 \ldots +2 \quad , \qquad J_i = 0 \ldots +36$$

Subregion 3b

$$\frac{T_{3b}(p,s)}{650\,\mathrm{K}} = \sum_{i=1}^{13} n_i \cdot \left(\frac{p}{23\,\mathrm{MPa}} - 0.128\right)^{I_i} \cdot \left(\frac{s}{5.2\,\mathrm{kJ\cdot kg^{-1}\cdot K^{-1}}} - 0.595\right)^{J_i}$$

$$I_i = 0 \ldots +8 \quad , \qquad J_i = 0 \ldots +20$$

Subregion 3c

$$\frac{T_{3c}(p,s)}{670\,\mathrm{K}} = \sum_{i=1}^{10} n_i \cdot \left(\frac{p}{23\,\mathrm{MPa}} - 0.705\right)^{I_i} \cdot \left(\frac{s}{5.3\,\mathrm{kJ\cdot kg^{-1}\cdot K^{-1}}} - 0.573\right)^{J_i}$$

$$I_i = 0 \ldots +3 \quad , \qquad J_i = 0 \ldots +10$$

Results for Numerical Consistencies

Numerical Consistency with IAPWS-IF97 Basic Equation

Equation	$\lvert \Delta T_{max} \rvert$	ΔT_{RMS}
$T_{3a}(p,h)$	22.9 mK	11.4 mK
$T_{3b}(p,h)$	24.8 mK	14.1 mK
$T_{3c}(p,h)$	23.8 mK	15.2 mK
$T_{3a}(p,s)$	23.4 mK	12.0 mK
$T_{3b}(p,s)$	19.6 mK	9.3 mK
$T_{3c}(p,s)$	20.4 mK	11.5 mK

ΔT_{tol} = 25 mK

Numerical Consistency with IAPWS-IF97 Basic Equation at the Critical Point

Equation	$\lvert \Delta T \rvert$
$T_{3b}(p,h)$	0.43 mK
$T_{3c}(p,h)$	0.40 mK
$T_{3b}(p,s)$	0.29 mK
$T_{3c}(p,s)$	0.34 mK

ΔT_{tol} = 0.49 mK

Computing Time in Relation to IAPWS-IF97

Measurement of the Computing Time

- Basis: IAPWS benchmark program NIFBENCH
- Specifications of the test platform:
  - Computer: PC with Pentium 4, 1500 MHz, 400 MHz front side bus
  - Operation System: Windows 2000®
  - Compiler: Compaq Visual Fortran 6.1®, standard options
  - Kind of executable file: Fortran Console Application

Computing Time Ratio (*CTR* Value)

$$CTR = \frac{\text{Computing time using IF97 equations only}}{\text{Computing time using the new } T_3(p,h) \text{ or } T_3(p,s) \text{ equations}}$$

Computing Time using $T_3(p,h)$ in Relation to IAPWS-IF97

	Calculation of T using		
	$T = T_3(p,h)$	Two-dimensional Iteration of T and ρ from: $p = p_3^{97}(\rho,T)$ and $h = h_3^{97}(\rho,T)$	
Subregion	**Computing Time**	**Computing Time** [a)]	**CTR**
3a	0.26 μs/call	3.94 μs/call	15.0
3b	0.19 μs/call	3.94 μs/call	21.0
3c	0.15 μs/call	3.94 μs/call	25.7

Computing Time using $T_3(p,s)$ in Relation to IAPWS-IF97

	Calculation of T using		
	$T = T_3(p,s)$	Two-dimensional Iteration of T and ρ from: $p = p_3^{97}(\rho,T)$ and $s = s_3^{97}(\rho,T)$	
Subregion	**Computing Time**	**Computing Time** [a)]	**CTR**
3a	0.28 μs/call	4.52 μs/call	16.0
3b	0.20 μs/call	4.49 μs/call	23.0
3c	0.14 μs/call	4.55 μs/call	33.1

a) Program Package: Property Database for the Calculation of Heat Cycles and Turbines, University of Applied Sciences of Zittau and Görlitz and Technical University of Dresden, 1998 - 2001

Conclusions

- Backward equations $T_3(p,h)$ and $T_3(p,s)$ for region 3 of IAPWS-IF97 are possible for required numerical consistency of ΔT_{tol} = 25 mK.

  ⇒ Confirmation of the specifications for numerical consistency necessary

- Calculation of T using backward equations $T_3(p,h)$ and $T_3(p,s)$:

  ⇒ Depending on iteration method and starting values CTR-values between 10 and 20 in comparison with IAPWS-IF97 are possible.

- For calculating further properties, the determination of ρ is necessary:

  ⇒ Investigations will be performed.

⇓

Final set of backward equations $T_3(p,h)$ and $T_3(p,s)$

for region 3 of IAPWS-IF97

will be presented next year.