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Fast and Accurate Calculation of Thermophysical Properties in Numerical Process Simulations with the Spline-Based Table Look-up Method (SBTL)

International Association for the Properties of Water and Steam (IAPWS)

Task Group "CFD Steam Property Formulation":

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"IAPWS Guideline on the Fast Calculation of Steam and Water Properties With the Spline-Based Table Look-Up Method (SBTL)"

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Contents:

Numerical Process Simulations – Requirements for Property Calculations

Computational Fluid Dynamics (CFD)

Flow analysis of power plant components

Heat-Cycle Calculations

Power plant design

Refrigeration-Cycle Calculations

Refrigeration plant design

Real-Time Process Optimizations

Operation management

Demands on Algorithms for Property Calculations

⇨ **Accurate property calculations are required.**

⇨ **Property functions need to be extremely fast.**

⇨ **Inverse functions must be numerically consistent with their forward functions, e.g. $u(p,v)$ and $p(v,u)$.**

Available IAPWS-Formulations for Water and Steam

Scientific Formulation IAPWS-95

Fundamental equation: $$\Phi = \frac{f}{R_m \cdot T} = \Phi^0(\tau,\delta) + \Phi^r(\tau,\delta) \qquad \tau = \frac{T_c}{T} \qquad \delta = \frac{\rho}{\rho_c}$$

Ideal part: $$\Phi^0(\tau,\delta) = \ln(\delta) + n_1^0 + n_2^0 \cdot \tau + n_3^0 \cdot \ln(\tau) + \sum_{i=4}^{8} n_i^0 \cdot \ln\left[1 - \exp\left(-\gamma_i^0 \cdot \tau\right)\right]$$

Residual part: $$\Phi^r(\tau,\delta) = \sum_{i=1}^{7} n_i \cdot \delta^{d_i} \cdot \tau^{t_i} + \sum_{i=8}^{51} n_i \cdot \delta^{d_i} \cdot \tau^{t_i} \cdot \exp\left(-\delta^{c_i}\right) +$$

$$+ \sum_{i=52}^{54} n_i \cdot \delta^{d_i} \cdot \tau^{t_i} \cdot \exp\left[-\alpha_i \cdot (\delta - \varepsilon_i)^2 - \beta_i \cdot (\tau - \gamma_i)^2\right] + \sum_{i=55}^{56} n_i \cdot \Delta^{b_i} \cdot \delta \cdot \psi$$

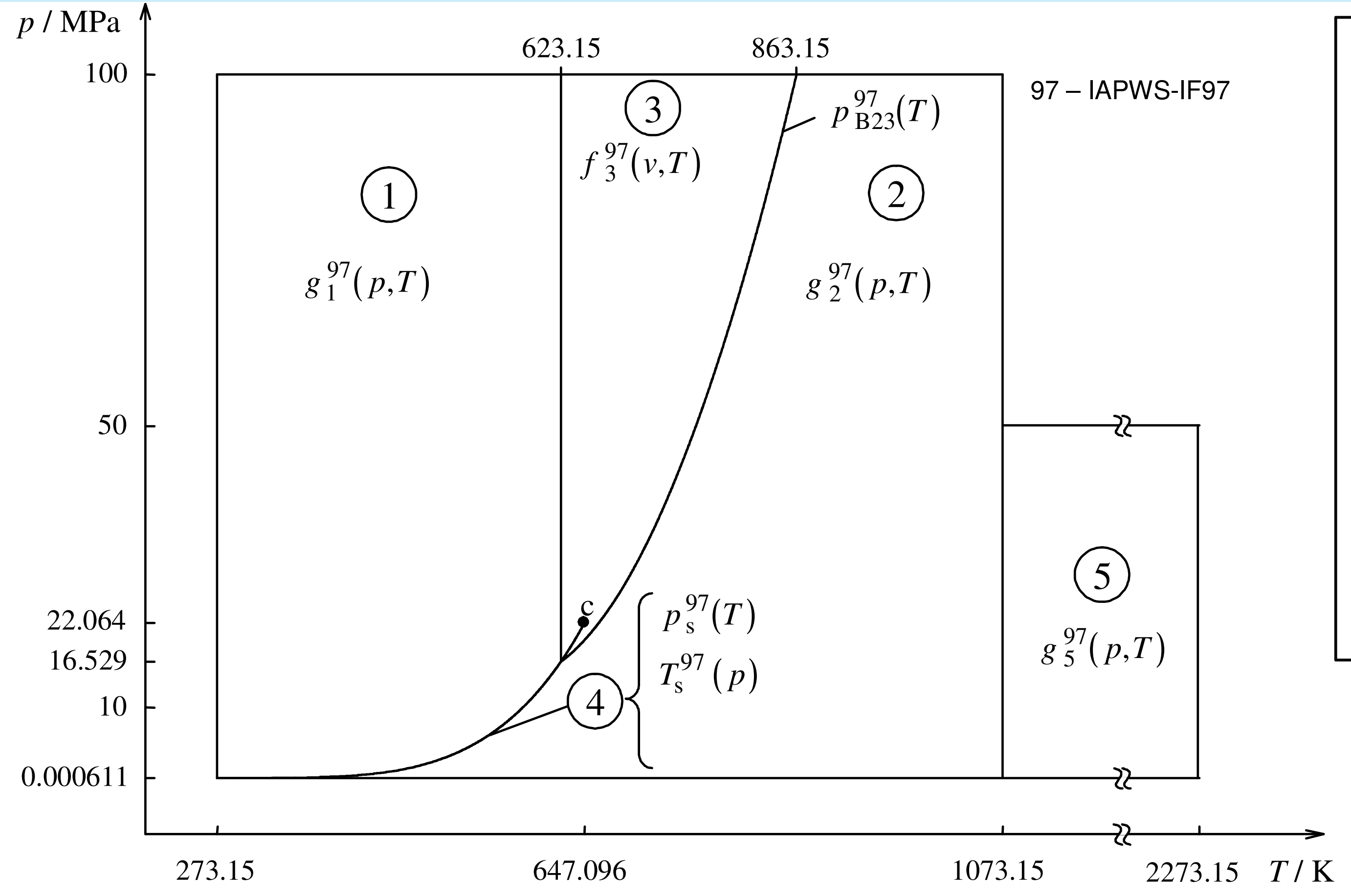
$$\Delta = \theta^2 + B_i \cdot \left[(\delta - 1)^2\right]^{a_i} \qquad \theta = (1 - \tau) + A_i \cdot \left[(\delta - 1)^2\right]^{\frac{1}{2 \cdot \beta_i}} \qquad \psi = \exp\left[-C_i \cdot (\delta - 1)^2 - D_i \cdot (\tau - 1)^2\right]$$

