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

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Motivation and Objectives

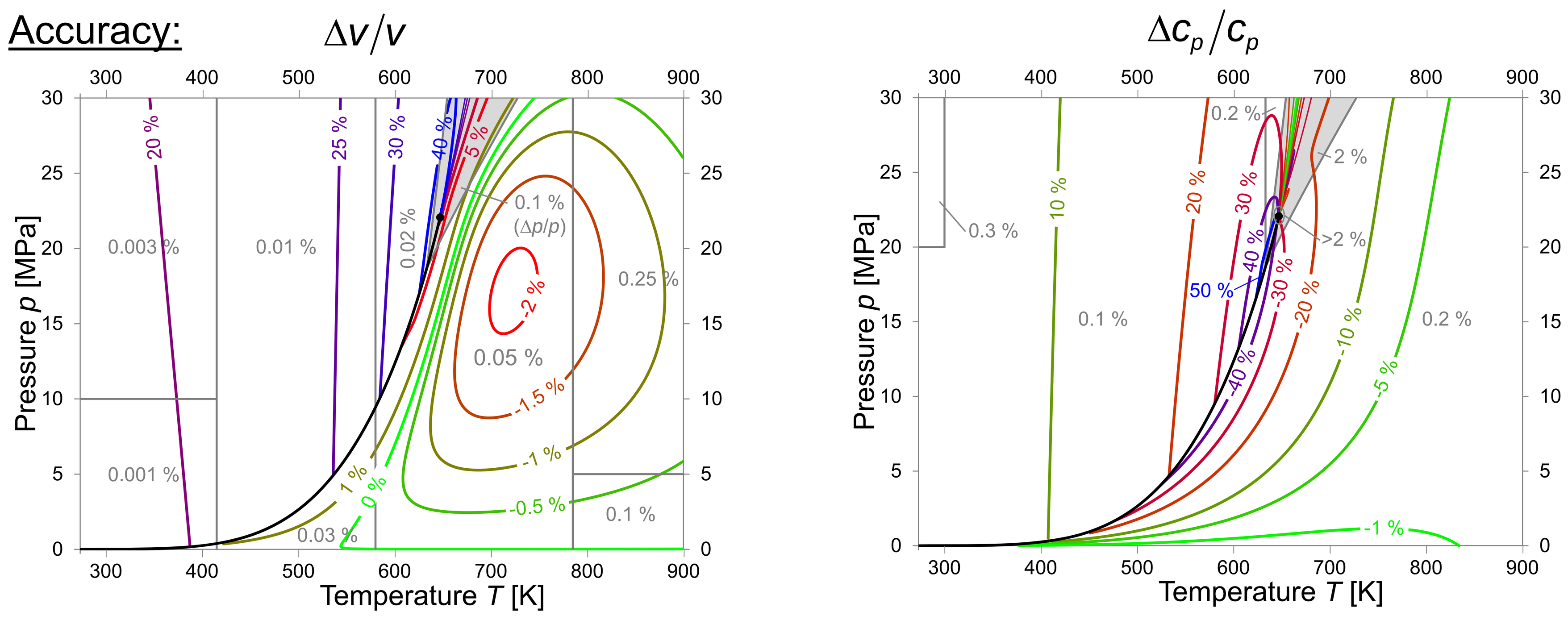
Problem Statement:

- Deviations in calculated fluid properties lead to inaccurate mass, energy, and entropy balances. → Property calculation algorithms need to be very accurate.
- Fluid properties are calculated extremely often, which consumes the majority of the computing time. → Property functions need to be extremely fast.
- Solvers require continuity and numerical consistency of the equations to be solved. → Property functions need to be continuous and consistent.

