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Fast and Accurate Calculation of Thermodynamic Properties in Process Simulations Using a Spline-Based Table Look-Up Method

Project of the International Association for the Properties of Water and Steam (IAPWS) -Task Group "CFD Steam Property Formulation"

Agenda:

- **Requirements for the Calculation of Thermodynamic Properties in Process Simulations**
- **Fundamentals of a Spline-Based Table Look-Up Method**
- **Property Calculations for Water and Steam in CFD-Simulations**
- **FluidSplines – a Tool to Generate Spline-Based Property Functions**
- **Summary and Outlook**

Symposium on Thermophysical Properties of Fluids, Zittau 2012

Requirements for Property Calculations in Process Simulations

Extensive Process Simulations:

- **Heat Cycle Calculations (HCC):**
  - calculation of non-stationary processes
  - heat cycle optimizations
- **Computational Fluid Dynamics (CFD) :**
  - 3D-flow analysis
  - consideration of real fluid behavior

Objectives/Conditions of Process Simulations	Requirements for Property Calculations
accurate results	high accuracy
small time steps, small volume elements (cells)	high numerical consistency (e.g., $u(p,v)$ must be numerically consistent to $p(u,v)$ in CFD-calculations)
application of numerical solvers	continuous functions and first derivatives
property functions are called frequently (millions of calls)	high computing speed

Requirements for Property Calculations in Process Simulations

Equations of State cannot meet the requirement for high computing speed because:

- **independent variables of Helmholtz-equations are temperature *T* and specific volume *v*,**
  - Heat Cycle Calculations: calculation from pressure *p* and specific enthalpy *h*
  - CFD: calculation from internal energy u and specific volume *v*
  - ➢ **iterative calculation of properties required**
- **equations of state contain numerous terms,**
- **complexity of terms (rational exponents, logarithms, …).**

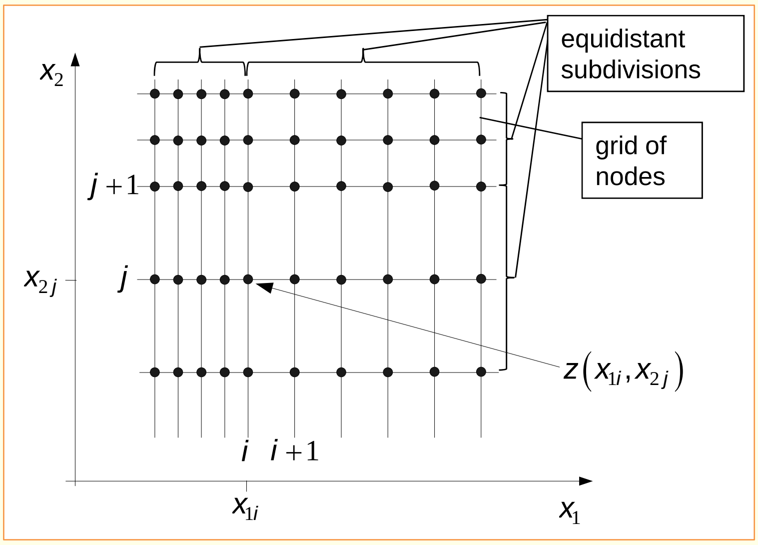
⇨ **Computing times must be reduced by factors >100…1000 to meet the requirements.**

It is advantageous for extensive process simulations to apply a spline-based table look-up method to existing equations of state because:

- **results of the equation of state can be reproduced with high accuracy and high computing speed,**
- **spline-functions represent property functions continuously,**
- **backward functions can be calculated with complete numerical consistency.**

Fundamentals of a Spline-Based Table Look-Up Method

Generation of a spline-function $z^{SPL}(x_1,x_2)$ from an existing equation of state $z^{EOS}(x_1,x_2)$:



- **Generation of a grid of nodes, optimized for:**
  - **required accuracy**
  - **maximal computing speed**
  - **minimal amount of data**
- **Calculation of node-values from equation of state**
- **Calculation of all spline-coefficients for all cells**

$$z_{ij}^{SPL}(x_1,x_2) = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ijkl}(x_1 - x_{1i})^{k-1}(x_2 - x_{2j})^{l-1}$$

To provide spline-based functions for property calculations:

- **save grid of nodes and spline-coefficients**
- **generate optimized source-code for the property function $z^{SPL}(x_1,x_2)$**

⇨ **Application of spline-functions in CFD and other extensive simulations**

Fundamentals of a Spline-Based Table Look-Up Method

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

$$z_{ij}^{\mathrm{SPL}}(x_1,x_2)=\sum_{k=1}^{3}\sum_{l=1}^{3}a_{ijkl}(x_1-x_{1i})^{k-1}(x_2-x_{2j})^{l-1}$$

$$\Rightarrow \quad x_{1,ij}^{\mathrm{INV}}(z,x_2)=\frac{\left(-B\pm\sqrt{B^2-4AC}\right)}{2A}+x_{1i}$$

in which $A=a_{ij31}+\Delta x_{2j}\left(a_{ij32}+a_{ij33}\Delta x_{2j}\right)$

$B=a_{ij21}+\Delta x_{2j}\left(a_{ij22}+a_{ij23}\Delta x_{2j}\right)$

$C=a_{ij11}+\Delta x_{2j}\left(a_{ij12}+a_{ij13}\Delta x_{2j}\right)-z$

and $\Delta x_{2j}=\left(x_2-x_{2j}\right)$

⇩

The inverse spline-function $x_{1,ij}^{\mathrm{INV}}(z,x_2)$ is numerically consistent to the spline-function $z_{ij}^{\mathrm{SPL}}(x_1,x_2)$.

Property Calculations for Water and Steam in CFD-Simulations

Application of inverse spline-functions (independent variables: *u*,*v*):

→ spline-functions with the variables *u* and *v*: $p^{\mathrm{SPL}}(u,v)$ $T^{\mathrm{SPL}}(u,v)$ $s^{\mathrm{SPL}}(u,v)$ $\eta^{\mathrm{SPL}}(u,v)$ $\lambda^{\mathrm{SPL}}(u,v)$

→ calculation from other pairs of variables using the spline-functions above:

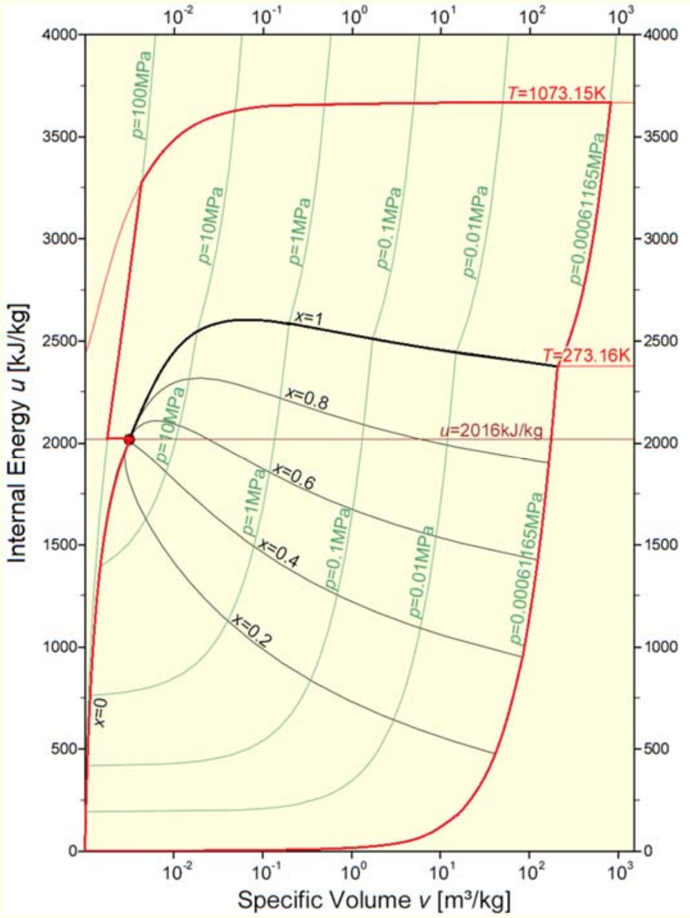
$T,s,u,\eta = \mathrm{f}(p,v)$	$T,v,s,\eta = \mathrm{f}(p,u)$	$p,T,v,\eta = \mathrm{f}(u,s)$
$u = u^{\mathrm{INV}}(p,v)$	$v = v^{\mathrm{INV}}(p,u)$	$v = v^{\mathrm{INV}}(u,s)$
$T = T^{\mathrm{SPL}}(u,v)$	$T = T^{\mathrm{SPL}}(u,v)$	$p = p^{\mathrm{SPL}}(u,v)$
$s = s^{\mathrm{SPL}}(u,v)$	$s = s^{\mathrm{SPL}}(u,v)$	$T = T^{\mathrm{SPL}}(u,v)$
$\eta = \eta^{\mathrm{SPL}}(u,v)$	$\eta = \eta^{\mathrm{SPL}}(u,v)$	$\eta = \eta^{\mathrm{SPL}}(u,v)$

