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Fast Calculation of Thermodynamic Properties in Process Modeling Using Spline-Interpolation

Agenda

- Calculation of Thermodynamic Properties: Requirements and Algorithms
- Spline-Interpolation of Thermodynamic Properties
- Example 1: A Set of Spline-Functions for Gaseous CO_2
- Example 2: Comparison of a Spline-Function $T_2^{\mathrm{SPL}}(p,h)$ with the Corresponding Backward-Equation $T_2^{\mathrm{IF97}}(p,h)$ for Region 2 of IAPWS-IF97 for Steam
- Software-Tool for Generating Spline-Based Property Libraries
- Summary and Outlook

Designing and Optimizing Advanced Power Cycles – Calculation of Thermodynamic Properties: Requirements and Algorithms

Requirements	Precise fundamental equations	Fast fundamental equations and backward equations	Table look-up methods
Accuracy	high	sufficient for industrial use	depends on table size and interpolation algorithm
Computing speed	low, because: • contain numerous transcendental terms • backward functions calculated iteratively	high, because: • contain integer exponents only (calculable using Horner's scheme) • backward functions calculated without iterations	very high, because: • simple interpolation equations are in use • backward functions calculated without iterations
Numerical consistency	depending on number of iterations	limited	complete numerical consistency is possible
Availability	available for most working fluids	for only a few working fluids backward equations are available	tables must be prepared in advance

Developments in computer technology

- Improvement of clock rate of CPU's stagnates
- Extremely large main memory available now

Advantages of Spline-Interpolation

- Continuous representation of one- or multi-dimensional functions and their derivatives
- High accuracy with small tables (grids) in comparison to linear interpolation
- Spline polynomials up to third degree can be solved analytically in terms of their variables

Spline-based table look-up methods are preferable.

Spline Interpolation of Thermodynamic Properties

Choice of spline polynomial and calculation method:

- → Demand for high computing speed leads to simple spline polynomials.
- → Spline polynomials up to third degree can be solved analytically in terms of their variables. This enables complete numerical consistency between forward and backward functions.
- → Example: bi-quadratic polynomial (to be defined in each cell (*i*,*j*))

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

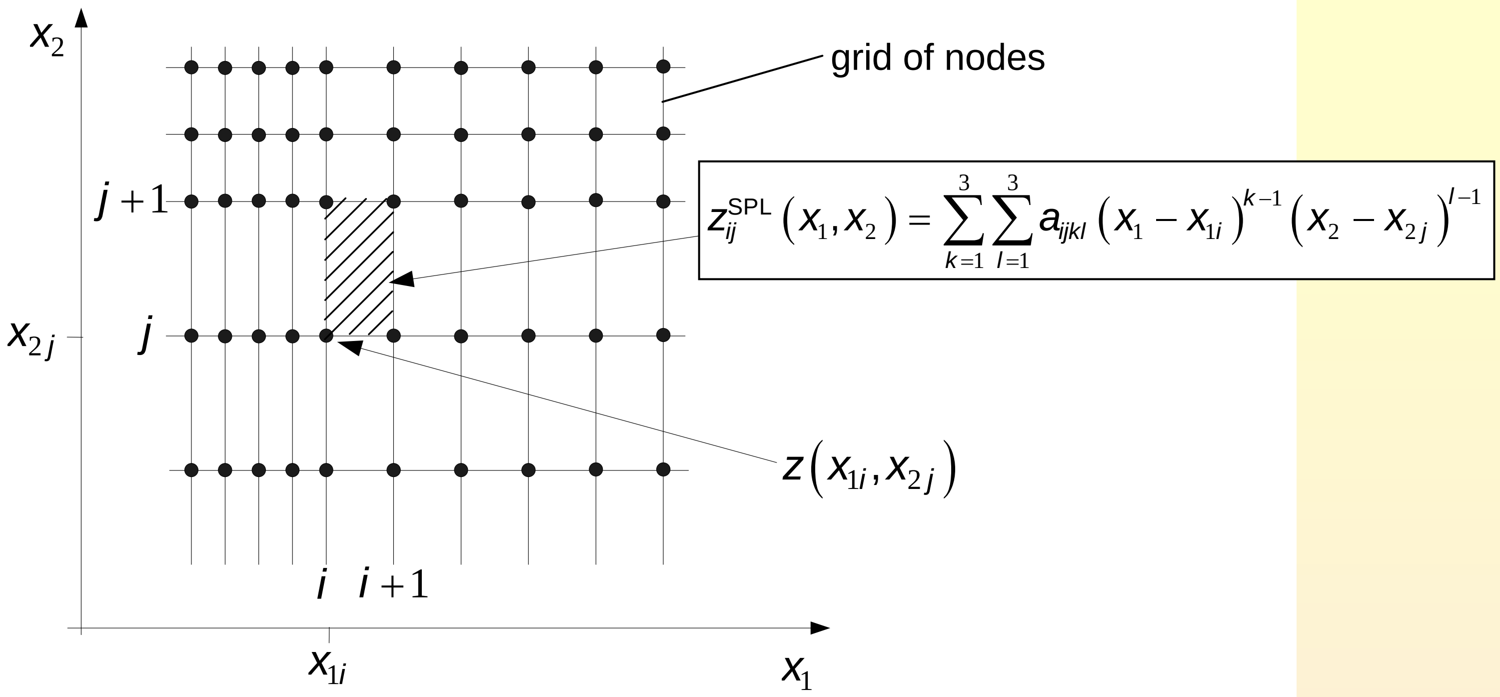
complete notation:

$$\begin{aligned} z_{ij}^{\mathrm{SPL}}\left(x_1, x_2\right) = {} & a_{ij11} + a_{ij21}\Delta x_{1i} + a_{31}\Delta x_{1i}^2 \\ & + a_{ij12}\Delta x_{2j} + a_{ij22}\Delta x_{1i}\Delta x_{2j} + a_{32}\Delta x_{1i}^2\Delta x_{2j} \\ & + a_{ij13}\Delta x_{2j}^2 + a_{ij23}\Delta x_{1i}\Delta x_{2j}^2 + a_{33}\Delta x_{1i}^2\Delta x_{2j}^2 \end{aligned}$$

with $\Delta x_{1i} = \left(x_1 - x_{1i}\right)$ and $\Delta x_{2j} = \left(x_2 - x_{2j}\right)$

- → Several calculation methods for determining the coefficients lead to different kinds of splines with differing characteristics.

Creating a spline function $z^{SPL}(x_1,x_2)$ from a given EOS $z^{EOS}(x_1,x_2)$:



→ Generation of a piecewise equidistant grid of nodes:

- density of nodes can be adjusted to the curvature of the property surface locally for desired accuracy
- simple search algorithms can be applied
- enables fast data handling which is important for high computing speed

→ Calculation of required function values and derivatives at all nodes from a given equation of state $z^{EOS}(x_1,x_2)$.

→ Determination of all spline coefficients a_{ijkl} for each polynomial $z_{ij}^{SPL}(x_1,x_2)$.

→ Store all coefficients in a look-up table.

Calculation of inverse spline functions:

→ Bi-quadratic polynomials can be solved analytically in terms of their variables

→ Inverse spline function $x_{1,ij}^{\mathrm{INV}}\left(z,x_2\right)$ of cell (i,j):

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

with
$$A=a_{ij31}+\Delta x_{2j}\left(a_{ij32}+a_{ij33}\Delta x_{2j}\right)$$
$$B=a_{ij21}+\Delta x_{2j}\left(a_{ij22}+a_{ij23}\Delta x_{2j}\right)$$
$$C=a_{ij11}+\Delta x_{2j}\left(a_{ij12}+a_{ij13}\Delta x_{2j}\right)-z$$

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

⇒ The inverse spline function is completely numerically consistent with the spline function $z_{ij}^{\mathrm{SPL}}\left(x_1,x_2\right)$.