Real Fluid Properties in Process Simulations (example: water and steam):

- **Equations of State (EOS):**
  - Cubic EOS, e.g., Peng-Robinson EOS (PR-EOS)
  - Fundamental EOS, e.g., IAPWS-95 [1] or IAPWS-IF97 [2]

Accuracy:



Colored contours: deviations of PR-EOS from IAPWS-95
Gray figures: uncertainties of IAPWS-95 (those of IAPWS-IF97 are slightly higher)

Computing-Time Ratio (CTR):

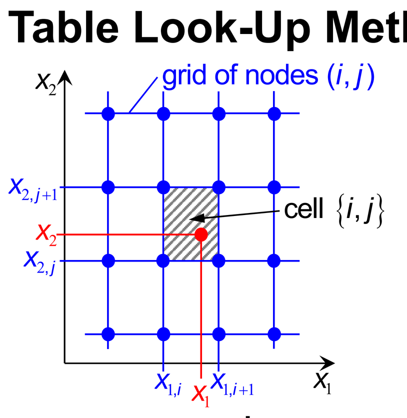
$$CTR = \frac{\text{Comp. Time of IAPWS-IF97 (-95)}}{\text{Comp. Time of PR-EOS}}$$

	IAPWS-IF97 Region	
Function	1 (liquid)	2 (vapor)
$p(v,u)$	4.8 (88)	9.0 (114)
$T(v,u)$	4.8 (91)	9.3 (115)
$T(p,h)$	0.41 a) (23)	0.60 a) (43)
$v(p,h)$	0.48 a) (23)	0.91 a) (43)

a) IAPWS-IF97 backward equation and one Newton step

Phase/region tests are not included in these CTR values and increase the computing times even further!

- **Table Look-Up Methods (interpolation from tabulated values):**



Calculation of any property $z(x_1,x_2)$:

- Discrete values $z_{ij}(x_{1,i},x_{2,j})$ are calculated at the nodes (i,j) from an equation of state and stored in a look-up table.
- During the process simulation, the cell $\{i,j\}$ in the grid of nodes is to be determined and $z(x_1,x_2)$ is interpolated.

Accuracy and computing speed depend on the structure of the grid of nodes and the applied interpolation algorithm.

Shortcomings of frequently applied methods:

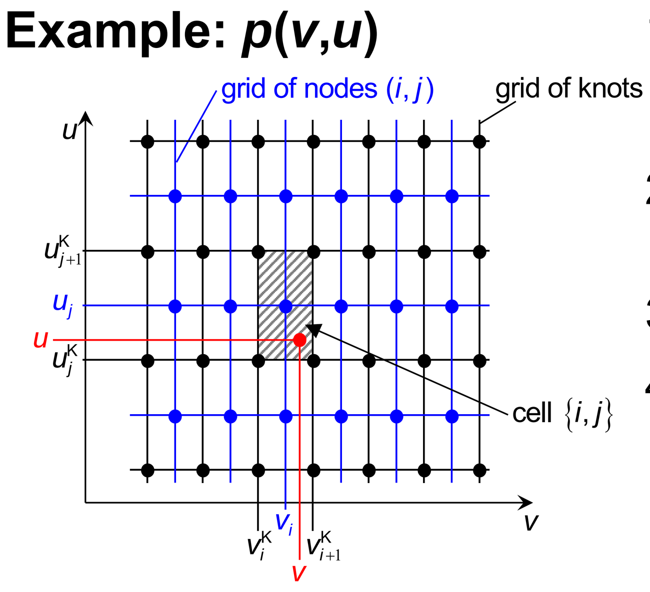
- Nodes are often clustered to consider the nonlinear behavior of the fluid property function, which leads to computationally intensive cell search algorithms.
- Most frequently applied property functions are often calculated from inverse functions, rather than from explicit forward functions.
- Bi-linear interpolation cannot provide continuous 1st derivatives.
- Bi-cubic interpolation leads to computationally intensive inverse functions.

Objectives of this Project:

Development of new table look-up algorithms that overcome the shortcomings outlined above and provide:
- fast and accurate property functions with cont. 1st derivatives
- fast and numerically consistent inverse functions

Spline-Based Table Look-up Method (SBTL)

Example: $p(v,u)$



1) Variable transformations (e.g., $v \to \bar{v}$) to:
   - enhance accuracy (linearization)
   - reshape the range of state
2) Definition of a rectangular, piecewise equidistant grid of nodes (fast cell search algorithm)
3) Definition of cells in the grid of knots
4) Calculation of all coefficients a_{ijkl} of the bi-quadratic spline-polynomial (continuous 1st derivatives):

$$p_{\{i,j\}}(\bar{v},u) = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ijkl}\left(\bar{v}-\bar{v}_i\right)^{k-1}\left(u-u_j\right)^{l-1}$$