→ inverse spline functions: $u = u^{\mathrm{INV}}(p,v)$, $v = v^{\mathrm{INV}}(p,u)$, $v = v^{\mathrm{INV}}(u,s)$

⇩

- **All thermodynamic properties, including backward-functions, can be calculated without iterations.**
- **Spline-functions can be calculated with complete numerical consistency.**

Property Calculations for Water and Steam in CFD-Simulations



Required Range of Validity:

Superheated vapor:

0.000612 MPa ≤ p ≤ 100 MPa

273.16 K ≤ T ≤ 1073.15 K

Two-phase region:

273.16 K ≤ T ≤ 647.096 K

0 kg/kg ≤ x ≤ 1 kg/kg

Available Equations of State:

IAPWS-IF97:

Single-phase region: $g(p,T)$

Critical and supercritical region: $f(T,v)$

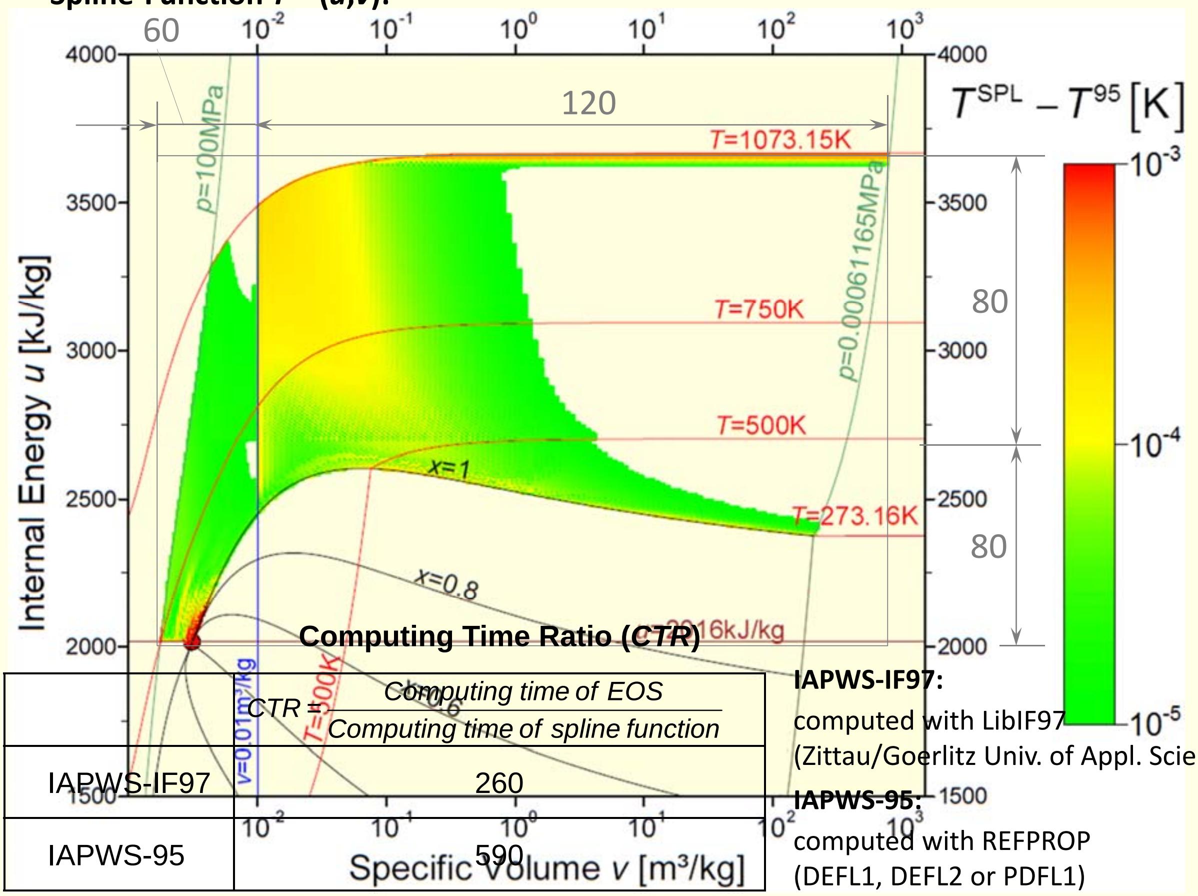
Two-phase region: $p_s(T)$

IAPWS-95:

Helmholtz-equation of state: $f(T,v)$

Property Calculations for Water and Steam in CFD-Simulations

→ **Spline-Function $T^{SPL}(u,v)$:**



Computing Time Ratio (*CTR*)

	$CTR = \dfrac{\text{Computing time of EOS}}{\text{Computing time of spline function}}$
IAPWS-IF97	260
IAPWS-95	590

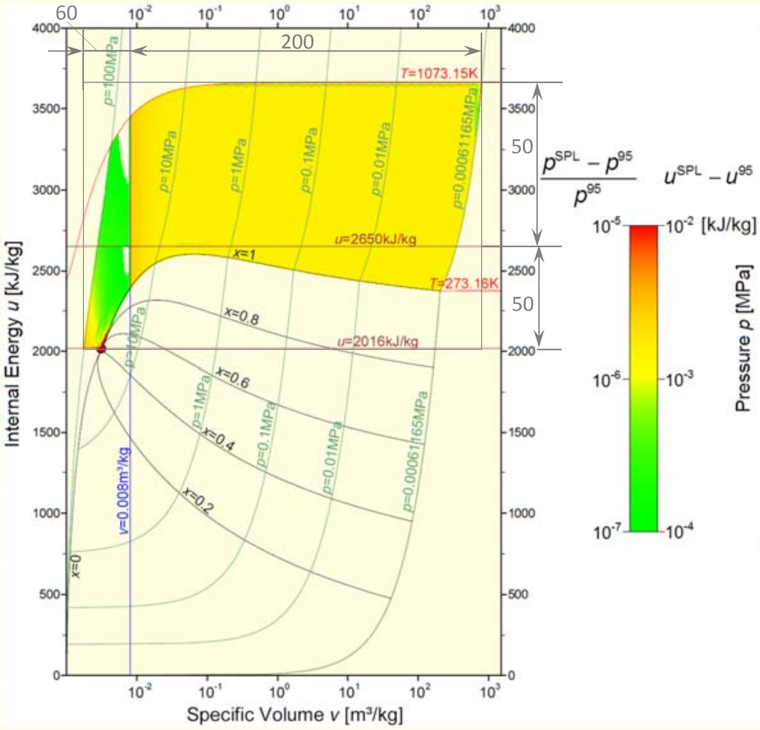
IAPWS-IF97:
computed with LibIF97
(Zittau/Goerlitz Univ. of Appl. Sciences)