Set of spline functions defined in a *p*-*h* grid:

- In process modeling properties are often calculated from (p,h).
- Spline Functions of p and h: $T^{SPL}(p,h)$ $s^{SPL}(p,h)$ $v^{SPL}(p,h)$ …
- Calculation from other pairs of variables using these spline functions:
- Inverse Spline Functions:

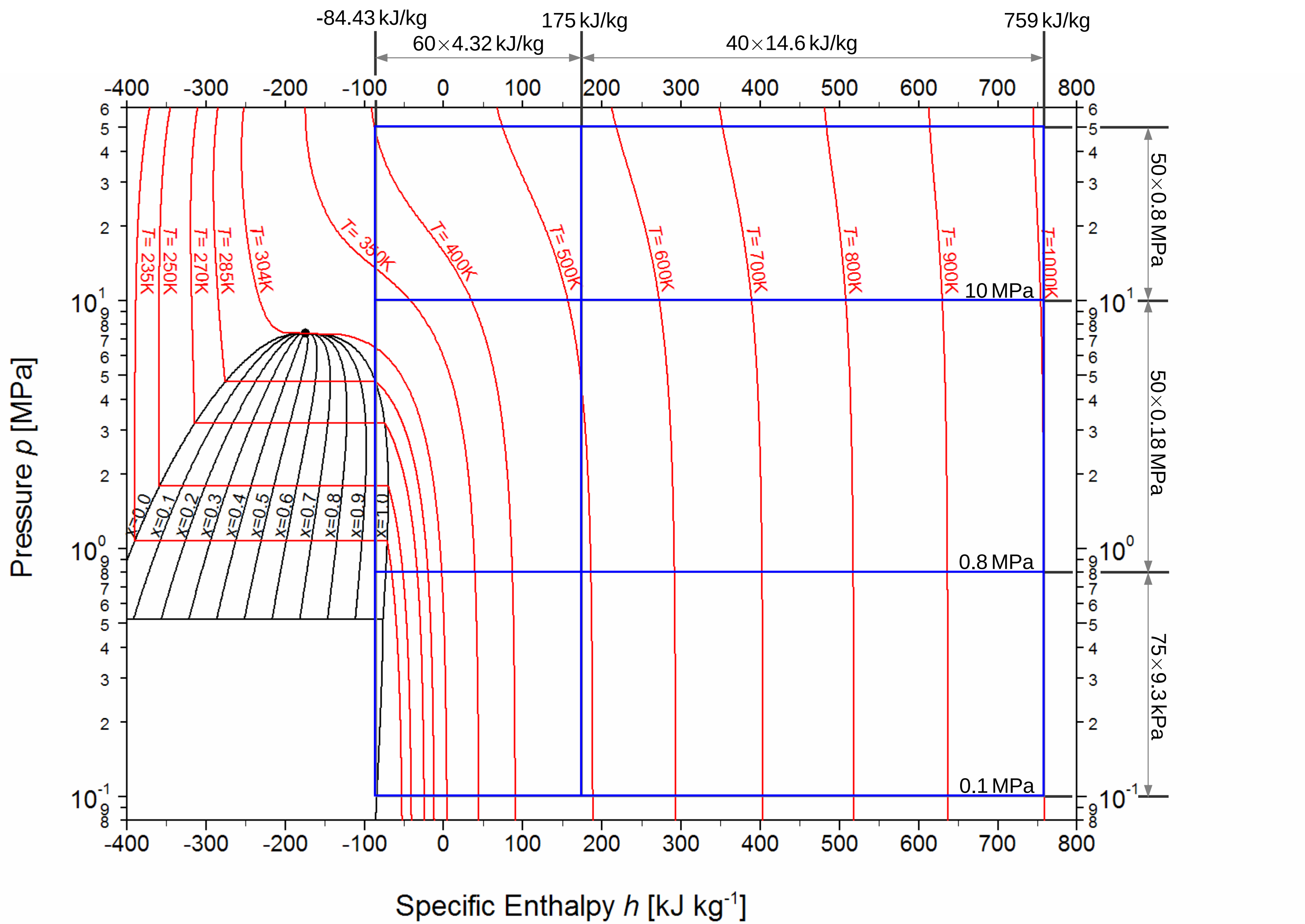
(p,T)	(p,s)	(h,s)
$h=h^{INV}(p,T)$	$h=h^{INV}(p,s)$	$p=p^{INV}(h,s)$
$s=s^{SPL}(p,h)$	$T=T^{SPL}(p,h)$	$T=T^{SPL}(p,h)$
$v=v^{SPL}(p,h)$	$v=v^{SPL}(p,h)$	$v=v^{SPL}(p,h)$
…	…	…

All thermodynamic properties, including backward functions, can be calculated without iterations.