- Represents the measurement data it is based on to within their uncertainties
- Contains numerous computationally intensive terms
- Property functions of (v,u) and (p,h) need to be calculated by iteration

⇨ **Computing speed is insufficient for extensive process simulations and needs to be accelerated by factors > 100…1000 to meet the requirements.**

Available IAPWS-Formulations for Water and Steam

Industrial Formulation IAPWS-IF97



Region 2:

$$\frac{g_2(p,T)}{R\cdot T} = \gamma^0(\pi,\tau) + \gamma^r(\pi,\tau)$$

$$\tau = \frac{T^*}{T} \qquad \pi = \frac{p}{p^*}$$

$$\gamma^0(\pi,\tau) = \ln\pi + \sum_{i=1}^{9} n_i^0 \tau^{J_i^0}$$

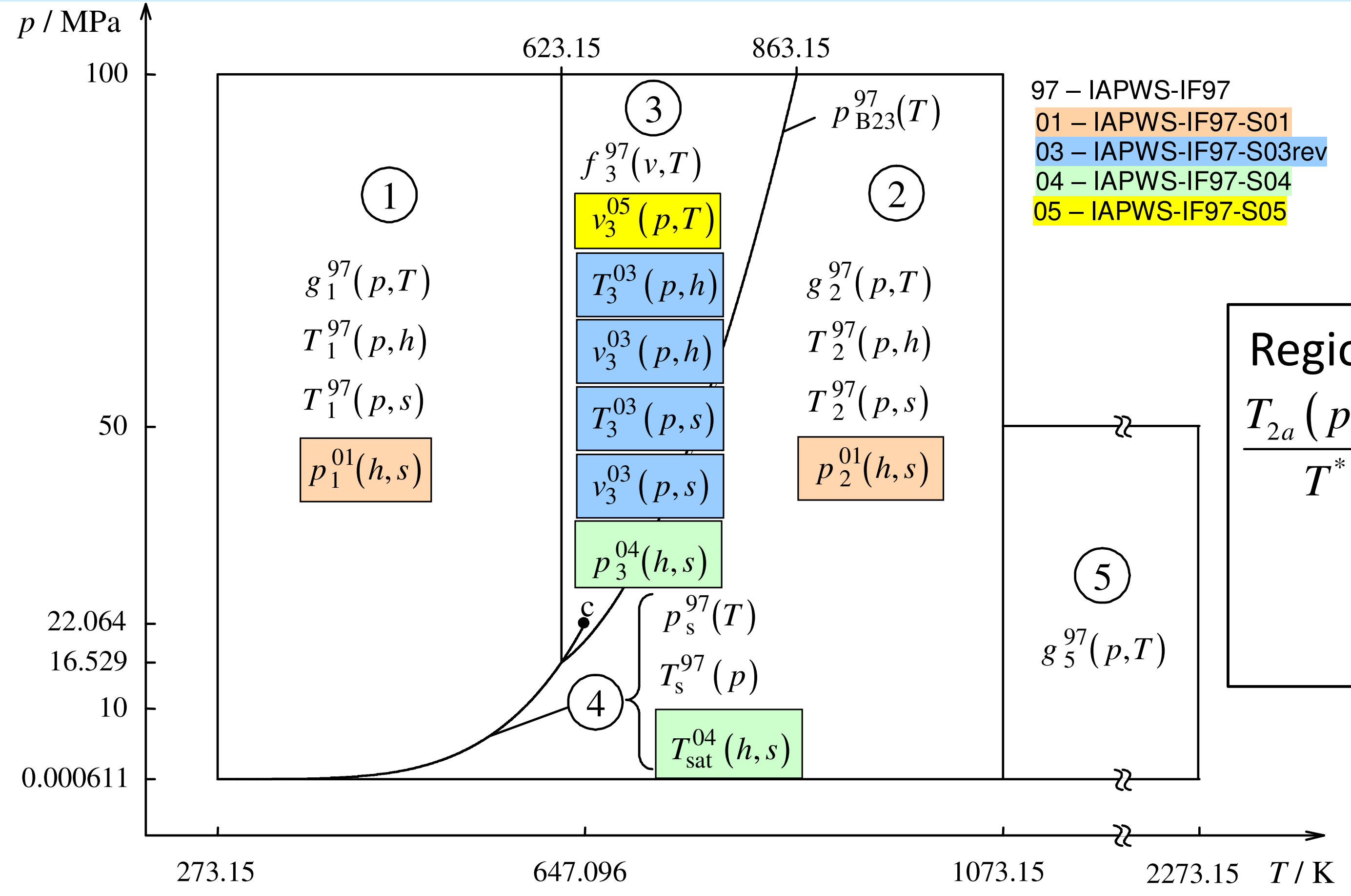
$$\gamma^r(\pi,\tau) = \ln\pi + \sum_{i=1}^{43} n_i \pi^{I_i} (\tau - 0.5)^{J_i}$$

- Basic equations are optimized for computing speed
- Accuracy is sufficient for industrial use
- Property functions of (*v*,*u*) need to be calculated by iteration

⇨ **Even IAPWS-IF97 is too slow for CFD simulations.**

Available IAPWS-Formulations for Water and Steam

Industrial Formulation IAPWS-IF97 – Backward Equations



Region 2:

$$\frac{T_{2a}(p,h)}{T^*} = \theta_{2a}(\pi,\eta) = \sum_{i=1}^{34} n_i \pi^{I_i} (\eta - 2.1)^{J_i}$$

