M. Kunick, H.-J. Kretzschmar, F. di Mare, U. Gampe

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

Project of the IAPWS Task Group “CFD Steam Property Formulation”

Task Group “CFD Steam Property Formulation”:
Hans-Joachim Kretzschmar, Matthias Kunick, Zittau/Goerlitz University of Applied Sciences
Jan Hrubý, Michal Duška, Václav Vinš, Czech Academy of Sciences, Prague
Francesca di Mare, German Aerospace Center (DLR), Cologne
Anurag Singh, General Electric, Schenectady

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

Evaluation Committee:
Adam Novy, Doosan Skoda Francisco Blangetti, Alstom Power Reiner Pawellek, STEAG
Julien Bonifay, Siemens Energy Ingo Weber, Siemens Energy

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- 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 \((v,u)\)
- Application of the SBTL Method in CFD (TRACE, developed at DLR)
- FluidSplines – Generation of SBTL Functions for Specific Demands
- Summary
Fluid Property Calculations in CFD Analyses of Steam Turbines

**Need for accurate fluid properties in CFD:**
- Density deviations $\Delta \rho$ result in:
  - inaccurate mass flows and velocities (speeds and directions)
- Deviations in caloric properties, e.g. the isobaric heat capacity $c_p$, result in:
  - inaccurate energy and entropy balances

**Available property calculation algorithms for water and steam:**
- Ideal gas model
- Cubic equations of state (Peng-Robinson, Redlich-Kwong, ...)
- Industrial standard IAPWS-IF97 (fundamental equations)
- Table look-up methods (such as the bi-linear interpolation in ANSYS CFX)

**Requirements for property calculations in CFD:**
- Accuracy
- Computing speed
Deviations in density from real fluid (water and steam): ideal gas

\[
\left( \frac{\rho_{\text{ideal}} - \rho_{\text{real}}}{\rho_{\text{real}}} \right) = p R T
\]

Typical live steam parameters:

\( T = 800 \, \text{K} \)
\( p = 25 \, \text{MPa} \)
Deviation in density from real fluid (water and steam):

cubic equation of state (Peng-Robinson)

\[
\left( \frac{\rho^{\text{PR}} - \rho^{\text{real}}}{\rho^{\text{real}}} \right)
\]

\[
p = \frac{RT}{v - b} - \frac{a(T)}{v^2 + 2bv - b^2}
\]
Uncertainties in density of water and steam: IAPWS-IF97

\[
\left( \rho_{\text{IF97}}^{\text{real}} - \rho^{\text{real}} \right) / \rho^{\text{real}}
\]

Region 2:

\[
\frac{g_2(p, T)}{RT} = \gamma^0(\pi, \tau) + \gamma'(\pi, \tau)
\]

\[
\tau = \frac{\tau^*}{T}, \quad \pi = \frac{p}{p^*}
\]

\[
\gamma^0(\pi, \tau) = \ln \pi + \sum_{i=1}^{9} n_i^0 \tau_i^0
\]

\[
\gamma'(\pi, \tau) = \ln \pi + \sum_{i=1}^{43} n_i \pi_i^j (\tau - 0.5)^j
\]

\[
v(\pi, \tau) \frac{p}{RT} = \pi \left( \gamma^0 + \gamma' \right)
\]
Deviations in isobaric heat capacity from real fluid (water and steam): ideal gas

$\left( \frac{c_p^{\text{ideal}} - c_p^{\text{real}}}{c_p^{\text{real}}} \right)$
Deviations in isobaric heat capacity from real fluid (water and steam):
cubic equation of state + $c_p^{\text{ideal}}(T)$

$$\left( c_p^{\text{PR}} - c_p^{\text{real}} \right) / c_p^{\text{real}}$$

$p^{\text{PR}}(T, v)$ and $c_p^{\text{ideal}}(T)$
Uncertainties in isobaric heat capacity of water and steam: IAPWS-IF97

\[ \left( C_p^{\text{IF97}} - C_p^{\text{real}} \right) / C_p^{\text{real}} \]

Region 2:

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

\[ \gamma^0(\pi,\tau) = \ln \pi + \sum_{i=1}^{9} n_i^0 \tau_i^0 \]

\[ \gamma^r(\pi,\tau) = \ln \pi + \sum_{i=1}^{43} n_i \pi_i (\tau - 0.5)^i \]

\[ C_p(p,T) = -\tau^2 \left( \gamma^0_{\tau \tau} + \gamma^r_{\tau \tau} \right) \]
### Fluid Property Calculations in CFD Analyses of Steam Turbines

<table>
<thead>
<tr>
<th>Requirements</th>
<th>Ideal gas</th>
<th>Cubic equation of state</th>
<th>Ind. standard IAPWS-IF97</th>
<th>Table look-up methods</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Accuracy</strong></td>
<td>(</td>
<td>\Delta \rho</td>
<td>\leq 20 %)</td>
<td>(</td>
</tr>
<tr>
<td>(</td>
<td>\Delta c_p</td>
<td>\leq 50 %)</td>
<td>(</td>
<td>\Delta c_p</td>
</tr>
<tr>
<td><strong>Computing speed</strong></td>
<td>very high</td>
<td>acceptable</td>
<td>too slow</td>
<td>high</td>
</tr>
</tbody>
</table>

**Application of a Spline-Based Table Look-Up Method to available equations of state (standards):**

- Results of the underlying formulation can be reproduced with high accuracy and high computing speed.
- Spline functions represent property functions continuously.
- Forward and backward functions, e.g. \(p(v,u)\) and \(u(p,v)\), can be calculated with complete numerical consistency.
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:
    $$ p_{i,j}(v_i,u_j) = p_{EOS}(v,u) $$

- **Variable transformations of $v$, $u$, and $p$:**
  - enhance accuracy
  - transform the range of state

- **Cell definition in the grid of knots:**
  - spline-polynomial:
    $$ p_{ij}^{SPL}(v,u) = \sum_{k=1}^{3} \sum_{l=1}^{3} a_{ijkl} (v-v_i)^{k-1} (u-u_j)^{l-1} $$
  - 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 within CFD:**
- transform $v$ and $u$
- cell $(i,j)$ determination
- computation of the spline polynomial
- inverse transformation of $p$
Fundamentals of the Spline-Based Table Look-Up Method (SBTL)

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

\[
p_{ij}^{SPL}(v,u) = \sum_{k=1}^{3} \sum_{l=1}^{3} a_{ijkl} (v - v_i)^{k-1} (u - u_j)^{l-1}
\]

\[
u_{ij}^{INV}(p,v) = \left( -B \pm \sqrt{B^2 - 4AC} \right) \frac{2A}{2A} + u_j
\]

where

\[A = a_{j13} + \Delta v_i \left( a_{j23} + a_{j33} \Delta v_i \right)\]

\[B = a_{j12} + \Delta v_i \left( a_{j22} + a_{j32} \Delta v_i \right)\]

\[C = a_{j11} + \Delta v_i \left( a_{j21} + a_{j31} \Delta v_i \right) - p\]

and

\[\Delta v_i = (v - v_i)\]

\[(\pm) = \text{sign}(B)\]

- The inverse spline function is numerically consistent with its forward function.
- The inverse function can be calculated without any iteration.
Spline Functions of \((v,u)\) and Inverse Spline Functions Based on IAPWS-IF97

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

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

Calculation of inverse spline functions:

- \((p,v)\):
  - \(u^{\text{INV}}(p,v)\)
- \((u,s)\):
  - \(v^{\text{INV}}(u,s)\)

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

- All thermodynamic and transport properties including derivatives and backward functions are calculated without iterations.
- Forward and backward functions are calculated with complete numerical consistency.
Spline function \( p_L(v,u) \):

\[
|\Delta p / p| < 10^{-7}
\]

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

Transformations:

\( \bar{v} = \ln(v) \)
Inverse spline functions are numerically consistent with their forward spline functions.

