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Fast Calculation of Real Fluid Properties with the New IAPWS Standard on the Spline-Based Table Look-Up Method (SBTL) and its Application in CFD

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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:

- Need for Fast and Accurate Property Calculations in CFD & Available Algorithms
- Fundamentals of the Spline-Based Table Look-Up Method (SBTL)
- Accuracy and Computing Speed of SBTL Functions of (*v*,*u*), (*p*,*h*), …
- Application of the SBTL Method in CFD (TRACE, developed at DLR)
- FluidSplines – Generation of SBTL Functions for Specific Demands
- Summary

Demands on Fluid Property Functions in CFD & Available Algorithms

Demands on Fluid Property Functions in CFD:

- **Inaccurate property calculations lead to inaccurate simulation results:**
  - Deviations in specific volume *v* result in inaccurate mass flows and velocities.
  - Deviations in caloric properties, *e.g*. internal energy *u* or entropy *s*, result in inaccurate energy and entropy balances.

  ⇨ **Accurate property functions are required.**
- **Property functions have a major influence on the overall computing time:**
  - Fluid properties need to be determined millions of times!

  ⇨ **Property functions need to be extremely fast.**
- **Numerical methods make high demands on property functions:**

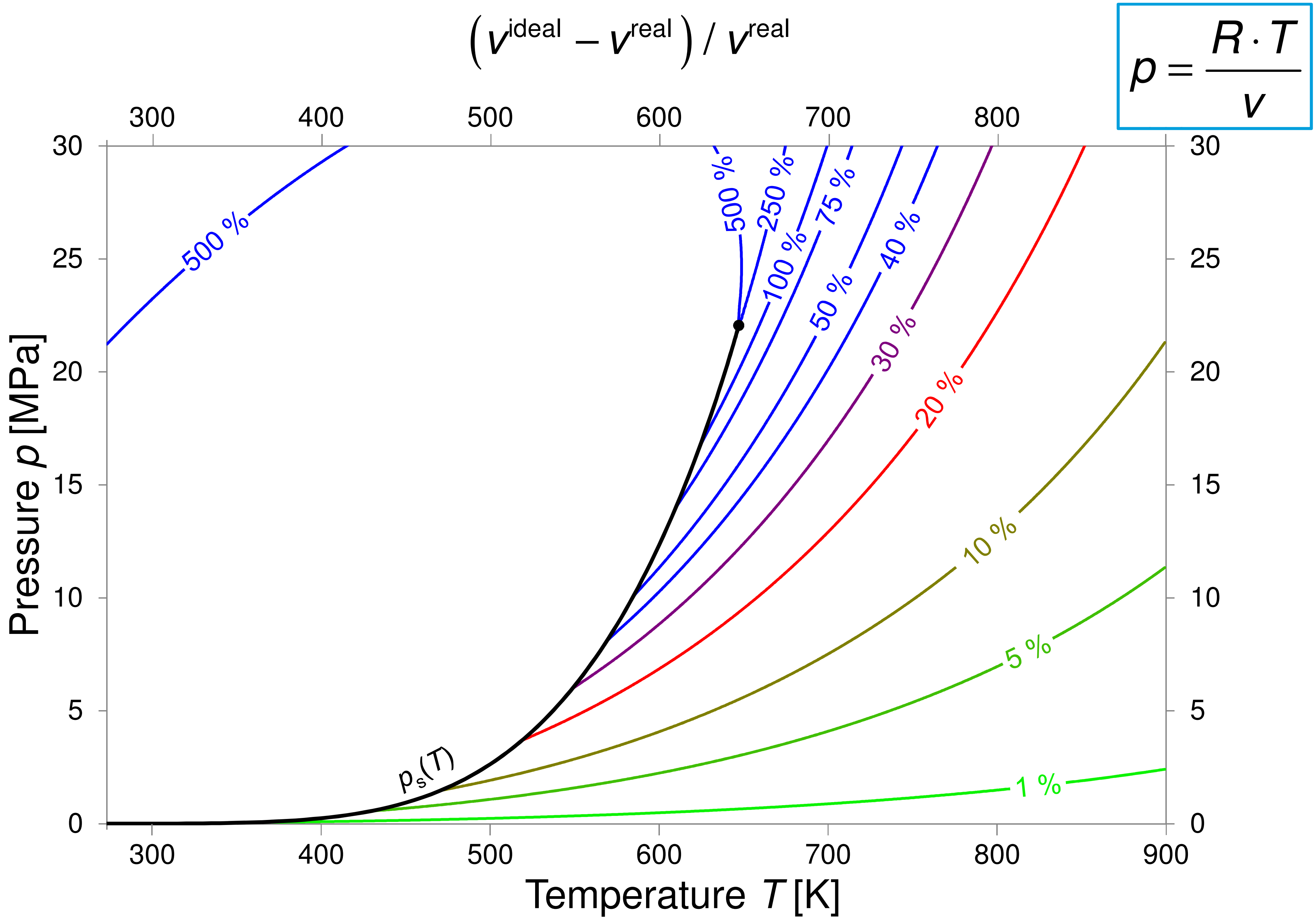
  ⇨ **Numerically consistent inverse functions are required, *e.g.*, *u*(*p*,*v*) and *p*(*v*,*u*).**

  ⇨ **Continuity of property functions and their first derivatives is required.**

Available Property Calculation Algorithms for Water and Steam:

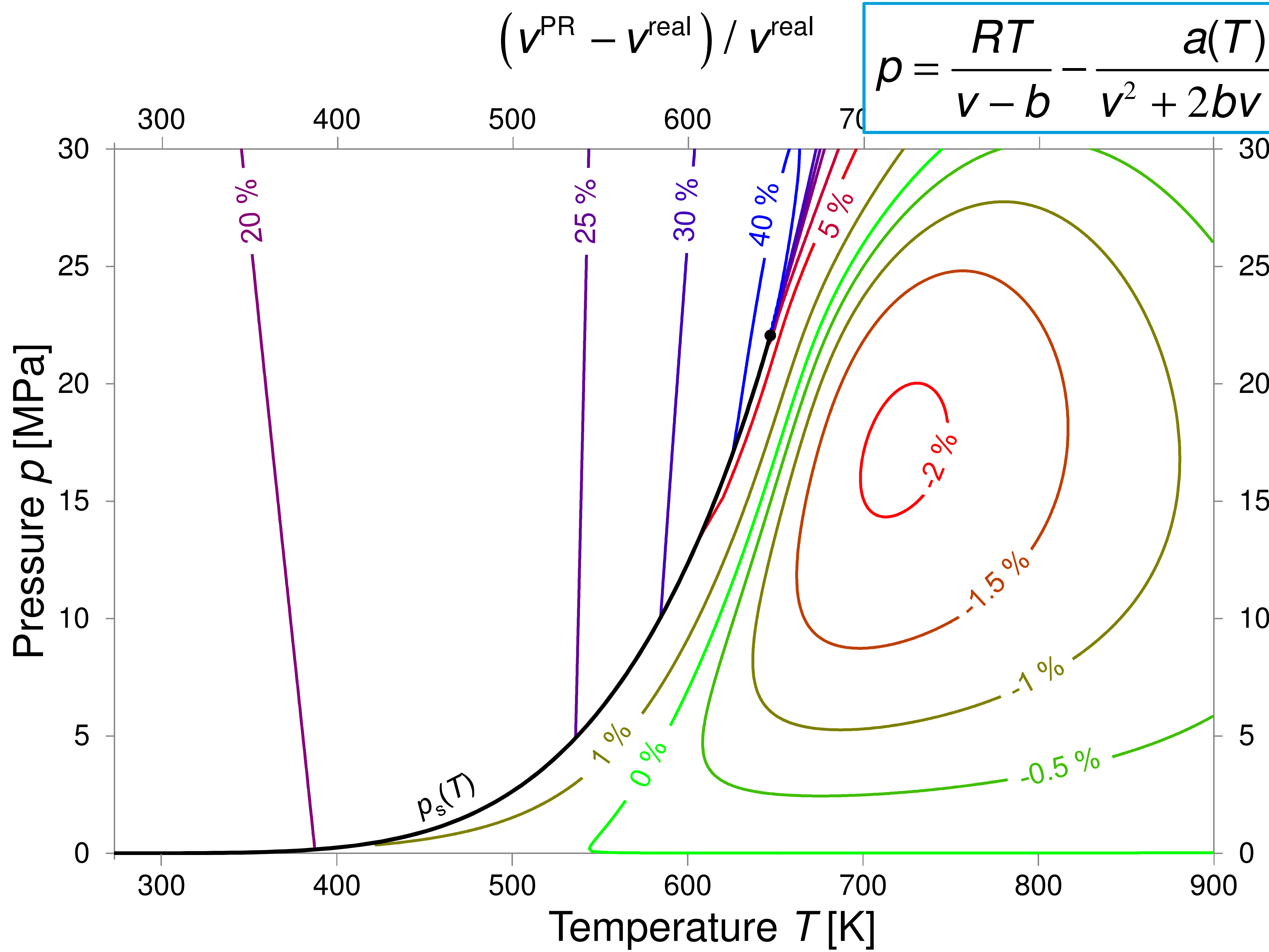
- Ideal-Gas Model
- Cubic Equations of State (Peng-Robinson, Redlich-Kwong, …)
- Industrial Formulation IAPWS-IF97 (fundamental equations)
- Table Look-Up Methods (such as bi-linear or bi-cubic interpolation)

Deviations in Specific Volume (Water and Steam): Ideal-Gas Model

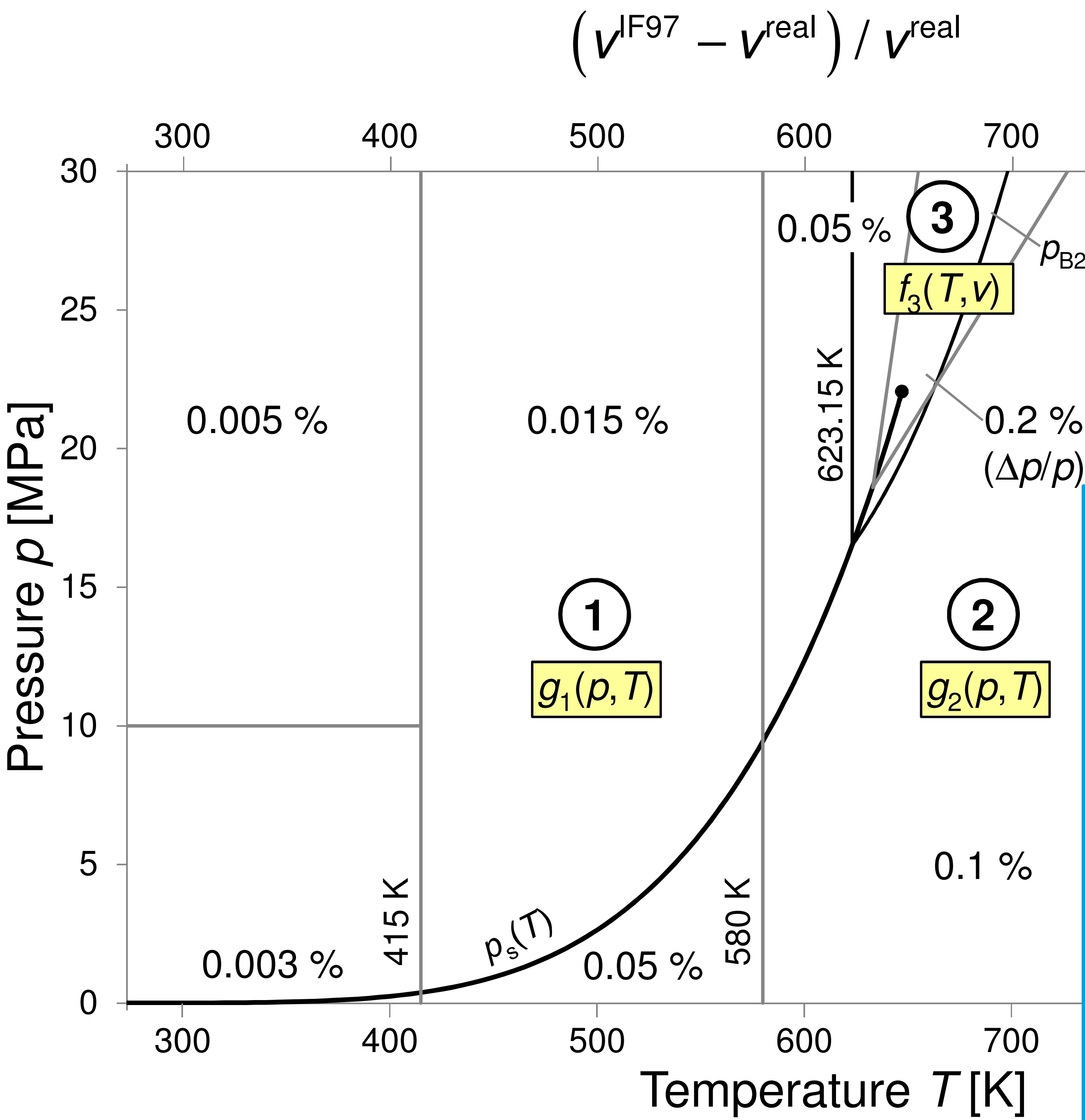


Deviations in Specific Volume (Water and Steam): Cubic Equation of State (Peng-Robinson)

$$p = \frac{RT}{v-b} - \frac{a(T)}{v^2 + 2bv - b^2}$$



Uncertainties in Specific Volume of IAPWS-IF97 for Water and Steam:



Region 2:

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

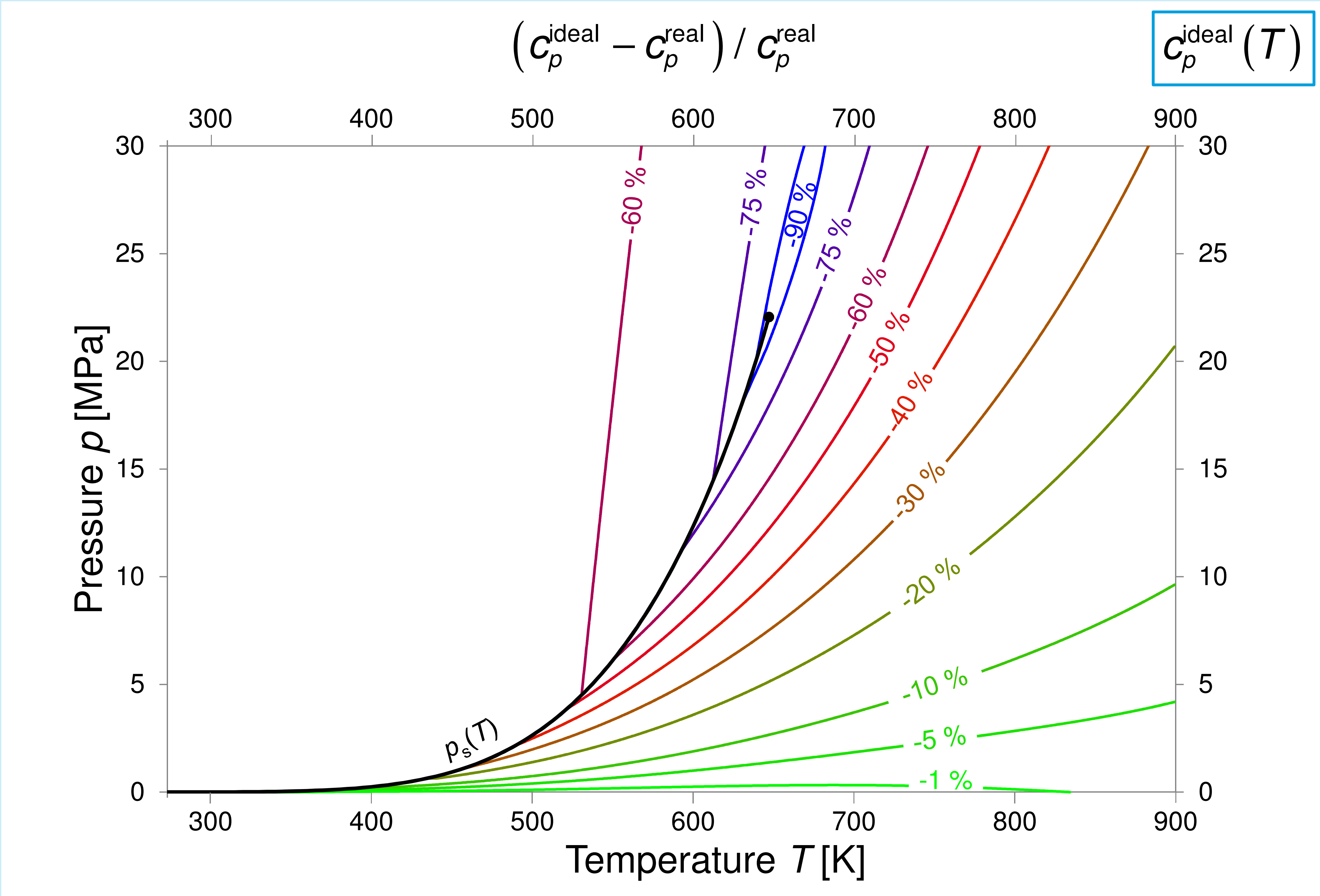
$$\pi = \frac{p}{p^*} \qquad \tau = \frac{T^*}{T}$$

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

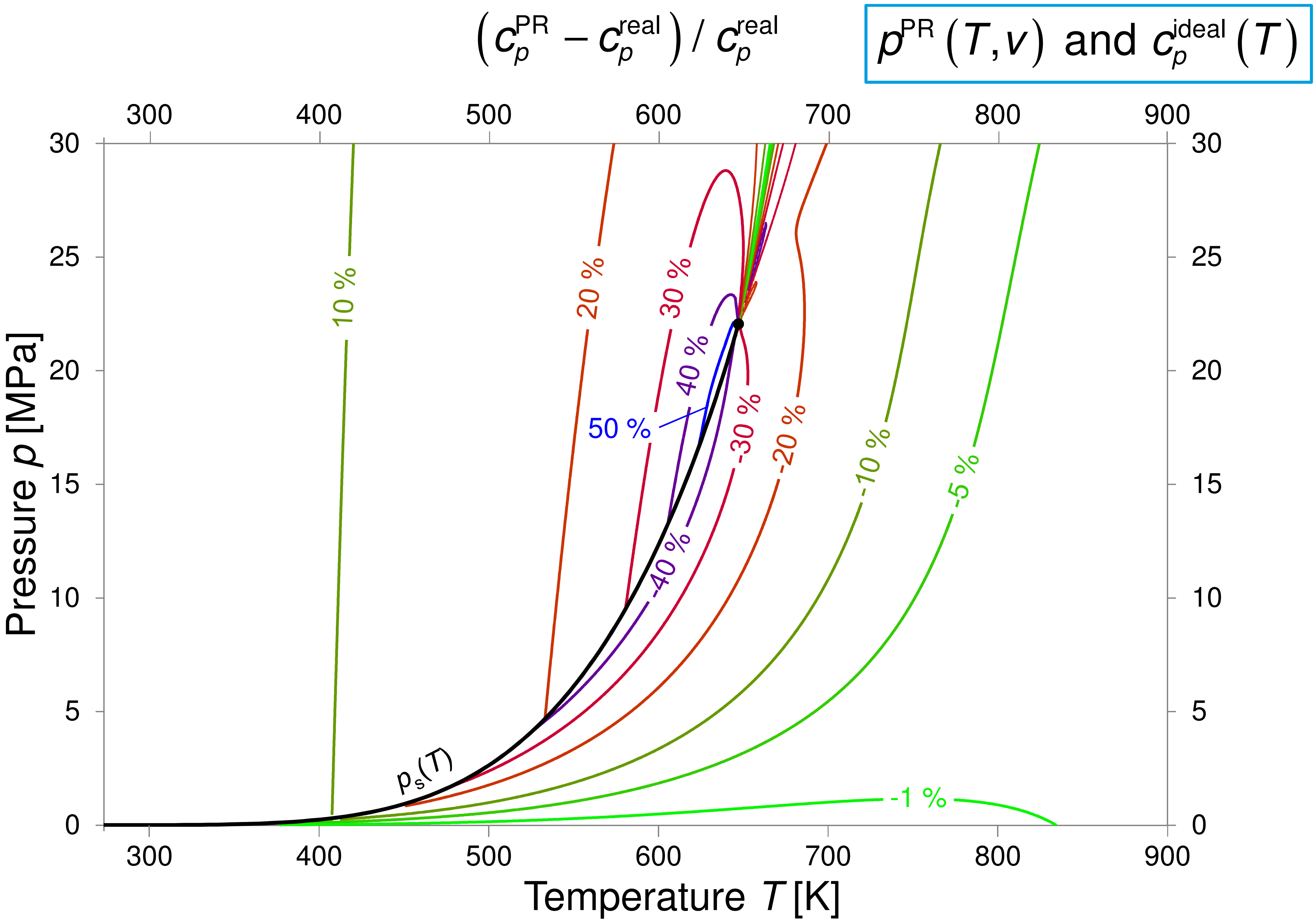
$$\gamma^r(\pi,\tau) = \ln\pi + \sum_{i=1}^{43} n_i \pi^{I_i} (\tau - 0.5)^{J_i}$$