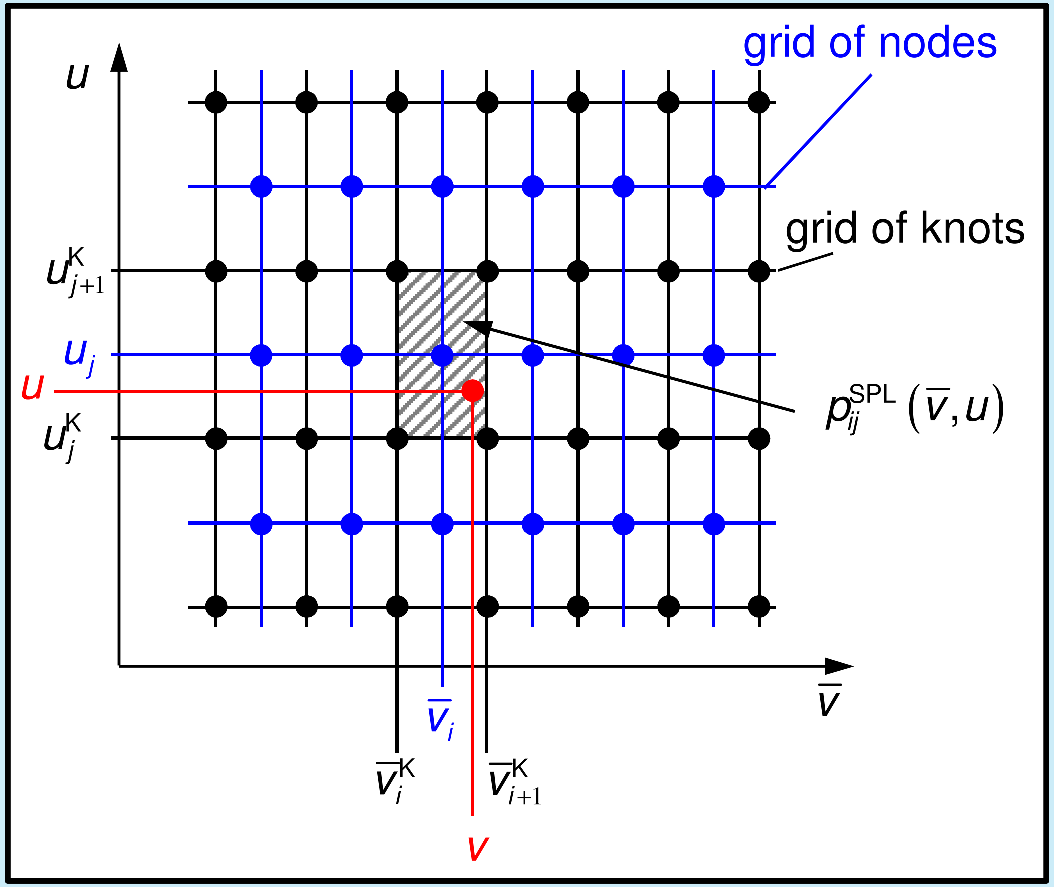
$$\pi = \frac{p}{p^*} \qquad \eta = \frac{h}{h^*}$$

- Numerical consistency of backward equations is not sufficient for small spatial and time steps in CFD calculations or the simulation of transient processes in heat-cycles
  → inverse functions need to be calculated from the basic equations by iteration

⇨ **Backward equations are not an option for CFD and the simulation of transient processes.**

Fundamentals of the Spline-Based Table Look-Up Method (SBTL)

Generation of a spline function $p^{SPL}(v,u)$ from an underlying eq. of state $p^{EOS}(v,u)$:



- **Generation of a rectangular grid of nodes:**
  - each node is calculated from the underlying equation of state:
    $$p_{i,j}(v_i,u_j) = p^{EOS}(v_i,u_j)$$
- **Variable transformation: $v \rightarrow \bar{v}$**
  - enhance accuracy
  - transform the range of state
- **Cell definition in the grid of knots:**
  - spline polynomial:
    $$p_{ij}^{SPL}(\bar{v},u) = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ijkl}\left(\bar{v}-\bar{v}_i\right)^{k-1}\left(u-u_j\right)^{l-1}$$
  - intersects the inner node
  - continuous function and first derivatives
- **Optimization for:**
  - required accuracy
  - maximum computing speed
  - minimum amount of data (table size)
- **Providing the look-up table with the determined spline coefficients**

Property calculation within CFD:

- transformation of v
- cell (i,j) determination
- computation of the spline polynomial

Fundamentals of the Spline-Based Table Look-Up Method (SBTL)

Calculation of inverse spline functions (Example: bi-quadratic polynomial):

Forward spline function: $p_{ij}^{\mathrm{SPL}}(\bar{v},u)=\sum_{k=1}^{3}\sum_{l=1}^{3}a_{ijkl}(\bar{v}-\bar{v}_i)^{k-1}(u-u_j)^{l-1}$

Inverse spline function: $u_{ij}^{\mathrm{INV}}(p,\bar{v})=\dfrac{\left(-B\pm\sqrt{B^2-4AC}\right)}{2A}+u_j$

where $A=a_{ij13}+\Delta\bar{v}_i\left(a_{ij23}+a_{ij33}\Delta\bar{v}_i\right)$

$B=a_{ij12}+\Delta\bar{v}_i\left(a_{ij22}+a_{ij32}\Delta\bar{v}_i\right)$

$C=a_{ij11}+\Delta\bar{v}_i\left(a_{ij21}+a_{ij31}\Delta\bar{v}_i\right)-p$

and $\Delta\bar{v}_i=\left(\bar{v}-\bar{v}_i\right)$

$(\pm)=\mathrm{sign}(B)$

- **The inverse spline function is numerically consistent with its forward function.**
- **The inverse spline function can be calculated without any iteration.**

SBTL Functions of (*v*,*u*) and Inverse Functions of (*p*,*v*) and (*u*,*s*) Based on IAPWS-IF97

Spline functions of (*v*,*u*):

Pressure $p^{SPL}(v,u)$

Temperature $T^{SPL}(v,u)$

Spec. entropy $s^{SPL}(v,u)$

Speed of sound $w^{SPL}(v,u)$

Dynamic viscosity $\eta^{SPL}(v,u)$

Therm. conductivity $\lambda^{SPL}(v,u)$

Calculation of inverse spline functions:

(*p*,*v*):

$p^{SPL}(v,u) \rightarrow u^{INV}(p,v) \rightarrow T^{SPL}, s^{SPL}, w^{SPL}, \eta^{SPL}, \lambda^{SPL}(v, u^{INV})$