Inverse Functions, e.g., $u(p,v)$:

$$u^{\mathrm{INV}}_{\{i,j\}}(p,\bar{v}) = \frac{-B \pm \sqrt{B^2-4AC}}{2A} + u_j$$

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

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

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

$$\Delta\bar{v}_i = \bar{v}_i\left(\bar{v}-\bar{v}_i\right) \qquad (\pm) = \mathrm{sign}(B)$$

SBTL functions of (v,u):

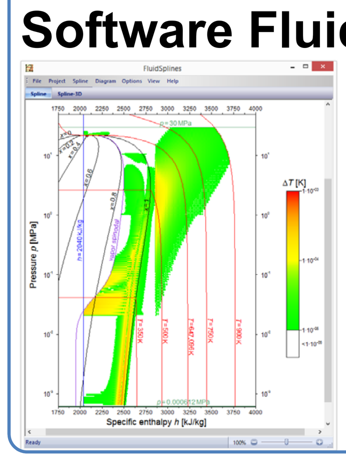
Pressure	$p^{SPL}(v,u)$
Temperature	$T^{SPL}(v,u)$
Spec. entropy	$s^{SPL}(v,u)$
Speed of sound	$w^{SPL}(v,u)$
Dynamic viscosity	$\eta^{SPL}(v,u)$

Calculation of inverse functions:

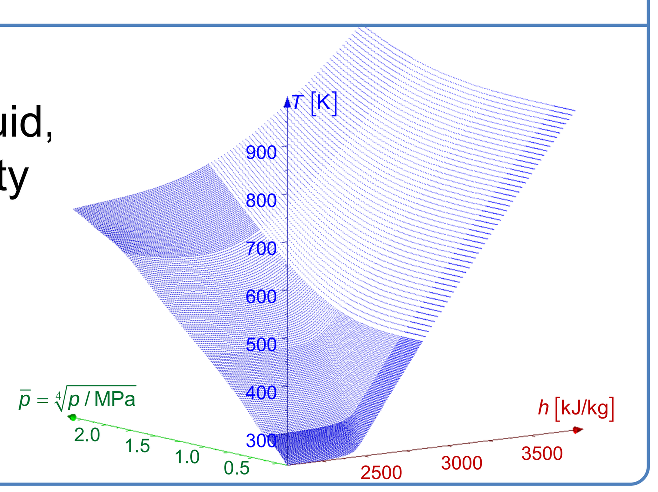
(p,v): $p^{SPL}(v,u) \to u^{INV}(p,v) \to T^{SPL}, s^{SPL}, w^{SPL}, \eta^{SPL}(v, u^{INV})$