$$v(\pi,\tau)\frac{p}{RT} = \pi\left(\gamma_\pi^0 + \gamma_\pi^r\right)$$

Deviations in Isobaric Heat Capacity (Water and Steam): Ideal-Gas Model

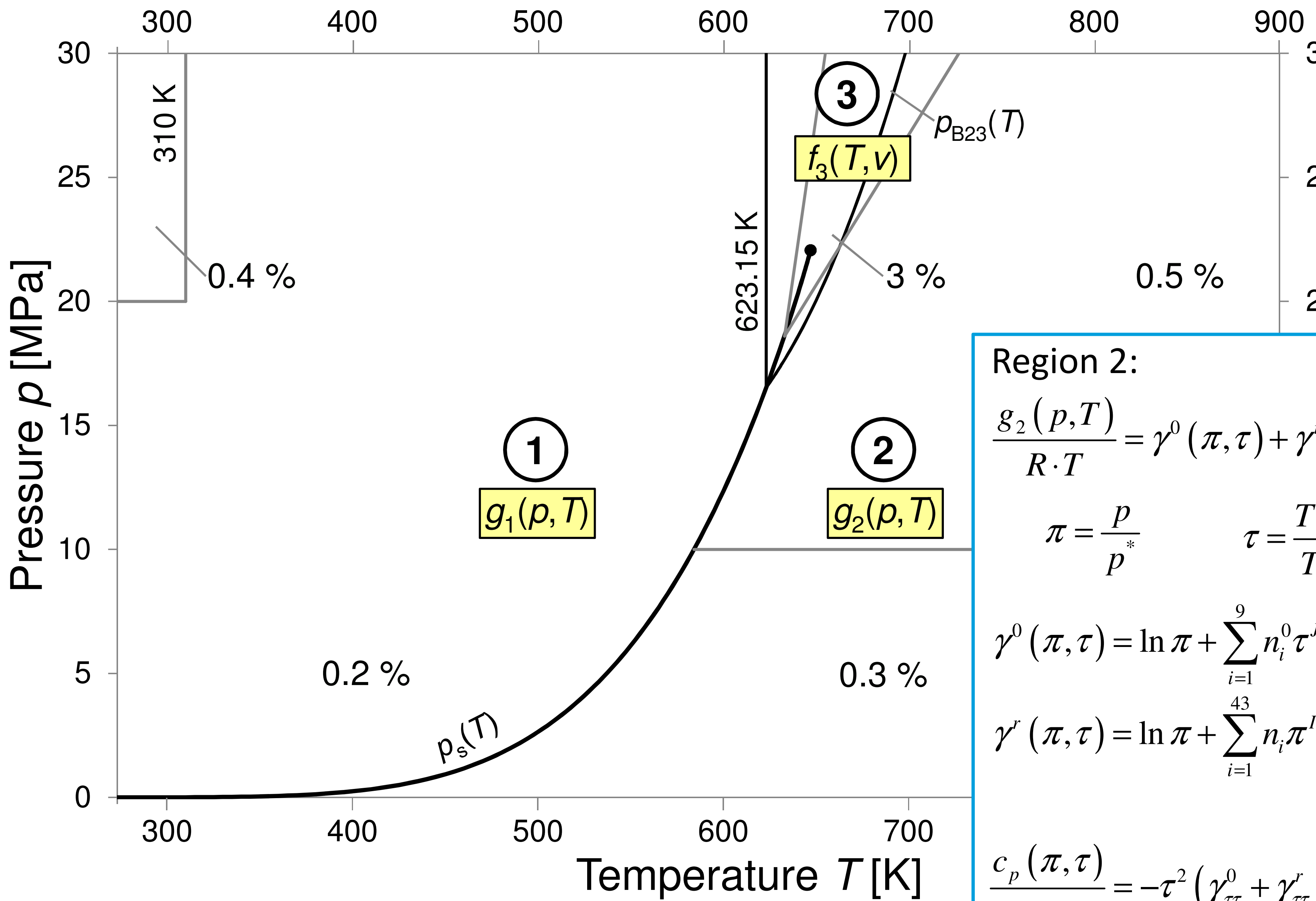


Deviations in Isobaric Heat Capacity (Water and Steam): Cubic Equation of State (Peng-Robinson) + $c_p^{\text{ideal}}(T)$



Uncertainties in Isobaric Heat Capacity of IAPWS-IF97 for Water and Steam:

$$\left(c_p^{\mathrm{IF97}} - c_p^{\mathrm{real}}\right) / c_p^{\mathrm{real}}$$



Region 2:

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

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

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

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

$$\frac{c_p(\pi,\tau)}{R} = -\tau^2\left(\gamma_{\tau\tau}^0 + \gamma_{\tau\tau}^r\right)$$

Fluid Property Calculations in CFD – Objectives

	Available Property Calculation Algorithms for Water and Steam			
Requirements	**Ideal gas**	**Cubic Equation of State**	**Ind. Standard IAPWS-IF97**	**Table Look-Up Methods**
Accuracy	$\lvert\Delta v\rvert \leq 50\ \%$ $\lvert\Delta c_p\rvert \leq 50\ \%$	$\lvert\Delta v\rvert \leq 5\ \%$ $\lvert\Delta c_p\rvert \leq 40\ \%$	$\lvert\Delta v\rvert \leq 0.3\ \%$ $\lvert\Delta c_p\rvert \leq 0.5\ \%$	depends on table size and algorithm
Computing speed	very high	slow	too slow	high

Table Look-Up Methods:

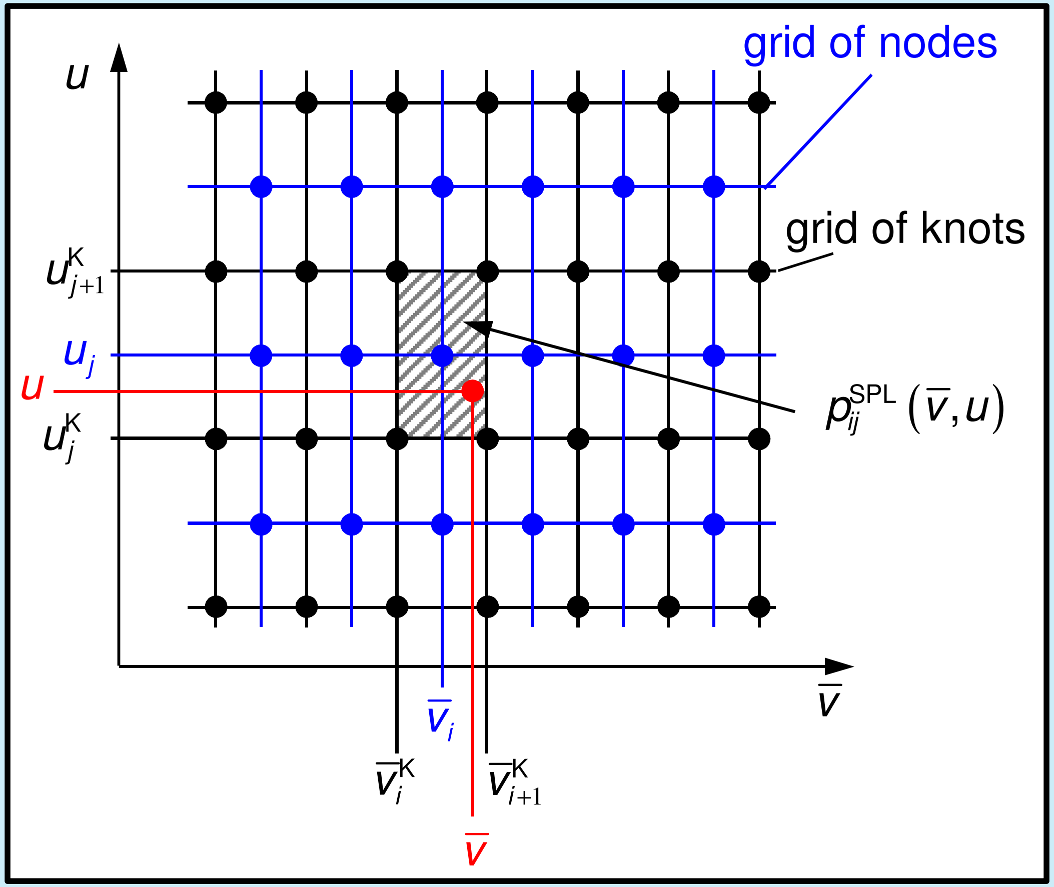
- Bi-linear interpolation:
  - requires comparatively large look-up tables for a certain accuracy
  - shows discontinuities in the first derivatives
  - clustered look-up tables → computationally intensive cell search
- Bi-cubic interpolation:
  - continuous first derivatives (local application)
  - calculation of inverse functions is computationally intensive

Objectives for the Development of a Spline-Based Table Look-Up Method (SBTL):

- property calculations with high accuracy at high computing speed
- continuous property functions and first derivatives
- fast and numerically consistent inverse functions, *e.g.*, $u(p,v)$ and $p(v,u)$

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:**
  - bi-quadratic spline polynomial:

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

- transformation of $v \rightarrow \bar{v}$
- 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: $$p_{ij}^{\mathrm{SPL}}(\bar{v},u)=\sum_{k=1}^{3}\sum_{l=1}^{3}a_{ijkl}\left(\bar{v}-\bar{v}_i\right)^{k-1}\left(u-u_j\right)^{l-1}$$

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

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.**

Spline Functions of (*v*,*u*) and Inverse Spline Functions Based on IAPWS-IF97

Calculation of inverse spline functions:

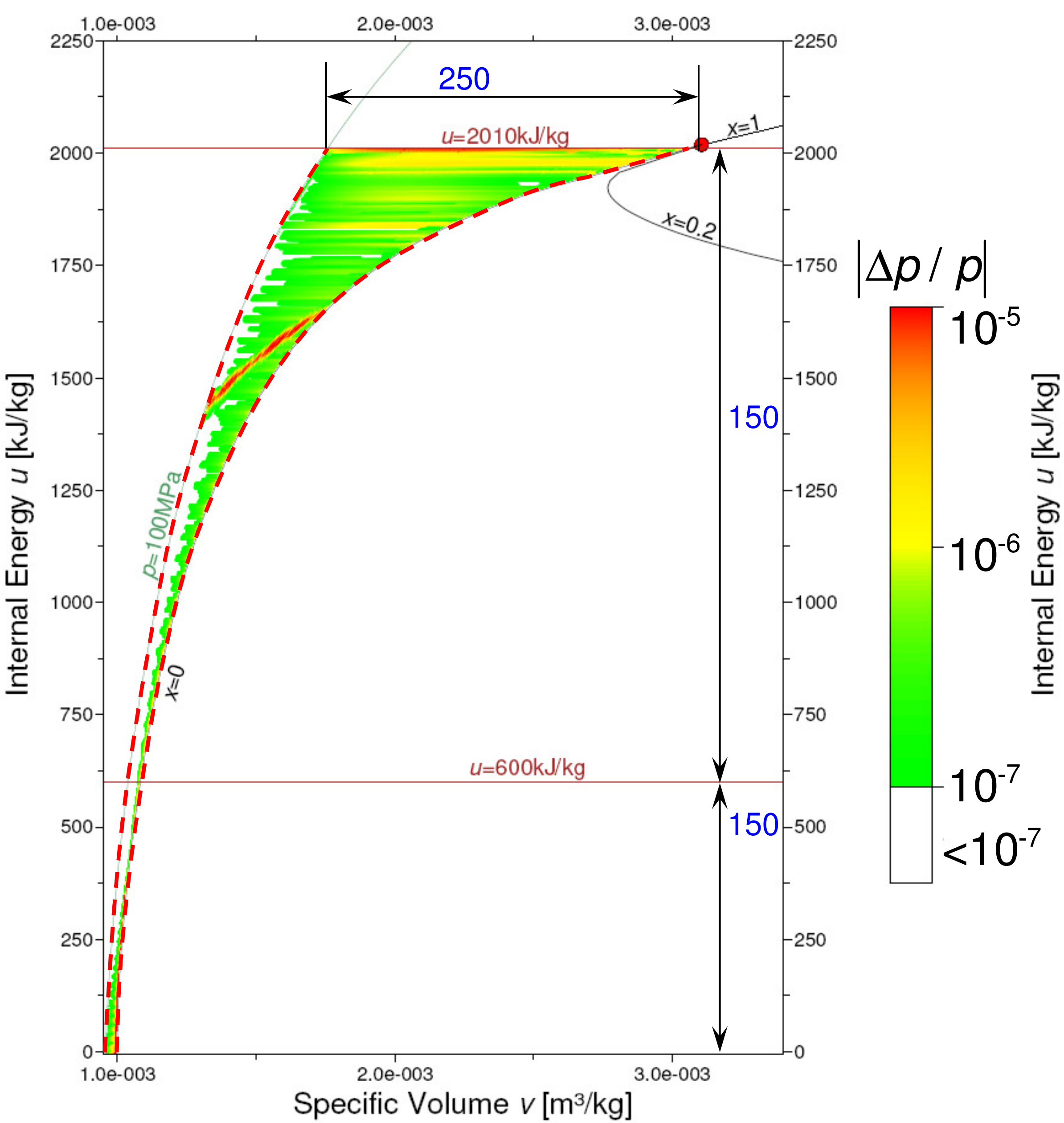
Spline functions of (*v*,*u*):

		(*p*,*v*)	(*u*,*s*)
Pressure	$p^{SPL}(v,u)$	→ $u^{INV}(p,v)$	
Temperature	$T^{SPL}(v,u)$	$T^{SPL}, s^{SPL}, w^{SPL}, \eta^{SPL}, \lambda^{SPL}(v, u^{INV})$	
Spec. entropy	$s^{SPL}(v,u)$		→ $v^{INV}(u,s)$
Speed of sound	$w^{SPL}(v,u)$		$p^{SPL}, T^{SPL}, w^{SPL}, \eta^{SPL}, \lambda^{SPL}(v^{INV},u)$
Dynamic viscosity	$\eta^{SPL}(v,u)$		
Therm. conductivity	$\lambda^{SPL}(v,u)$		