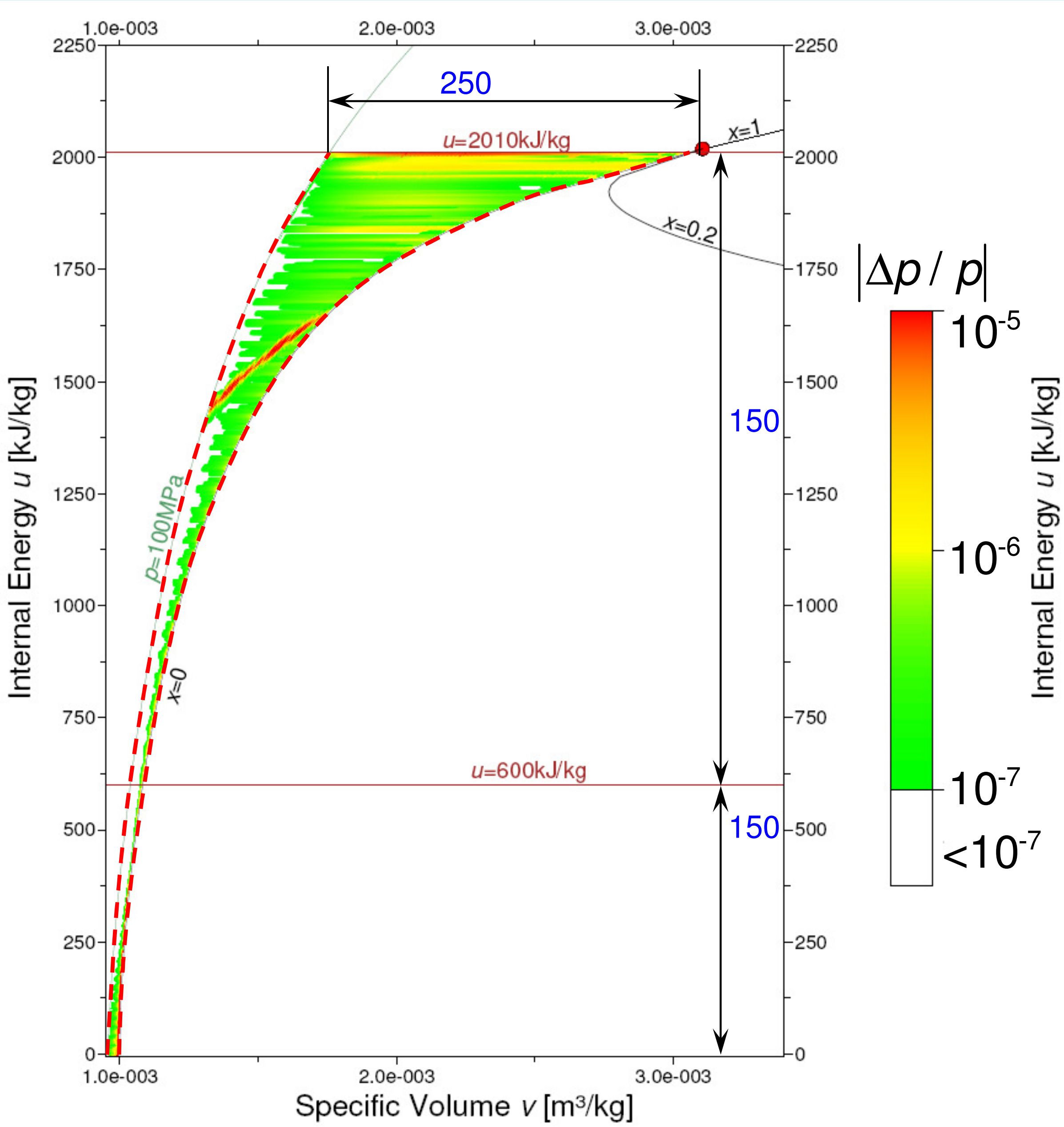
(*u*,*s*):

$s^{SPL}(v,u) \rightarrow v^{INV}(u,s) \rightarrow p^{SPL}, T^{SPL}, w^{SPL}, \eta^{SPL}, \lambda^{SPL}(v^{INV}, u)$

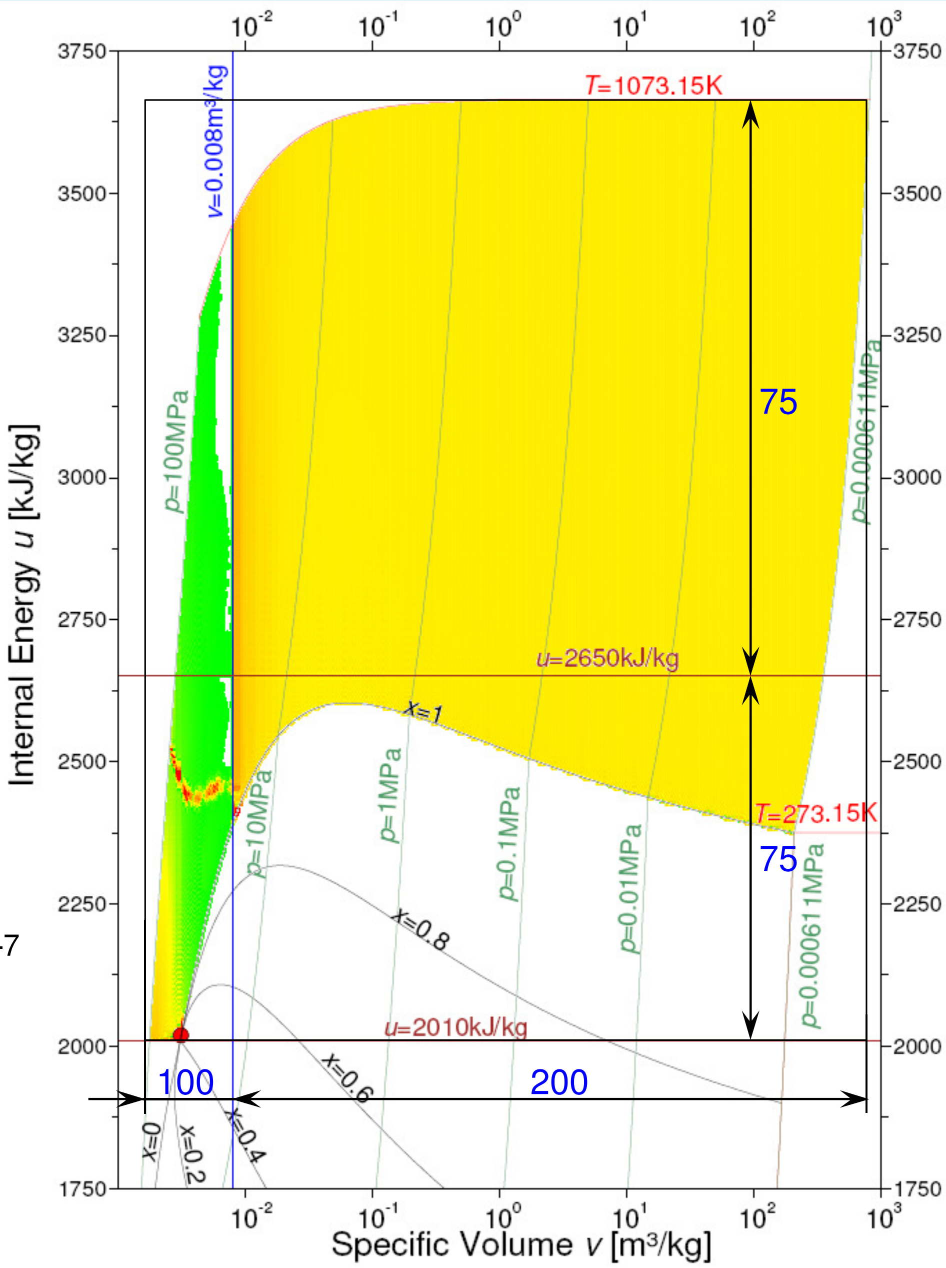
- **All thermodynamic and transport properties including derivatives and backward functions are calculated without iterations.**
- **Forward and backward functions are calculated with complete numerical consistency.**