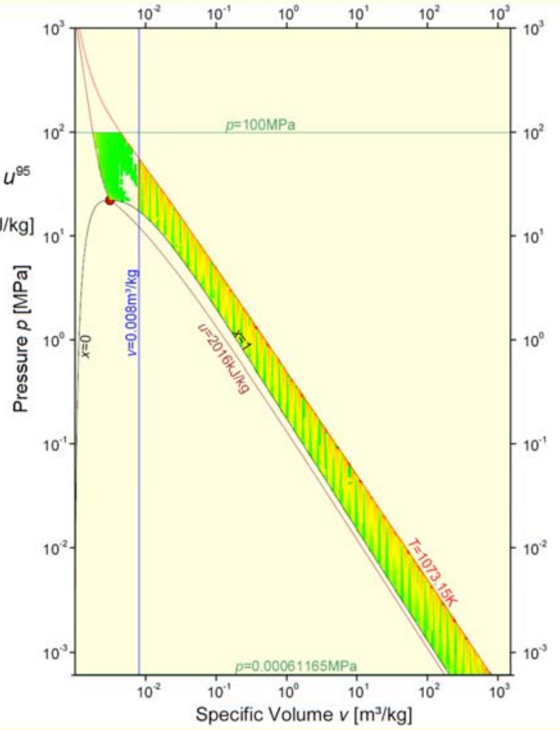
IAPWS-95:
computed with REFPROP
(DEFL1, DEFL2 or PDFL1)

Property Calculations for Water and Steam in CFD-Simulations

→ Spline-Function $p^{SPL}(u,v)$:

→ Inverse Spline-Function $u^{INV}(p,v)$:





Computing time ratio in comparison to IAPWS-IF97 (IAPWS-95):