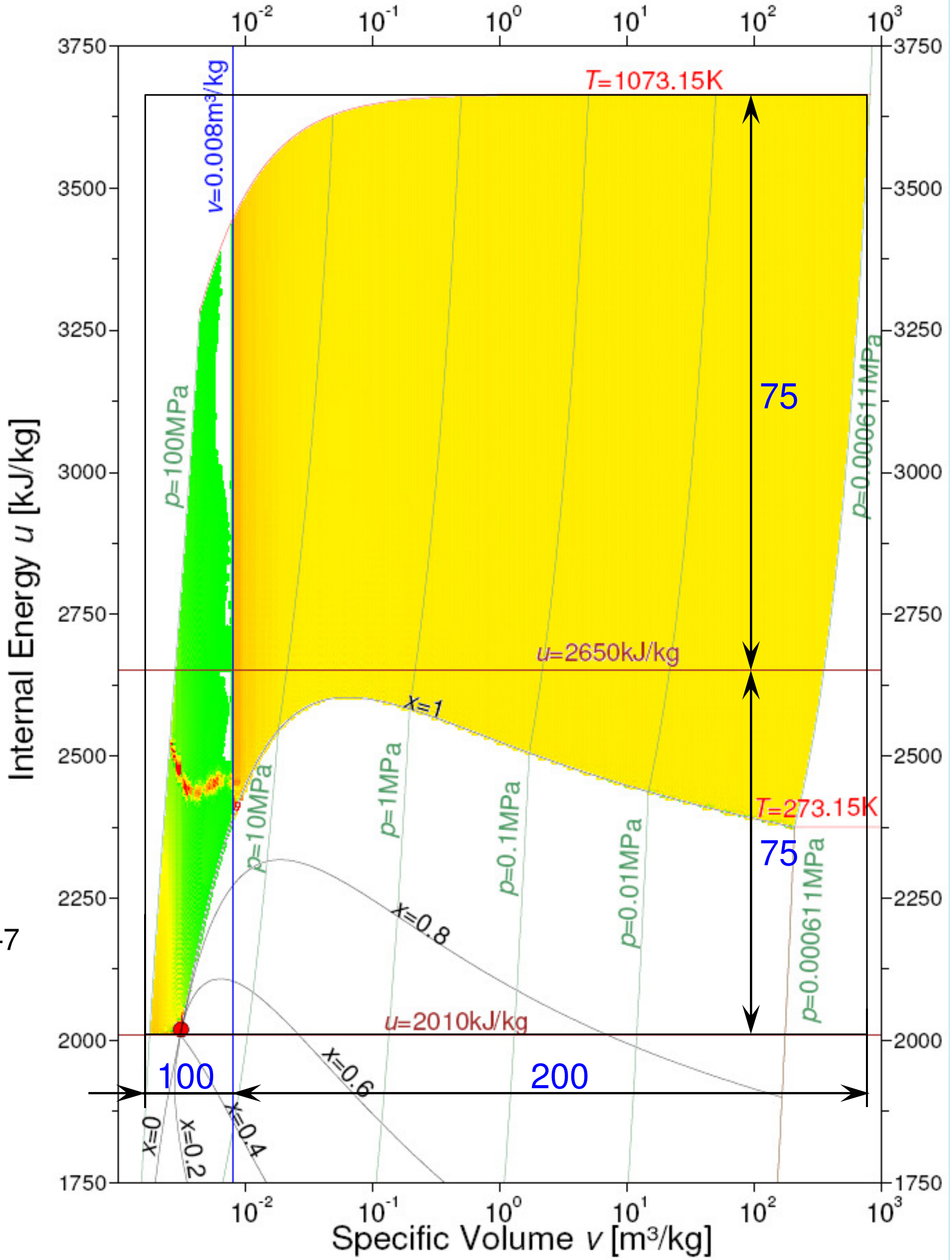
- **All thermodynamic and transport properties including derivatives and inverse functions are calculated without iterations.**
- **Property functions are numerically consistent with each other.**

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 $v'(u)$

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

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)
$p(v,u)$	$p \le 2.5$ MPa	$\lvert \Delta p / p \rvert < 0.12\ \%$	$\lvert \Delta p / p \rvert < 0.001\ \%$
	$p > 2.5$ MPa	$\lvert \Delta p \rvert < 0.6\ \mathrm{kPa}$	
$T(v,u)$		$\lvert \Delta T \rvert < 1\ \mathrm{mK}$	$\lvert \Delta T \rvert < 1\ \mathrm{mK}$
$s(v,u)$		$\lvert \Delta s \rvert < 10^{-6}\ \mathrm{kJ\ kg^{-1}\ K^{-1}}$	$\lvert \Delta s \rvert < 10^{-6}\ \mathrm{kJ\ kg^{-1}\ K^{-1}}$
$w(v,u)$		$\lvert \Delta w / w \rvert < 0.001\ \%$	$\lvert \Delta w / w \rvert < 0.001\ \%$
$\eta(v,u)$		$\lvert \Delta \eta / \eta \rvert < 0.001\ \%$	$\lvert \Delta \eta / \eta \rvert < 0.001\ \%$

- **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.**

SBTL Functions of (v,u) and Inverse Functions of (p,v) and (u,s) – Computing time comparisons with IAPWS-IF97

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

	IAPWS-IF97 Region				
SBTL function	**1 (liquid)**	**2 (vapour)**	**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