SBTL Functions *p*(*v*,*u*) – Deviations from IAPWS-IF97

→ Spline function $p_L(v,u)$:



→ Spline function $p_G(v,u)$:



Transformations:

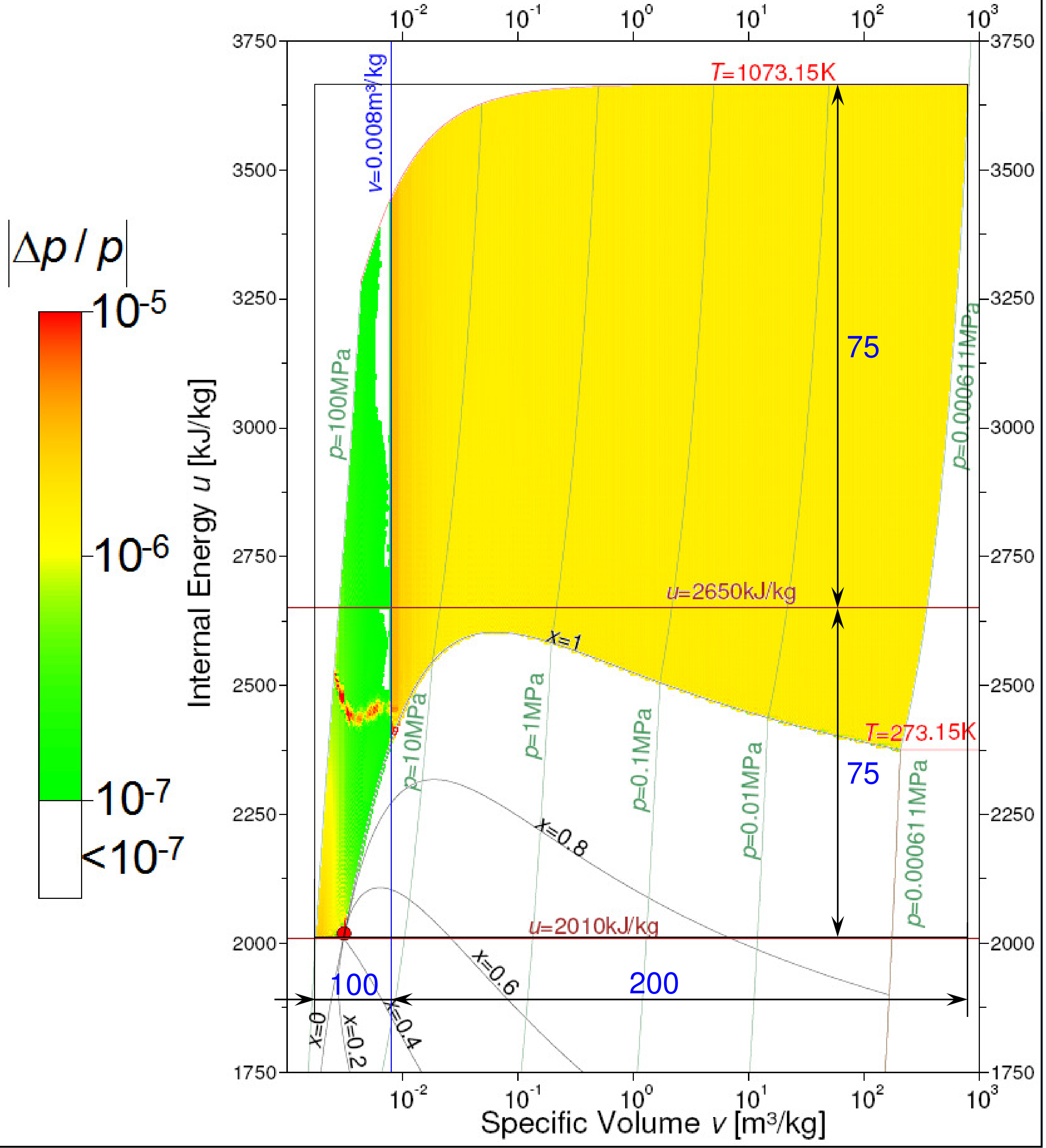
$\bar{v}$ scaled between $v(100\text{MPa},u)$ and $v'(u)$

$\bar{v} = \ln(v)$

→ **Spline function $p_G(v,u)$:**

Maximum deviation from IAPWS-IF97:

$$\left|\Delta p / p\right|_{max} = 0.00095\%$$

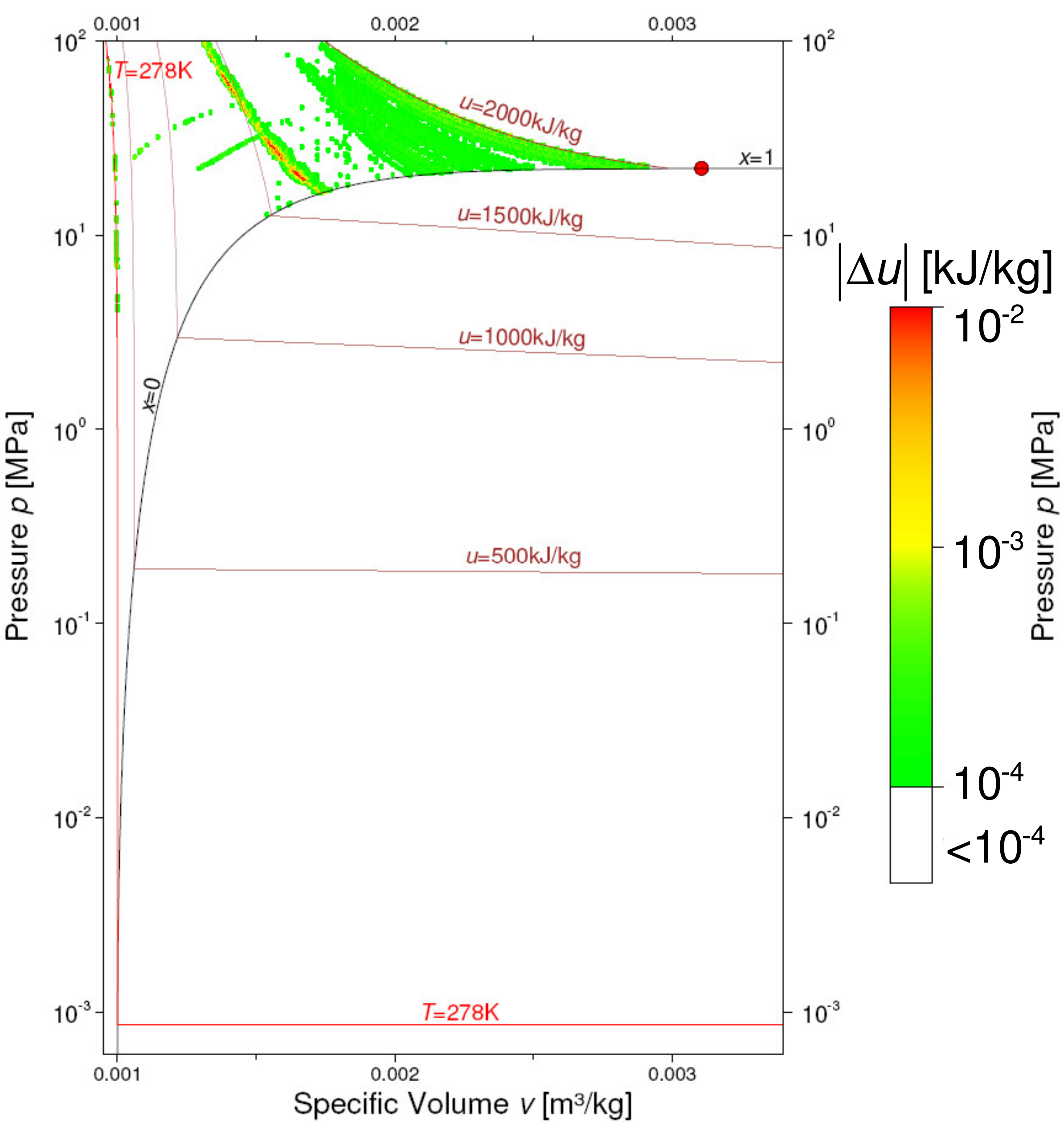


Transformation:

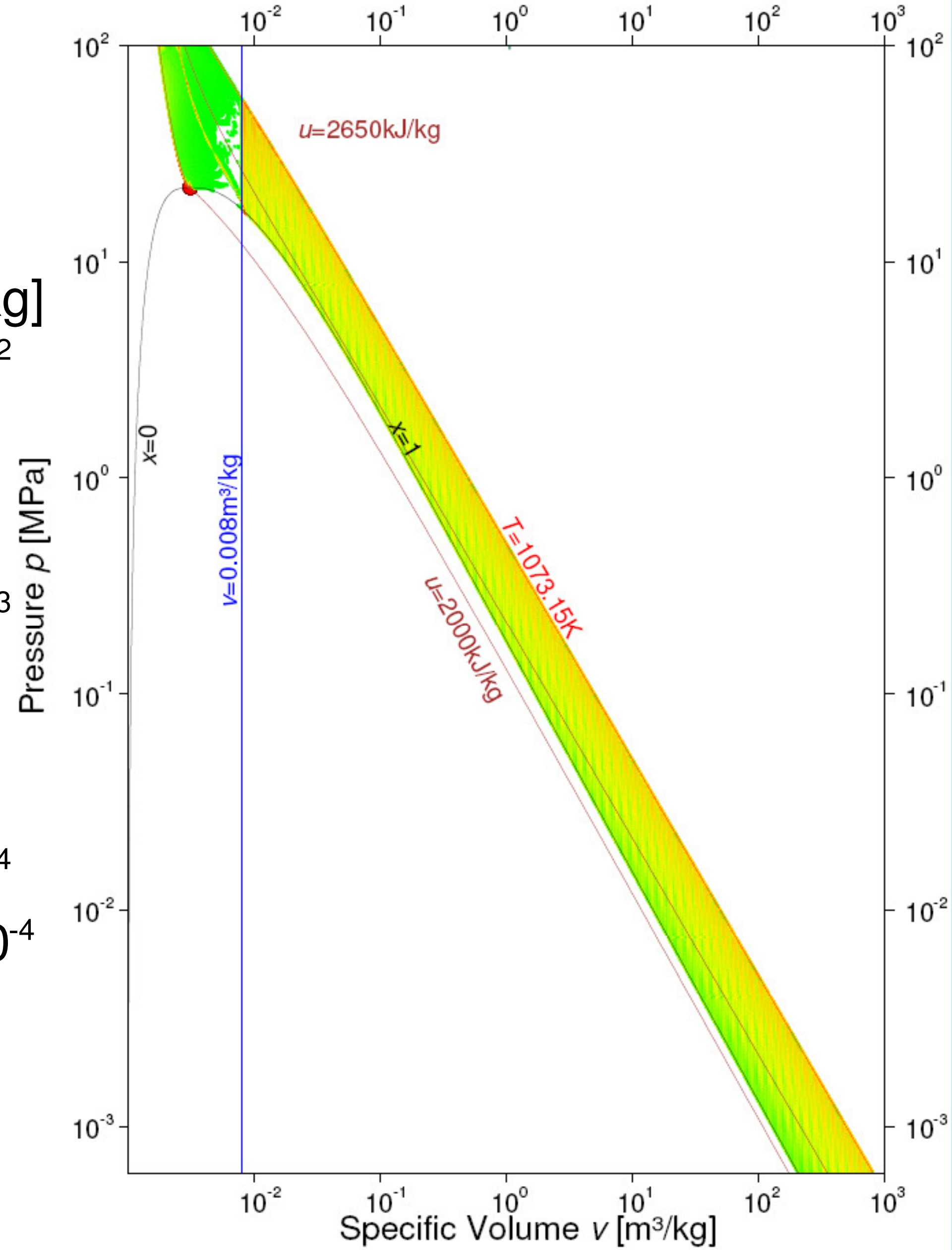
$$\overline{v}(v) = \ln(v)$$

Inverse Functions $u(p,v)$ – Deviations from IAPWS-IF97

→ **Inverse spline function $u_L(p,v)$:**



→ **Inverse spline function $u_G(p,v)$:**



➢ **Inverse spline functions are numerically consistent with their forward spline functions.**