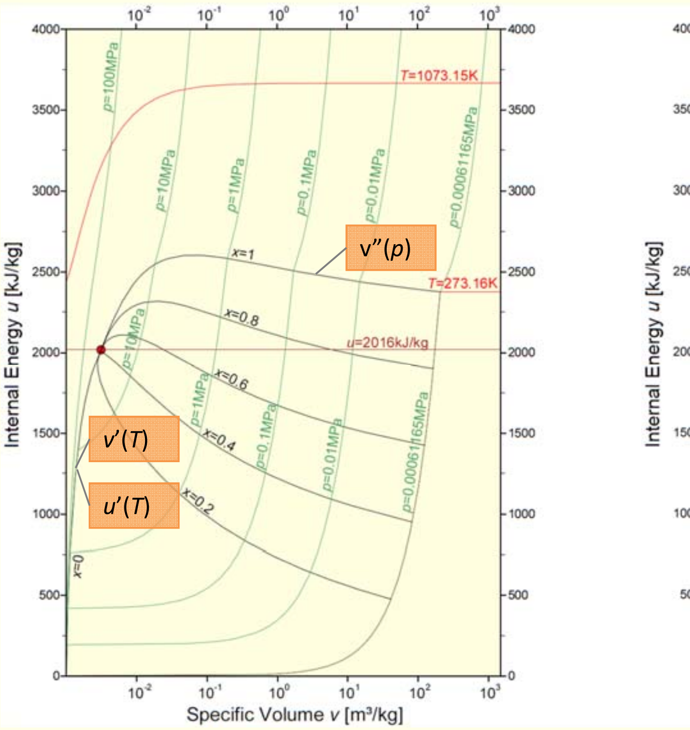
***CTR* ≈ 260 (590)**

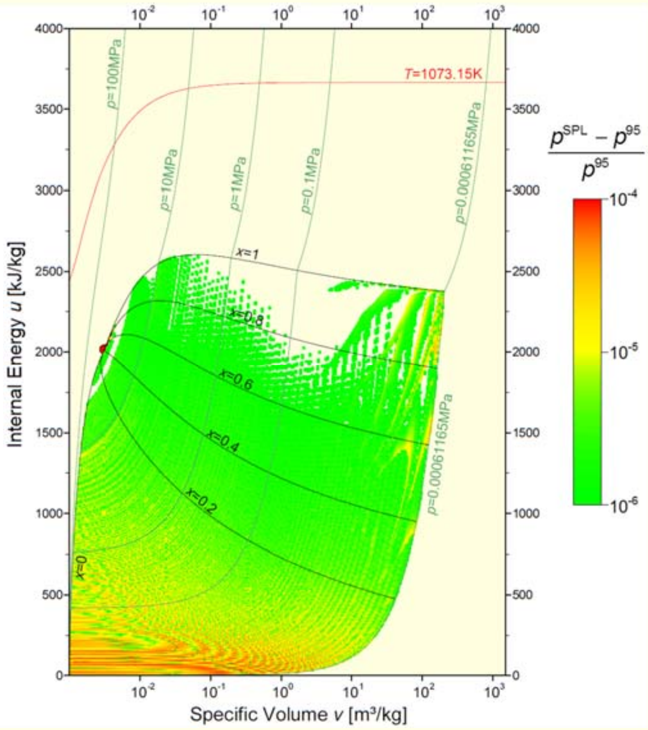
***CTR* ≈ 19 (160)**

Property Calculations for Water and Steam in CFD-Simulations

→ Auxiliary Functions for Two-Phase Region:

→ Saturation Pressure $p_s(u,v)$:





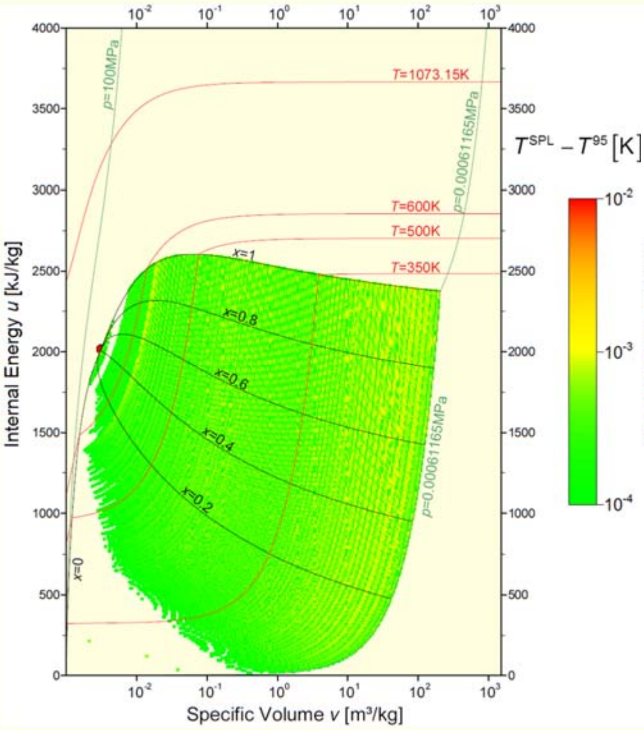
- High numerical consistency at dew curve
- Distinct phase test

Computing time ratio in comparison to IAPWS-IF97 (IAPWS-95):

