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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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16th International Symposium on Transport Phenomena and Dynamics of Rotating Machinery, April 10 – 15, Honolulu
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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 \((v,u), (p,h), \ldots\)
- Application of the SBTL Method in CFD (TRACE, developed at DLR)
- FluidSplines – Generation of SBTL Functions for Specific Demands
- Summary

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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

\[
\left( \frac{v^{\text{ideal}} - v^{\text{real}}}{v^{\text{real}}} \right) \]

\[ p = \frac{R \cdot T}{v} \]
Deviations in Specific Volume (Water and Steam): Cubic Equation of State (Peng-Robinson)

\[
\left( \nu^{\text{PR}} - \nu^{\text{real}} \right) / \nu^{\text{real}}
\]

\[
p = \frac{RT}{\nu - b} - \frac{a(T)}{\nu^2 + 2bv - b^2}
\]
Uncertainties in Specific Volume of IAPWS-IF97 for Water and Steam:

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

Region 2:

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

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

\[
\gamma^0(\pi, \tau) = \ln \pi + \sum_{i=1}^{9} n_i \pi^{i_0} (\tau - 0.5)^{i_1}
\]

\[
\gamma^r(\pi, \tau) = \ln \pi + \sum_{i=1}^{43} n_i \pi^{i_0} (\tau - 0.5)^{i_1}
\]

\[
v(\pi, \tau) \frac{p}{RT} = \pi \left( \gamma^0_{\pi} + \gamma^r_{\pi} \right)
\]
Deviations in Isobaric Heat Capacity (Water and Steam):
Ideal-Gas Model

\[
\left( \frac{c_p^{\text{ideal}} - c_p^{\text{real}}}{c_p^{\text{real}}} \right) 
\]

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

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

$p^{\text{PR}}(T, v)$ and $c_p^{\text{ideal}}(T)$

-1% to 50% deviation

Pressure $p$ [MPa]
Temperature $T$ [K]
Uncertainties in Isobaric Heat Capacity of IAPWS-IF97 for Water and Steam:

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

Region 2:

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

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

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

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

\[
C_p(\pi, \tau) = -\tau^2 \left( \gamma^0_{\tau \pi} + \gamma^r_{\tau \pi} \right)
\]
### Fluid Property Calculations in CFD – Objectives

<table>
<thead>
<tr>
<th>Requirements</th>
<th>Ideal gas</th>
<th>Cubic Equation of State</th>
<th>Ind. Standard</th>
<th>Table Look-Up Methods</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Accuracy</strong></td>
<td>$</td>
<td>\Delta V</td>
<td>\leq 50%$</td>
<td>$</td>
</tr>
<tr>
<td></td>
<td>$</td>
<td>\Delta c_p</td>
<td>\leq 50%$</td>
<td>$</td>
</tr>
<tr>
<td><strong>Computing speed</strong></td>
<td>very high</td>
<td>slow</td>
<td>too slow</td>
<td>high</td>
</tr>
</tbody>
</table>

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

- **Generation of a rectangular grid of nodes:**
  - each node is calculated from the underlying equation of state:
    $$p_{i,j}(v_i, u_j) = p^{\text{EOS}}(v_i, u_j)$$

- **Variable transformation:** $v \rightarrow \bar{v}$
  - enhance accuracy
  - transform the range of state

- **Cell definition in the grid of knots:**
  - bi-quadratic spline polynomial:
    $$p_{ij}^{\text{SPL}}(\bar{v}, u) = \sum_{k=1}^{3} \sum_{l=1}^{3} a_{ijkl} (\bar{v} - \bar{v}_i)^{k-1} (u - u_j)^{l-1}$$
  - intersects the inner node
  - continuous function and first derivatives

- **Optimization for:**
  - required accuracy
  - maximum computing speed
  - minimum amount of data (table size)

**Property calculation in CFD:**
- transformation of $v \rightarrow \bar{v}$
- cell $(i,j)$ determination
- computation of the spline polynomial

**Providing the look-up table with the determined spline coefficients**
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

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

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

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

- **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 $p_L(v,u)$:

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

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

→ Spline function $p_G(v,u)$:
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 \((u,s)\) – Deviations from IAPWS-IF97

<table>
<thead>
<tr>
<th>SBTL function</th>
<th>Max. deviation (liquid phase)</th>
<th>Max. deviation (vapor phase)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(p(v,u))</td>
<td>(</td>
<td>\Delta p / p</td>
</tr>
<tr>
<td>(p &gt; 2.5 \text{ MPa})</td>
<td>(</td>
<td>\Delta p</td>
</tr>
<tr>
<td>(T(v,u))</td>
<td>(</td>
<td>\Delta T</td>
</tr>
<tr>
<td>(s(v,u))</td>
<td>(</td>
<td>\Delta s</td>
</tr>
<tr>
<td>(w(v,u))</td>
<td>(</td>
<td>\Delta w / w</td>
</tr>
<tr>
<td>(\eta(v,u))</td>
<td>(</td>
<td>\Delta \eta / \eta</td>
</tr>
</tbody>
</table>
SBTL Functions of \((v,u)\) and Inverse Functions of \((p,v)\) and \((u,s)\) – Computing time comparisons with IAPWS-IF97

### Computing-Time Ratio

\[ CTR = \frac{\text{Computing time of the calculation from IAPWS-IF97}}{\text{Computing time of the calculation from the spline function}} \]

<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)  
**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:

\[ x = \frac{m''}{m' + m''} \]

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

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

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

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 subcooling considered)
- homogeneous two-phase flow

**Pressure coefficient along the blade profile:**

![Graph showing pressure coefficient along the blade profile](image)
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
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

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Thank you for your attention!