SBTL Functions of (*v*,*u*) and Inverse Functions of (*p*,*v*) and (*u*,*s*) – Deviations from IAPWS-IF97

SBTL function		Max. deviation (liquid phase)	Max. deviation (vapor phase)
$p(v,u)$	$p \leq 2.5$ MPa	$\lvert \Delta p / p \rvert < 0.12$ %	$\lvert \Delta p / p \rvert < 0.001$ %
	$p > 2.5$ MPa	$\lvert \Delta p \rvert < 0.6$ kPa	
$T(v,u)$		$\lvert \Delta T \rvert < 1$ mK	$\lvert \Delta T \rvert < 1$ mK
$s(v,u)$		$\lvert \Delta s \rvert < 10^{-6}$ kJ kg^{-1} K^{-1}	$\lvert \Delta s \rvert < 10^{-6}$ kJ kg^{-1} K^{-1}
$w(v,u)$		$\lvert \Delta w / w \rvert < 0.001$ %	$\lvert \Delta w / w \rvert < 0.001$ %
$\eta(v,u)$		$\lvert \Delta \eta / \eta \rvert < 0.001$ %	$\lvert \Delta \eta / \eta \rvert < 0.001$ %

- **Spline-based property functions reproduce the industrial standard IAPWS-IF97 with high accuracy.**
- **Differences between the results of process simulations using the SBTL method and those obtained through the use of IAPWS-IF97 are negligible.**

Computing Time Comparisons with IAPWS-IF97

Computing Time Ratio $CTR = \dfrac{\text{Computing time of the calculation from IAPWS - IF97}}{\text{Computing time of the calculation from the spline function}}$

	IAPWS-IF97 Region				
SBTL function	**1 (liquid)**	**2 (vapor)**	**3 (critical)**	**4 (two-phase)**	**5 (high-temp.)**
$p(v,u)$	130	271	161	19.6	470
$T(v,u)$	161	250	158	20.6	442
$s(v,u)$	164	261	160	17.8	449
$w(v,u)$	199	310	234	-	471
$\eta(v,u)$	197	309	239	-	-
$u(p,v)$	2.0	6.4	2.8	5.6	3.2
$v(u,s)$	43.5	66.4	78.8	16.2	134

- **Computing time for region determination is included in these values.**

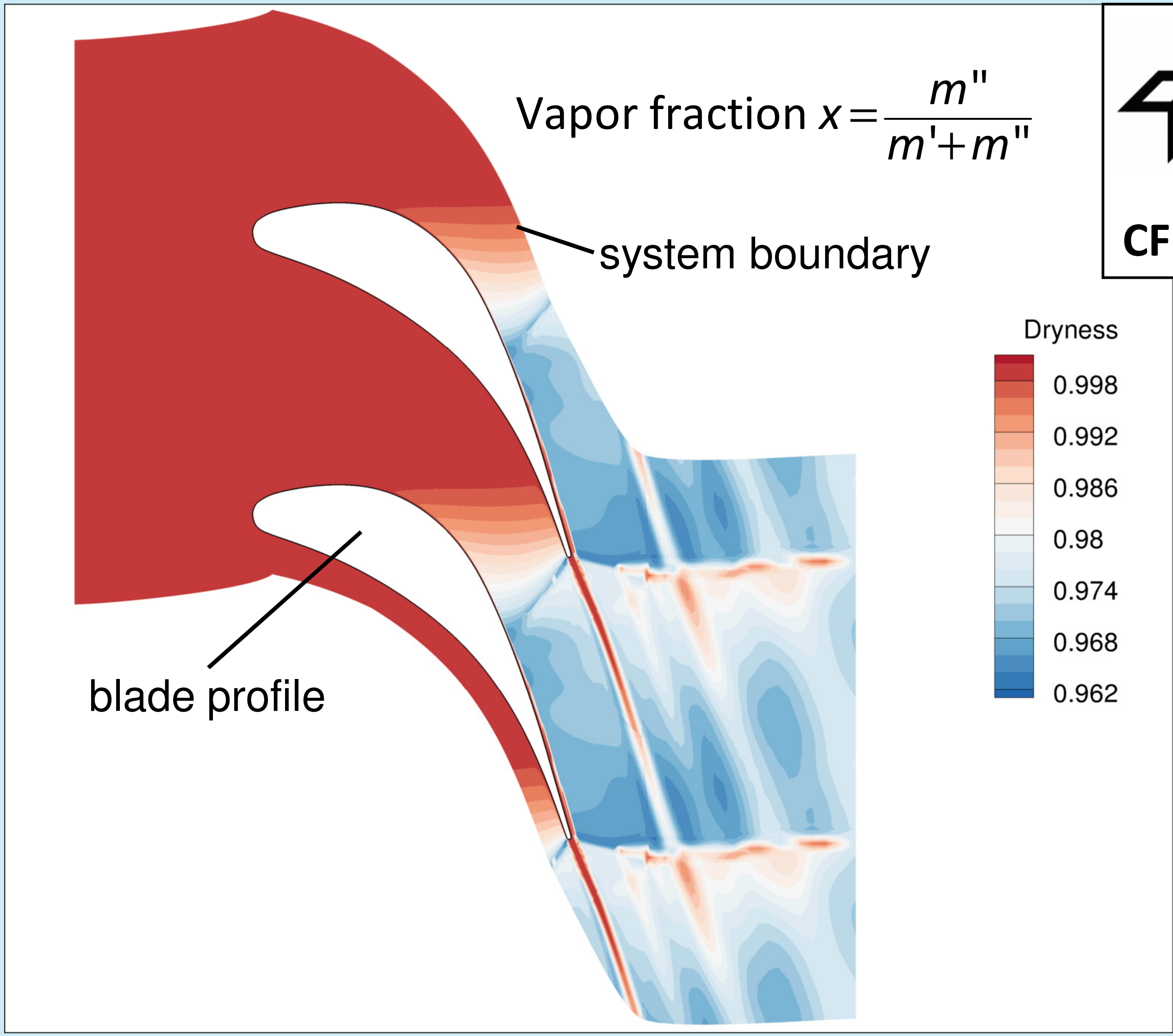
Processor: Intel Xeon – 3.2GHz

Operating system: Windows7 (32 Bit)

Compiler: Intel Composer XE 2011

- **Computing times are reduced by factors up to 300 (500)!**

Application of the SBTL Method in CFD – Condensing Steam Flow Around a Fixed Blade (White et al.)