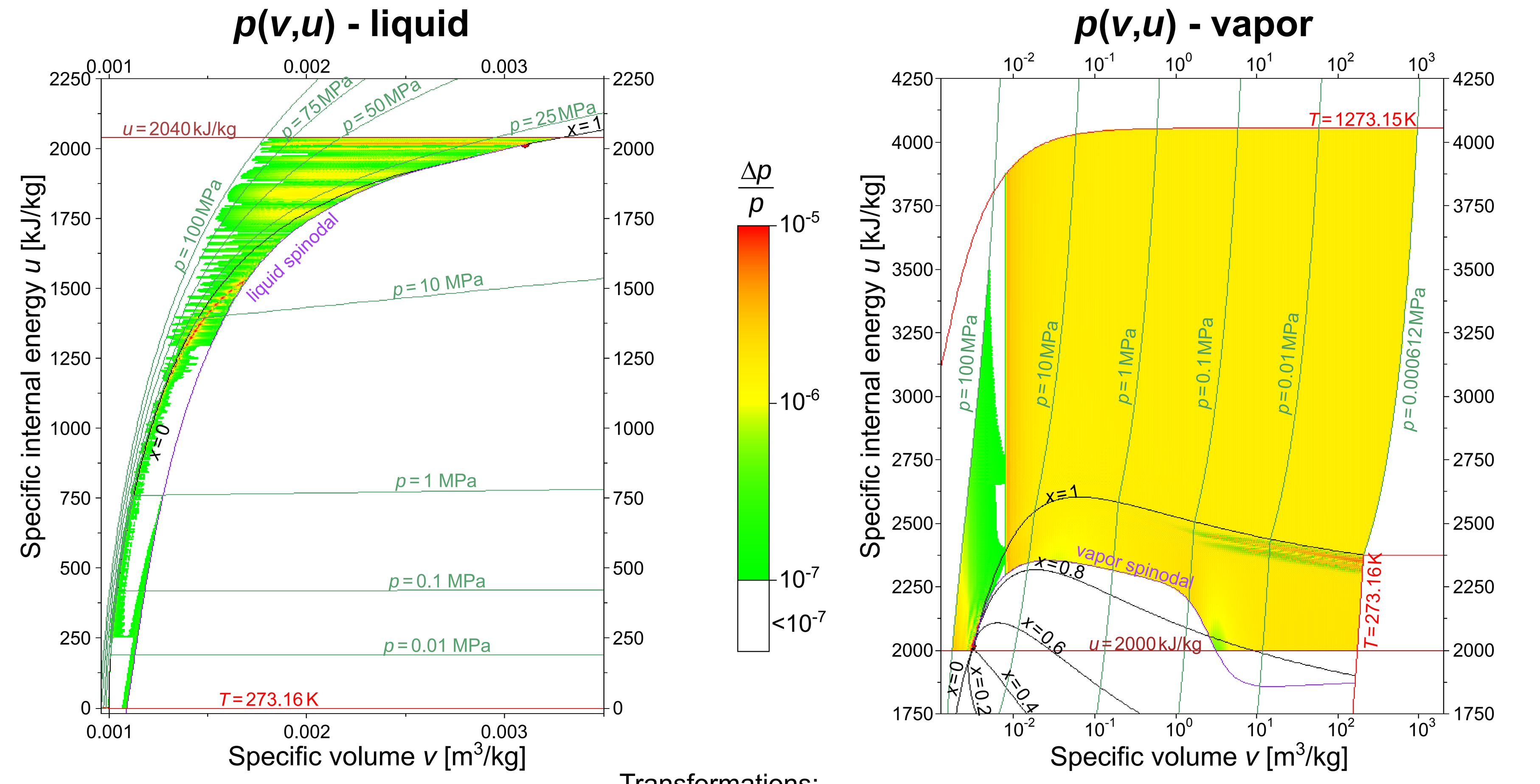
(u,s): $s^{SPL}(v,u) \to v^{INV}(u,s) \to p^{SPL}, T^{SPL}, w^{SPL}, \eta^{SPL}(v^{INV},u)$

Software FluidSplines:



- Generation of SBTL functions for any fluid, optimized for:
  - specified range of validity
  - desired accuracy
  - computational speed
- Underlying property functions are calculated from:
  - REFPROP
  - HSZG libraries





Transformations:

$$\bar{v}(v,u) = \frac{v - v(u)_{p\_max}}{v(u)_{\mathrm{Spinodal}} - v(u)_{p\_max}}\left(\bar{v}_{\max} - \bar{v}_{\min}\right) + \bar{v}_{\min}$$

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

Accuracy and Computing-Time Ratio (CTR):

		Max. deviation from IAPWS-IF97			
Function		liquid		vapor	
$p(v,u)$	≤2.5 MPa	$\lvert\Delta p/p\rvert$	<0.12 %	$\lvert\Delta p/p\rvert$	<0.001 %
	>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 %

