ZITTAU/GÖRLITZ UNIV. OF APPL. SCIENCES,
FACULTY OF MECHANICAL ENGINEERING,
DEPT. OF TECHNICAL THERMODYNAMICS

DRESDEN UNIVERSITY OF TECHNOLOGY,
FAC. OF MECHANICAL SCIENCE AND ENGINEERING,
CHAIR OF THERMAL POWER MACHINERY AND PLANTS

DLR

GERMAN AEROSPACE CENTER,
INSTITUTE OF PROPULSION TECHNOLOGY,
NUMERICAL METHODS

A New IAPWS Guideline on the Fast Calculation of Real Fluid Properties with the Spline-Based Table Look-Up Method (SBTL) for CFD Applications

Matthias Kunick, Hans-Joachim Kretzschmar, Francesca di Mare, and Uwe Gampe

Motivation & Objectives

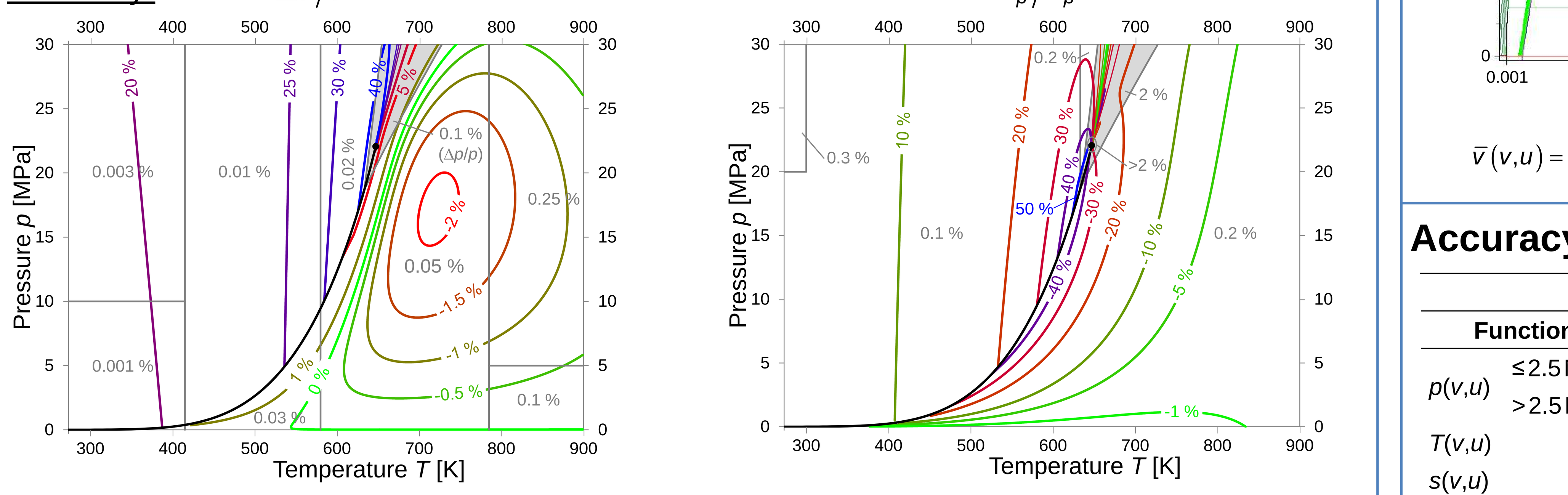
Problem Statement:

- 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.
- CFD solvers require continuity and numerical consistency of the equations to be solved. → Property functions need to be continuous and consistent.

Real Fluid Properties in CFD (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: $\Delta v/v$ $\Delta c_p/c_p$



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*):

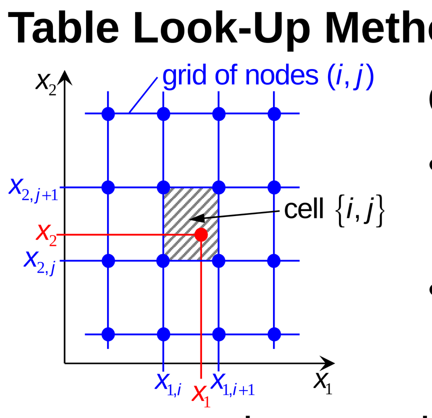
$$CTR = \frac{\text{Comp. Time of IAPWS-IF97 (-95)}}{\text{Comp. Time of PR-EOS}}$$

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

	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

- **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 CFD 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 currently 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.