German Aerospace Center (DLR)
Institute of Propulsion Technology
Numerical Methods,
Cologne, Germany

CFD-Software TRACE (DLR)

Inlet conditions:

- Total pressure: 41.7 kPa
- Total temperature: 357.5 K (ΔT_s=+7.5 K)

Outlet conditions:

- Static pressure: 20.6 kPa

Assumptions:

- equilibrium condensation (no sub-cooling considered)
- homogeneous two-phase flow

➢ **In comparison to simulations with IAPWS-IF97, the computing times are reduced by factors of 6 - 10 through the use of the SBTL method.**

➢ **With regard to simulations with the ideal-gas model, the computing times are increased by a factor of 1.4 only.**

Application of the SBTL Method in Other Software Products

- **RELAP-7** – Idaho National Laboratory (INL)
  international reference code for
  nuclear-reactor system safety analysis
  - SBTL functions of (v,u) based on IAPWS-95
    (incl. metastable liquid/vapor)

- **DYNAPLANT** – SIEMENS
  simulation of non-stationary processes in power plants
  - SBTL functions of (v,h) based on IAPWS-IF97

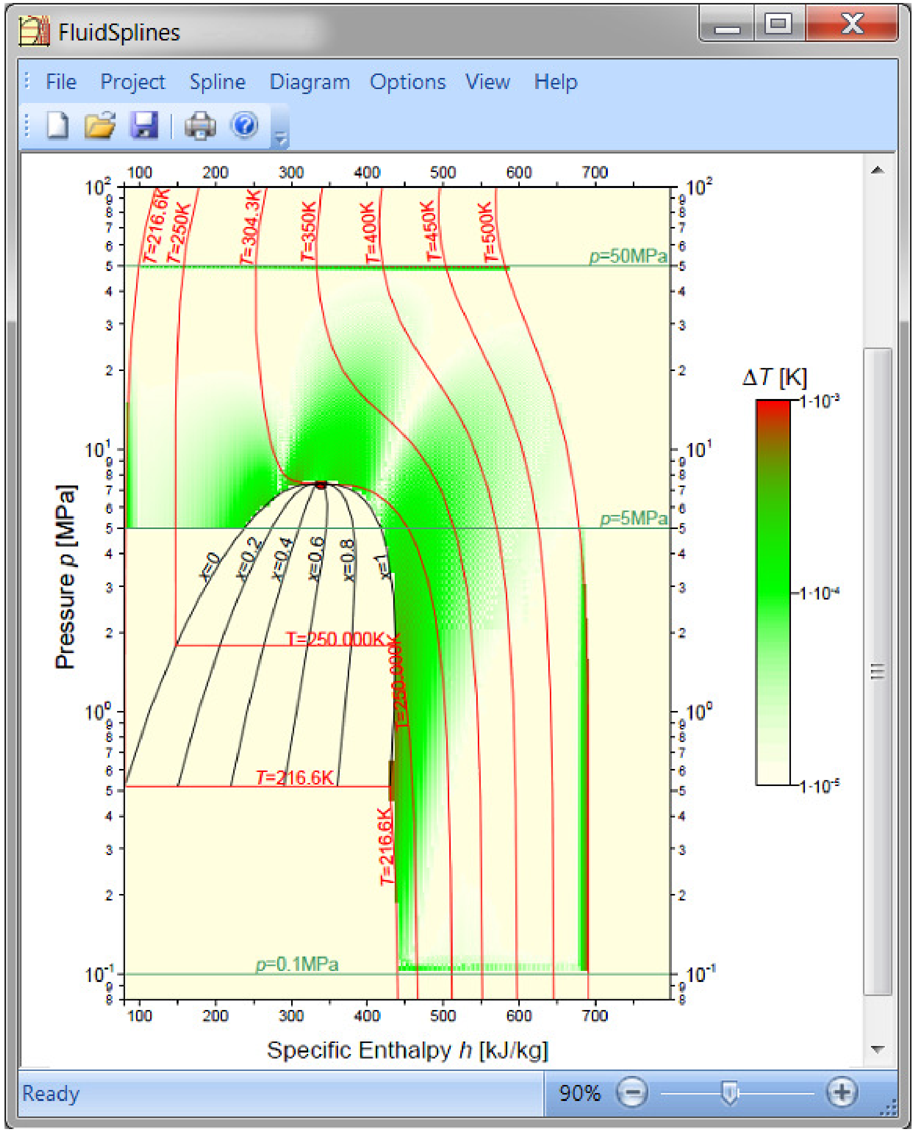
- **KRAWAL** – SIEMENS
  heat-cycle calculations for power plant design
  - SBTL functions of (p,h) based on IAPWS-IF97

- **EBSILON Professional** – STEAG Energy Services
  commercial heat-cycle simulation software
  - SBTL functions of (p,h) based on IAPWS-IF97

Generation of SBTL Functions for Specific Demands

FluidSplines

Software for generating
spline-based property functions



Input:

(Thermodynamic Properties)

REFPROP©

Property-Libraries
(Zittau/Goerlitz Univ.)

Generation of SBTL-Functions for:

- specified range of validity
- required accuracy

Additional Features:

- generation of inverse spline-functions
- accuracy tests
- computing time tests

Output:

- optimized source code for high computing speed
- static/dynamic libraries
- documentation of accuracy and computing speed

Summary

- **Spline-Based Table Look-up Method (SBTL) – a supplement to existing standards:**
  - Reproduces existing standards with high accuracy at high computing speed
  - Inverse spline functions are numerically consistent with their forward functions
  - Property functions and their first derivatives are continuous

- **SBTL functions based on IAPWS-IF97 and IAPWS-95:**
  - Property functions of IAPWS Standards are reproduced with an accuracy of 10 – 100 ppm
  - Computing speeds are considerably increased
    (SBTL functions of (v,u) up to 300 times faster than IAPWS-IF97)

- **Applicability in Computational Fluid Dynamics (CFD) has been demonstrated**
  - 6-10 times faster than simulations with IAPWS-IF97
  - Enables consideration of the real fluid behavior with high accuracy
  - Only 40% slower than simulations with the ideal gas model

- **SBTL functions for specific demands can be generated with FluidSplines:**
  - Tailored for the required range of validity and accuracy
  - Applicable for any property function and any fluid

Summary

The International Association for the Properties of Water and Steam

Stockholm, Sweden
July 2015

Guideline on the Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL)

President:
Dr. David Guzonas
Canadian Nuclear Laboratories
Chalk River, Ontario, Canada

Thank you for your attention!