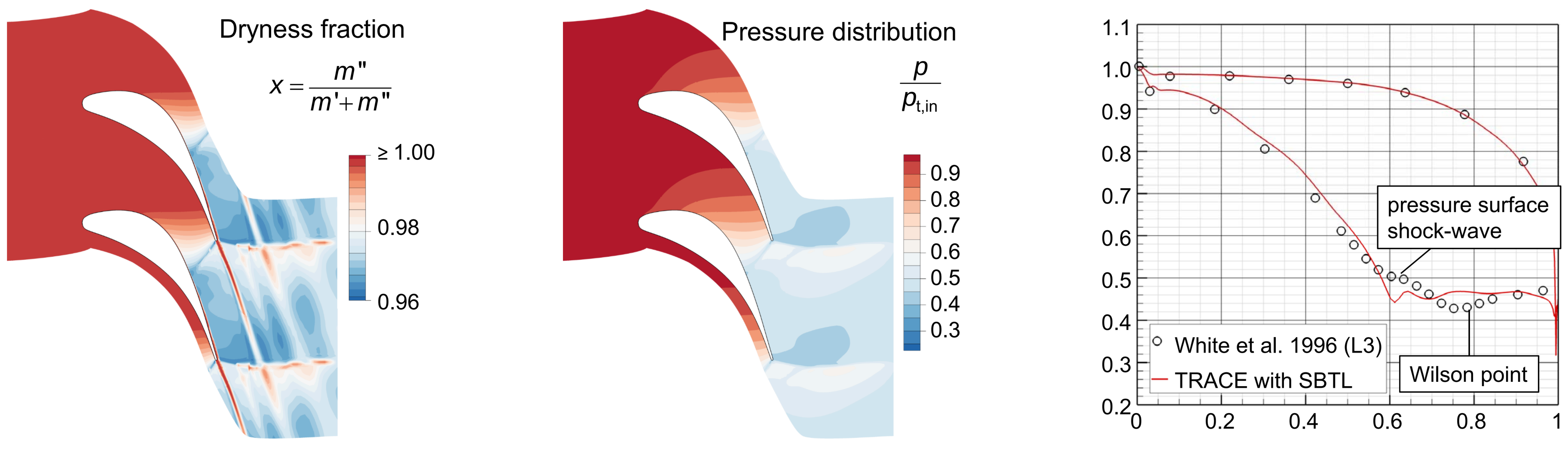
$$CTR = \frac{\text{Comp. Time of IAPWS-IF97}}{\text{Comp. Time of SBTL Function}}$$

	IAPWS-IF97 Region		
Func.	1 (liquid)	2 (vapor)	4 (two-phase)
$p(v,u)$	130	271	19.6
$T(v,u)$	161	250	20.6
$\eta(v,u)$	197	309	-
$u(p,v)$	2.0	6.4	5.6
$v(u,s)$	43.5	66.4	16.2

Application of the SBTL Method

- **TRACE (CFD-Software, developed at DLR):**

Simulation of condensing steam flow around a fixed blade [3]:



Inlet: • $p_{t,in}$ = 41.7 kPa • $T_{t,in}$ = 357.5 K (ΔT_s = +7.5 K)

Outlet: • p_{out} = 20.6 kPa

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

→ The numerical results show negligible differences from those obtained with the direct application of IAPWS-IF97.

→ Computing times for flow simulations considering the real fluid behavior are reduced by a factor of 10 with regard to simulations based on IAPWS-IF97.

→ With regard to the application of the ideal-gas model, the computing times are increased by a factor of 1.4 only.

- **KRAWAL (software for power plant design, developed at SIEMENS PG):**

→ The overall computing time is reduced by 50% with regard to calculations based on IAPWS-IF97, whereas the differences in the numerical results are negligible.

- **RELAP-7 (Nuclear-Reactor System Safety Analysis Code, developed at INL):**

→ Simplified property calculation algorithms have been replaced with fast and accurate SBTL functions; applied in a 7-equation non-equilibrium two-phase model [4].

→ New SBTL property libraries are being developed for various pure fluids and mixtures.

Conclusions and Outlook

The newly developed SBTL method [5,6,7]:
- enables the consideration of the real fluid behavior in computationally intensive process simulations with high accuracy and low computing times.
- can be applied to any fluid (SBTL functions can be generated with FluidSplines).
- is being applied successfully in a variety of software tools for process simulations.
- is being extended for mixtures, e.g., humid air and humid combustion gases.

References/Publications

[1] IAPWS, *Revised Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use* (2014), available at http://www.iapws.org.

[2] IAPWS, *Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam* (2007), available at http://www.iapws.org.

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[4] Kunick, M., Berry, R. A., Martineau, R. C., Kretzschmar, H.-J., Gampe, U., Application of the new IAPWS Guideline on the fast and accurate calculation of steam and water properties with the Spline-Based Table Look-Up Method (SBTL) in RELAP-7, *KERNTECHNIK*, **82** (3) , 264-279 (2017).

[5] IAPWS, *Guideline on the Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL)*, available at http://www.iapws.org.

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[7] Kunick, M., Fast Calculation of Thermophysical Properties in Extensive Process Simulations with the Spline-Based Table Look-Up Method (SBTL), *Fortschritt-Berichte VDI , Reihe 6*, ISBN: 978-3-18-361806-4 (2018).