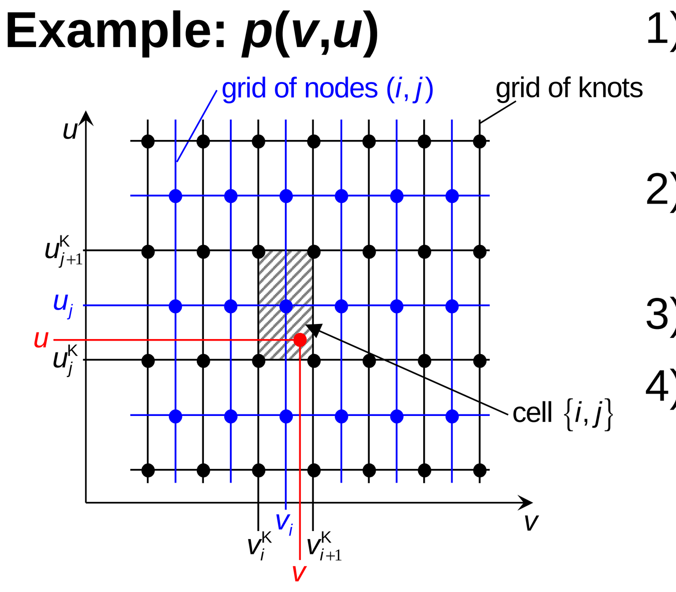
Objectives of this Project:

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., $v \rightarrow \bar{v}$) 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., $u(p,v)$:

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

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

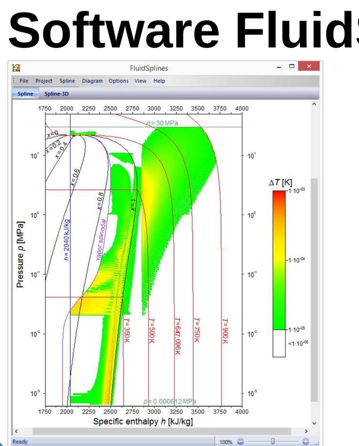
$$B = a_{ij12} + \Delta\bar{v}_i\left(a_{ij22} + a_{ij32}\Delta\bar{v}_i\right)$$

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

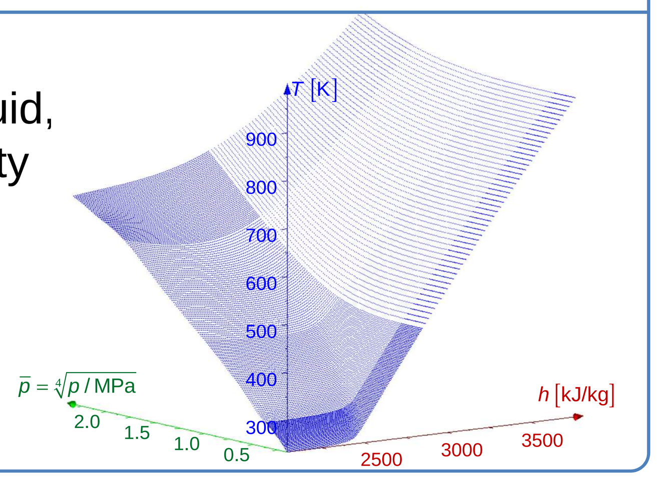
$$\Delta\bar{v}_i = \bar{v}_i(\bar{v}-\bar{v}_i) \qquad (\pm) = \text{sign}(B)$$