Accuracy and Computational Speed of SBTL Functions for Water and Steam – Deviations from IAPWS-IF97
## Accuracy and Computational Speed of SBTL Functions for Water and Steam – Deviations from IAPWS-IF97

<table>
<thead>
<tr>
<th>SBTL function</th>
<th>Max. deviation (L)</th>
<th>Max. deviation (G)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p(v,u)$</td>
<td>$\frac{\Delta p_L}{p} &lt; 0.12%$</td>
<td>$\frac{\Delta p_G}{p} &lt; 0.001%$</td>
</tr>
<tr>
<td></td>
<td>$\Delta p_L &lt; 0.6\text{ kPa}$</td>
<td></td>
</tr>
<tr>
<td>$T(v,u)$</td>
<td>$\Delta T_L &lt; 1\text{ mK}$</td>
<td>$\Delta T_G &lt; 1\text{ mK}$</td>
</tr>
<tr>
<td>$s(v,u)$</td>
<td>$\Delta s_L &lt; 10^{-6}\text{ kJ kg}^{-1}\text{ K}^{-1}$</td>
<td>$\Delta s_G &lt; 10^{-6}\text{ kJ kg}^{-1}\text{ K}^{-1}$</td>
</tr>
<tr>
<td>$w(v,u)$</td>
<td>$\frac{\Delta w_L}{w} &lt; 0.001%$</td>
<td>$\frac{\Delta w_G}{w} &lt; 0.001%$</td>
</tr>
<tr>
<td>$\eta(v,u)$</td>
<td>$\frac{\Delta \eta_L}{\eta} &lt; 0.001%$</td>
<td>$\frac{\Delta \eta_G}{\eta} &lt; 0.001%$</td>
</tr>
</tbody>
</table>

- Spline-based property functions reproduce the industrial standard IAPWS-IF97 with high accuracy (10 – 100 ppm).
Accuracy and Computational Speed of SBTL Functions for Water and Steam – Computing time comparisons with IAPWS-IF97

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

<table>
<thead>
<tr>
<th>SBTL function</th>
<th>1 (liquid)</th>
<th>2 (vapour)</th>
<th>3 (critical)</th>
<th>4 (two-phase)</th>
<th>5 (high-temp.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p(v,u) )</td>
<td>130</td>
<td>271</td>
<td>161</td>
<td>19.6</td>
<td>470</td>
</tr>
<tr>
<td>( T(v,u) )</td>
<td>161</td>
<td>250</td>
<td>158</td>
<td>20.6</td>
<td>442</td>
</tr>
<tr>
<td>( s(v,u) )</td>
<td>164</td>
<td>261</td>
<td>160</td>
<td>17.8</td>
<td>449</td>
</tr>
<tr>
<td>( w(v,u) )</td>
<td>199</td>
<td>310</td>
<td>234</td>
<td>-</td>
<td>471</td>
</tr>
<tr>
<td>( \eta(v,u) )</td>
<td>197</td>
<td>309</td>
<td>239</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>( u(p,v) )</td>
<td>2.0</td>
<td>6.4</td>
<td>2.8</td>
<td>5.6</td>
<td>3.2</td>
</tr>
<tr>
<td>( v(u,s) )</td>
<td>43.5</td>
<td>66.4</td>
<td>78.8</td>
<td>16.2</td>
<td>134</td>
</tr>
</tbody>
</table>

Processor: Intel Xeon – 3,2GHz
Operating system: Windows7 (32 Bit) ➤ Computing times are reduced by factors up to 300 (500)!
Compiler: Intel Composer XE 2011
Dryness fraction: \[ x = \frac{m''}{m' + m''} \]

Test-case L3:

**Inlet conditions:**
- Tot. press.: 41.7 kPa
- Tot. temp.: 357.5 K (\(\Delta T_s = +7.5 \text{ K}\))

**Outlet conditions:**
- Stat. pressure: 20.6 kPa

**Assumptions:**
- equilibrium condensation (no sub-cooling considered)
- homogeneous two-phase flow
Test-case L3:

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- 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:

Test-case L3:

Inlet conditions:
• Tot. press.: 41.7 kPa
• Tot. temp.: 357.5 K ($\Delta T_s = +7.5$ 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.)

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
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
Spline-Based Table Look-Up Method (SBTL):
- Provides high accuracy and high computing speed at the same time
- Property functions of available fundamental equations/standards are reproduced with an accuracy of 10 – 100 ppm - the results of a process simulation will not change
- Computing speeds can be increased by factors > 100 in comparison to the calculation from fundamental equations
- Complete numerical consistency of forward and backward functions is possible

Applicability in Computational Fluid Dynamics (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
- Next step: implementation of a nucleation model, heterogeneous two-phase flow

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

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

Thank you for your attention!