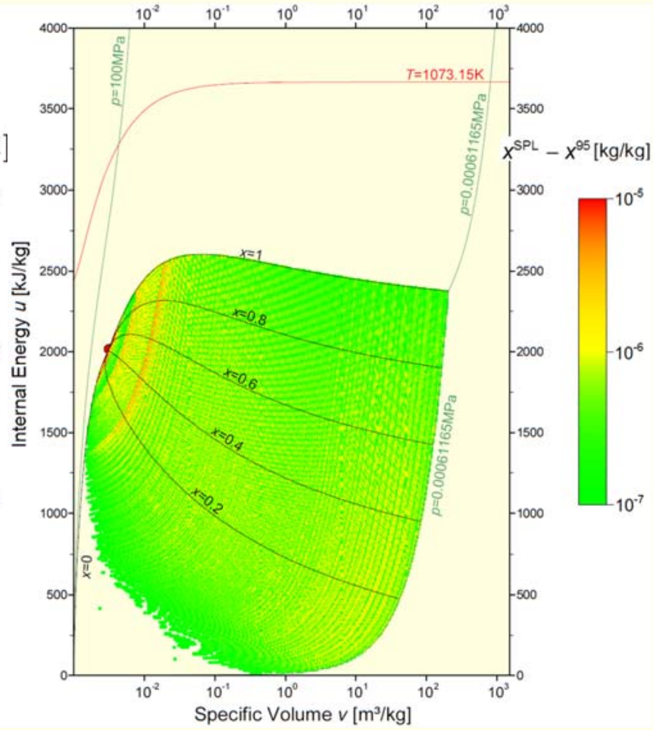
***CTR* ≈ 3 (490)**

Property Calculations for Water and Steam in CFD-Simulations

→ Saturation Temperature $T_s(u,v)$:



→ Vapor Fraction $x(u,v)$:



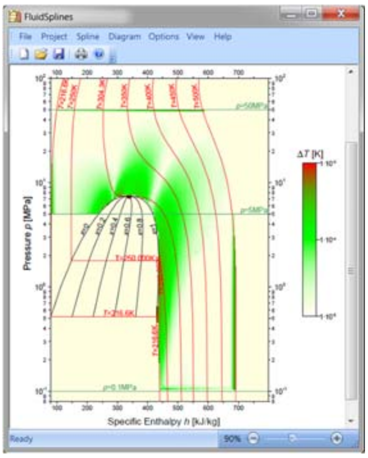
Computing time ratio in comparison to IAPWS-IF97 (IAPWS-95):

***CTR* ≈ 3 (490)**

FluidSplines – a Tool to Generate Spline-Based Property Functions

FluidSplines

Software for generating property functions based on spline-interpolation



Generation of Spline-Functions for:

- specified range of validity
- required accuracy

Additional Features:

- generation of inverse spline-functions
- accuracy check
- computing time check

Thermodynamic Properties:
(Database)

REFPROP©

Property-Libraries (Zittau/Goerlitz Univ.)

Output:

- optimized source code for high computing speed
- static/dynamic libraries
- documentation of accuracy and computing speed

Application of Property-Functions Based on Spline-Interpolation:

- Computational Fluid Dynamics (CFD)
- extensive heat-cycle calculations (optimization of heat cycles)
- calculation of non-stationary processes
- other applications

Summary and Outlook

Summary:

- Spline-based table look-up methods provide high accuracy and high computing speed at the same time
  (CTR=100...>1000 in comparison to equations of state)
- Complete numerical consistency of forward and backward functions is possible
- Requirements of Computational Fluid Dynamics and the calculation of non-stationary processes can be fulfilled (numerical consistency, continuity)
- Spline-functions can be fitted to existing equations of state of any fluid

Outlook:

- Further development of spline-algorithms and tools
- Test-calculations in CFD-Programs (TRACE, developed by DLR)
- Test-calculations in heat-cycle simulations (EBSILON, developed by STEAG Energy Services)
- Test-calculations with non-stationary simulation tools (Vattenfall Power Consult VPC)
- This method will be presented at the IAPWS-meeting in October, 1st-5th (Boulder, CO)

Thank you for your attention.