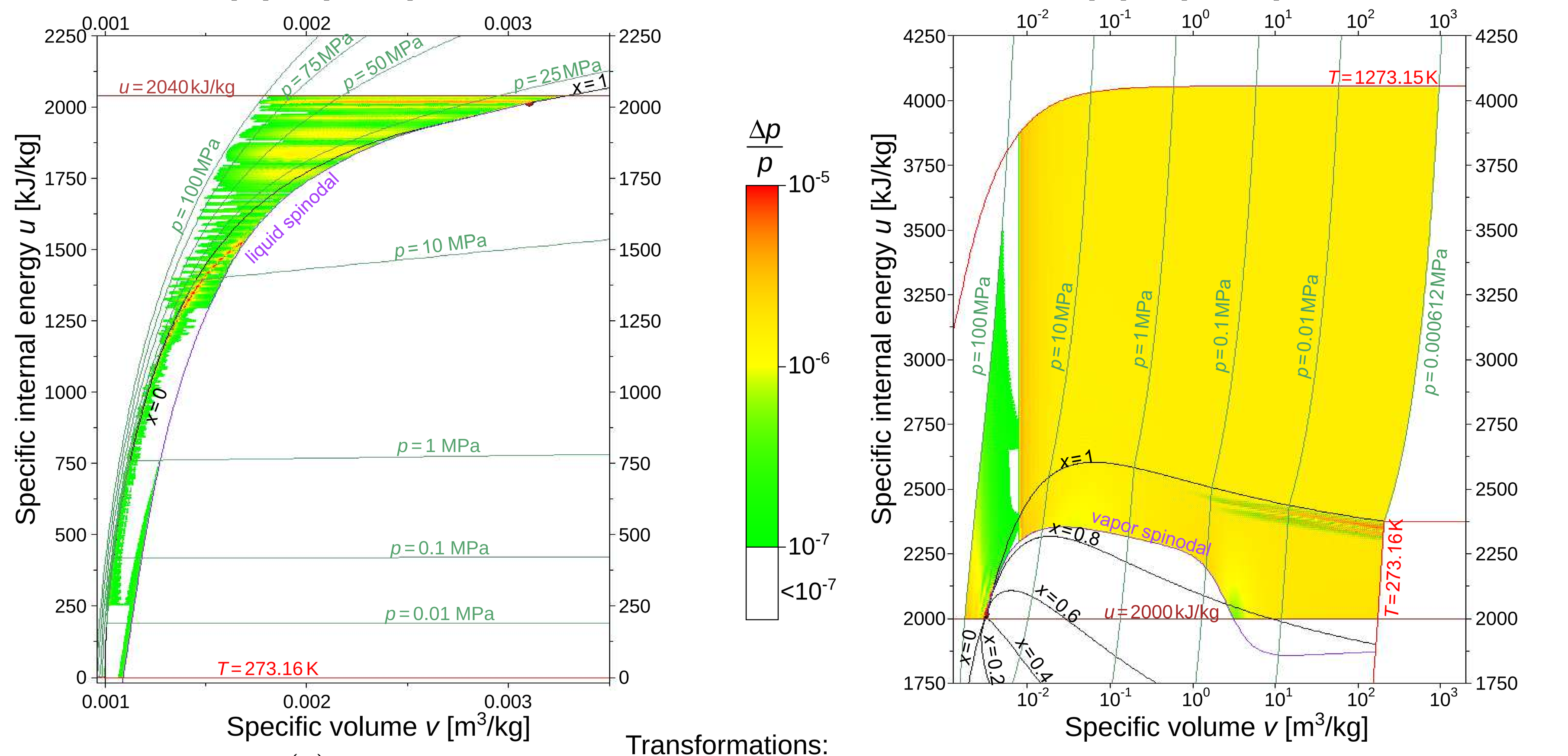
SBTL functions of (v,u):		Calculation of inverse functions: (p,v):	(u,s):
Pressure	$p^{\text{SPL}}(v,u)$	$u^{\text{INV}}(p,v)$	
Temperature	$T^{\text{SPL}}(v,u)$	$T^{\text{SPL}}, s^{\text{SPL}}, w^{\text{SPL}}, \eta^{\text{SPL}}(v, u^{\text{INV}})$	
Spec. entropy	$s^{\text{SPL}}(v,u)$		$v^{\text{INV}}(u,s)$
Speed of sound	$w^{\text{SPL}}(v,u)$		$p^{\text{SPL}}, T^{\text{SPL}}, w^{\text{SPL}}, \eta^{\text{SPL}}(v^{\text{INV}},u)$
Dynamic viscosity	$\eta^{\text{SPL}}(v,u)$		

Software FluidSplines:



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





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

Accuracy and Computing-Time Ratio (*CTR*):