Processor: Intel Xeon – 3,2GHz

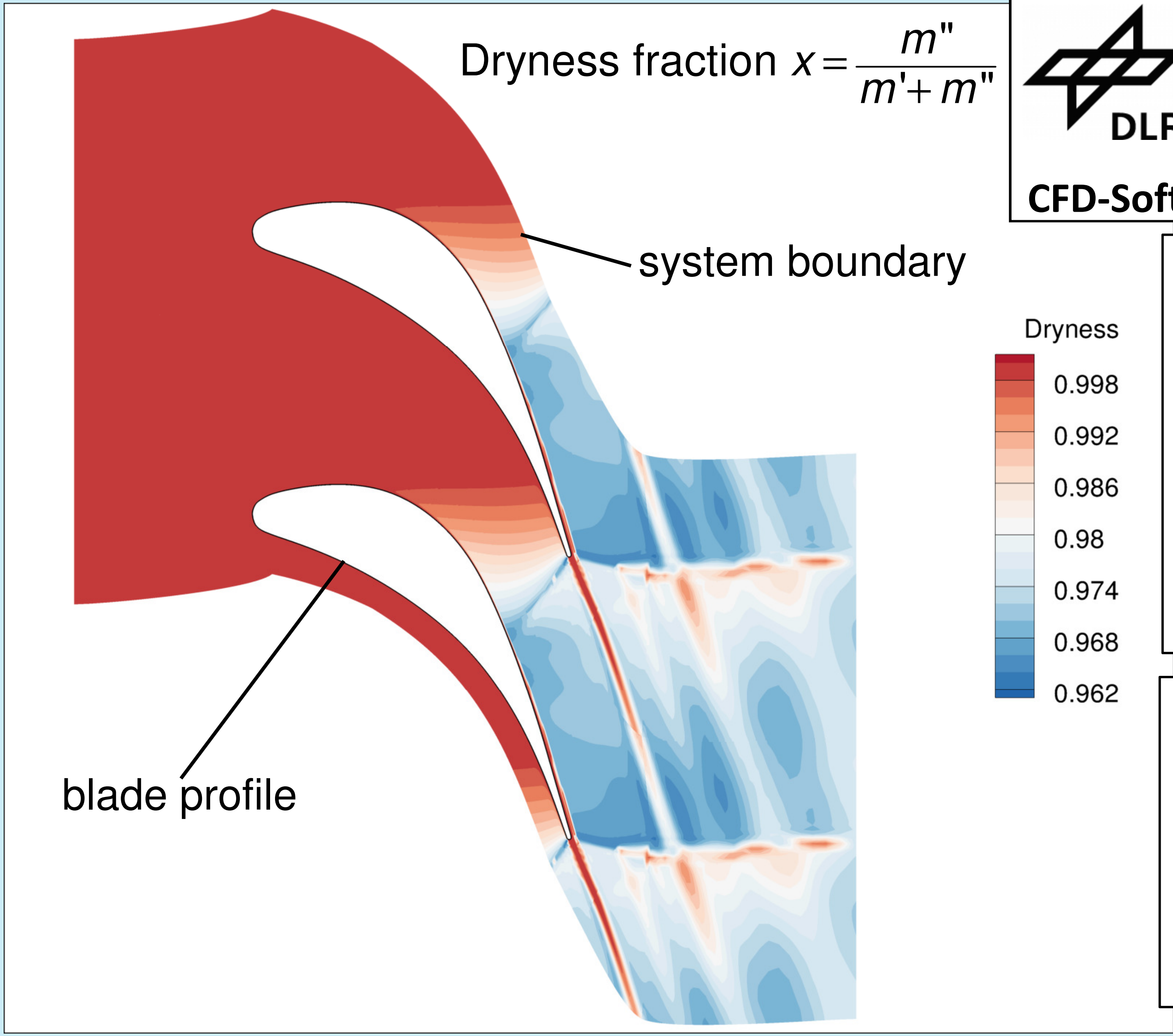
Operating system: Windows7 (32 Bit)

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.)

Dryness fraction:



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

CFD-Software TRACE (DLR)

Test-case L3:

Inlet conditions:

- Tot. press.: 41.7 kPa
- Tot. temp.: 357.5 K (ΔT_s=+7.5 K)

Outlet conditions:

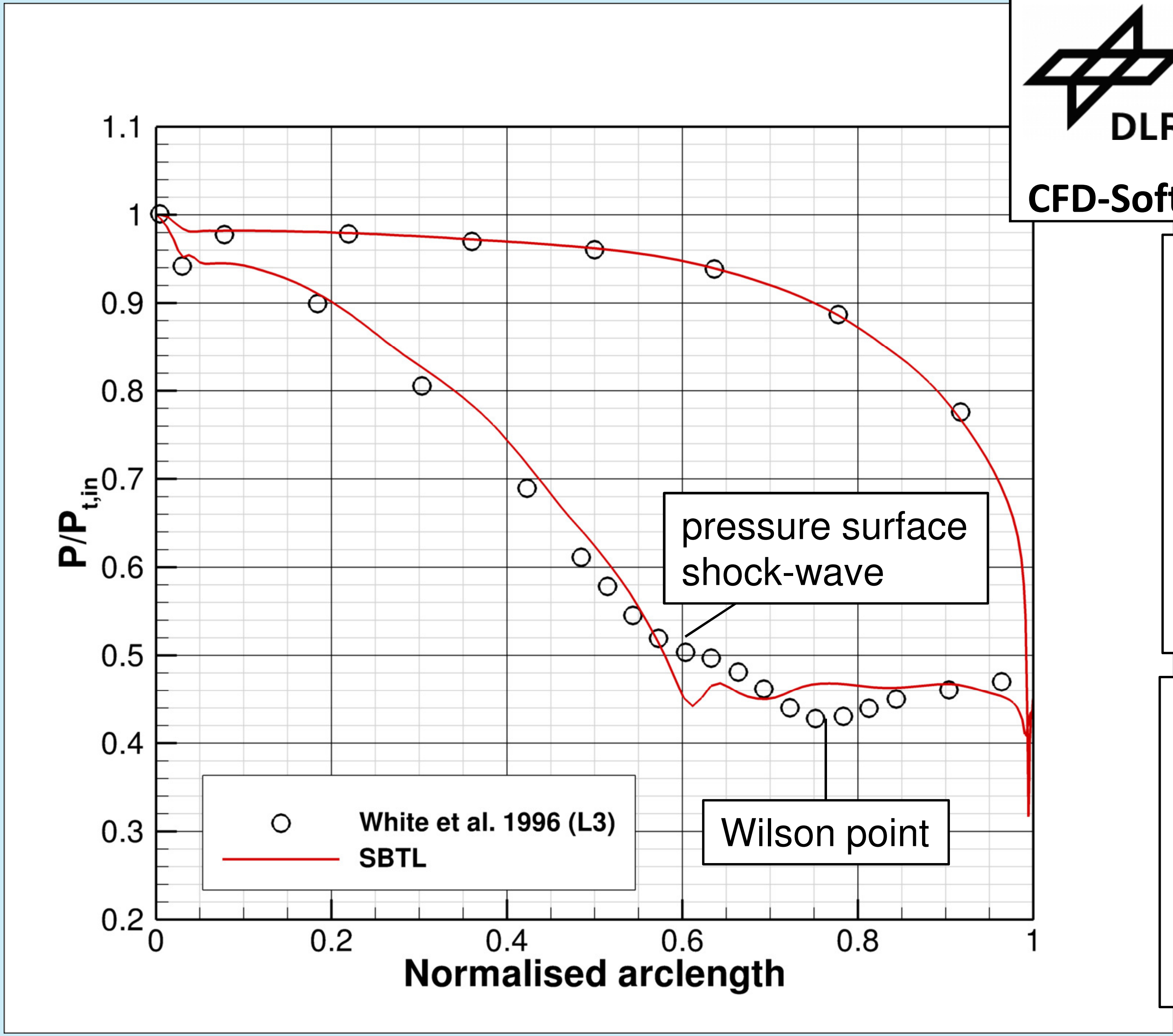
- Stat. pressure: 20.6 kPa

Assumptions:

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

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

Pressure coefficient along the blade profile:



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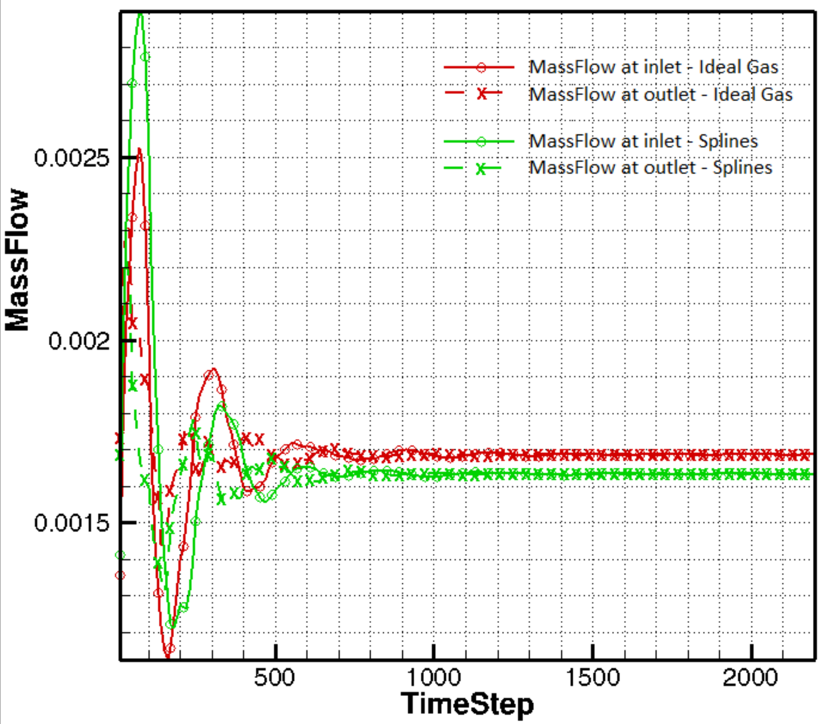
Application of the SBTL Method in CFD – Condensing Steam Flow Around a Fixed Blade (White et al.; L3)

Convergence:



CFL-Factor (Courant–Friedrichs–Lewy-Factor)=20

- **Calculation with SBTL functions:**
  - high speed of convergence because of complete numerical consistency
  - calculation accomplished after 1:50min/1000 steps

- **Comparison to calculation with ideal gas model:**
  - calculation accomplished after 1:20min/1000 steps

- **Calculation is approx. 6-10 times faster than the IAPWS-IF97 implementation in TRACE.**
- **Consideration of real fluid behavior with the SBTL Method requires only 40% additional computing time in comparison to a calculation with the ideal gas model.**
- **Practical calculations:**
  - **stage groups in 3D**
  - **non-stationary processes**

Computing time: several hours/days

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)

  ⇨ **Simplified property calculation algorithms have been replaced:**

    - Accuracy is enhanced
    - 7-equation non-equilibrium two-phase flow model is enabled

- **DYNAPLANT** – SIEMENS

  simulation of non-stationary processes in power plants

  - SBTL functions of (v,h) based on IAPWS-IF97

  ⇨ **Computing times have been considerably reduced with regard to the direct application of IAPWS-IF97. Differences in the numerical results are negligible.**

- **KRAWAL** – SIEMENS

  heat-cycle calculations for power-plant design

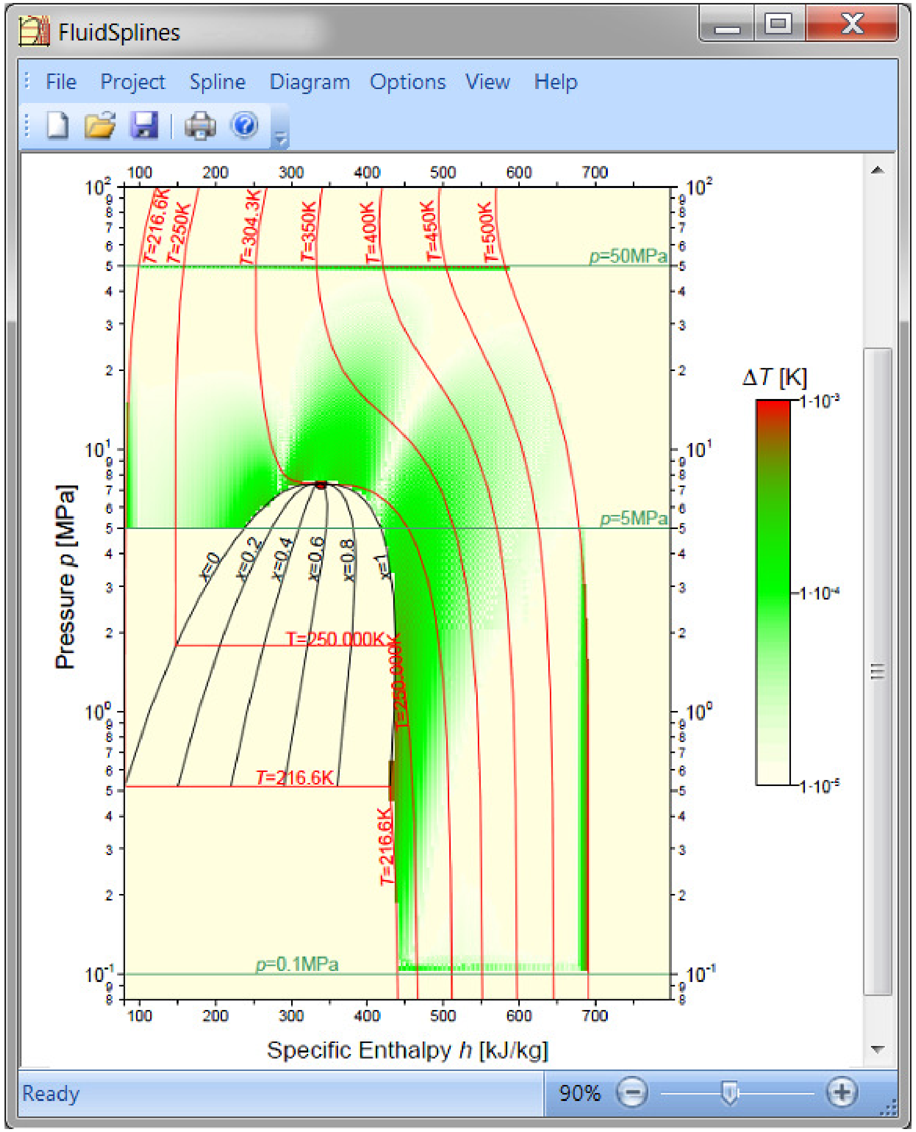
  - SBTL functions of (p,h) based on IAPWS-IF97

  ⇨ **Computing times have been reduced by factors >2 with regard to the direct application of IAPWS-IF97. Differences in the numerical results are negligible.**

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 fluid property formulations:**
  - Reproduces underlying formulations with high accuracy at high computing speed
  - Provides fast and numerically consistent inverse 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) are up to 300 times faster than IAPWS-IF97)
- **Applicability in CFD has been demonstrated:**
  - Enables consideration of the real fluid behavior with high accuracy
  - 6-10 times faster than simulations with IAPWS-IF97
  - Only 40% slower than simulations with the ideal-gas model
- **SBTL property functions can be generated for any fluid with FluidSplines**
- **SBTL method can be implemented into any CFD software to consider the real fluid behavior at high computing speeds**

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

Available at: www.iapws.org

Thank you for your attention!