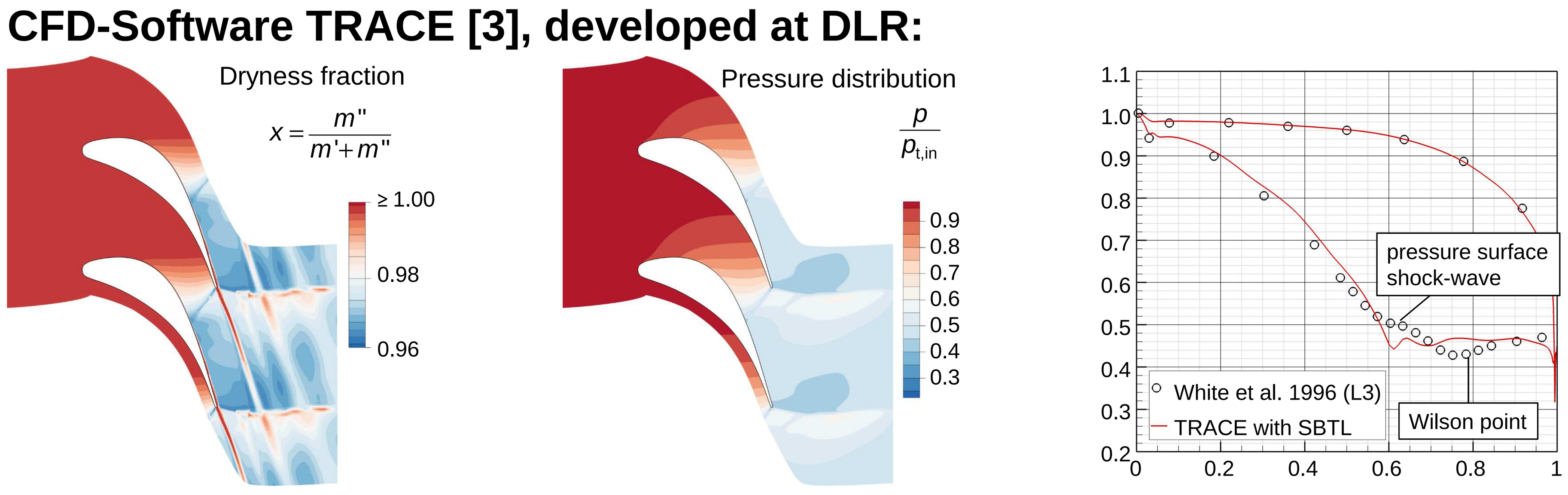
Function		Max. deviation from IAPWS-IF97: liquid		vapor	
$p(v,u)$	≤2.5 MPa	$\lvert\Delta p/p\rvert$	<0.12 %	$\lvert\Delta p/p\rvert$	<0.001 %
	>2.5 MPa	$\lvert\Delta p\rvert$	<0.6 kPa		
$T(v,u)$		$\lvert\Delta T\rvert$	<1 mK	$\lvert\Delta T\rvert$	<1 mK
$s(v,u)$		$\lvert\Delta s\rvert$	$<10^{-6}$ kJ 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 %

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

Func.	IAPWS-IF97 Region: 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

Simulation of Condensing Steam Flow Around a Fixed Blade with the CFD-Software TRACE [3], developed at DLR:



Inlet: • $p_{\text{t,in}}$ = 41.7 kPa • $T_{\text{t,in}}$ = 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

Key Results:

- 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.

Further Applications (Selection):

- **RELAP-7 (nuclear-reactor system safety analysis code, developed at the Idaho National Laboratory (INL)):**
  → simplified property calculation algorithms have been replaced with fast and accurate SBTL functions; applied in a 7-eq. non-equilibrium two-phase model
- **KRAWAL (heat-cycle calculation 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

Conclusions and Outlook

The newly developed SBTL method [4,5,6]:

- enables the consideration of the real fluid behavior in CFD and other 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 numerical process simulations.
- is being extended for mixtures, e.g., humid air and humid combustion gases.

A nucleation model is being implemented in TRACE to consider sub-cooling.

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.

[3] Kunick, M., Kretzschmar, H.-J., di Mare, F., and Gampe, U., CFD Analysis of Steam Turbines with the IAPWS Standard on the Spline-Based Table Look-Up Method (SBTL) for the Fast Calculation of Real Fluid Properties, *ASME Turbo Expo 2015: Turbine Technical Conference and Exposition, Vol.* **8**: *Microturbines, Turbochargers and Small Turbomachines; Steam Turbines*, ISBN: 978-0-7918-5679-6 (2015).

[4] 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

[5] Kunick, M., Kretzschmar, H.-J., Gampe, U., di Mare, F., Hrubý, J., Duška, M., Vinš, V., Singh, A., Miyagawa, K., Weber, I., Pawellek, R., Novi, A., Blangetti, F., Friend, D.G., and Harvey, A.H., Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL), *J. Eng. Gas Turbines & Power*, in preparation.

[6] Kunick, M., Fast Calculation of Thermophysical Properties in Extensive Process Simulations with the Spline-Based Table Look-Up Method (STBL), *VDI Fortschritt-Berichte*, in preparation.