Set of spline functions defined in a *v*-*u* grid can be created analoguously.

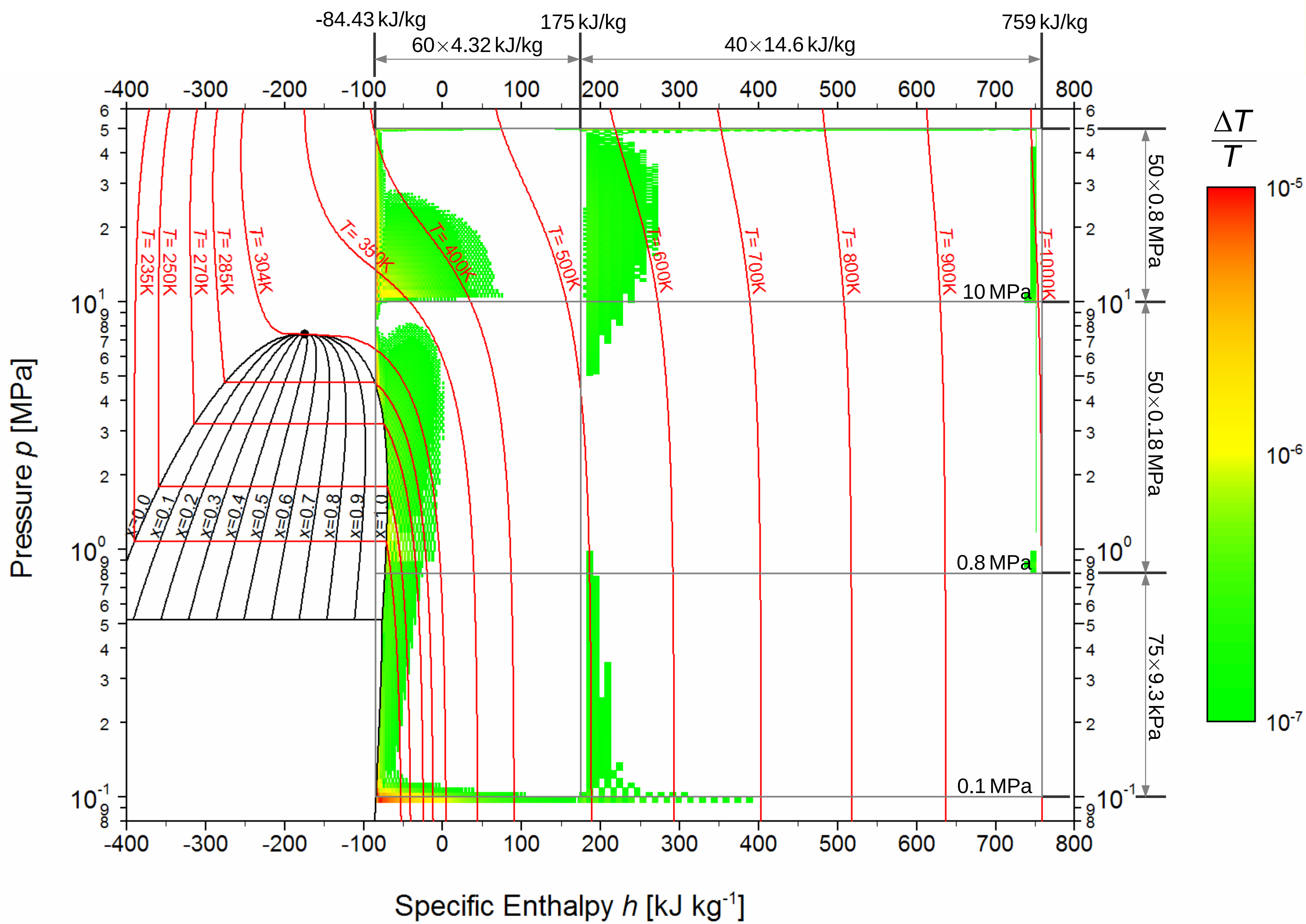
Example 1: A Set of Spline-Functions for gaseous CO_2

→ $T^{SPL}(p,h)$ and the *p*-*h* grid (calculated from scientific EOS of Span, R. and Wagner, W. (1996)):



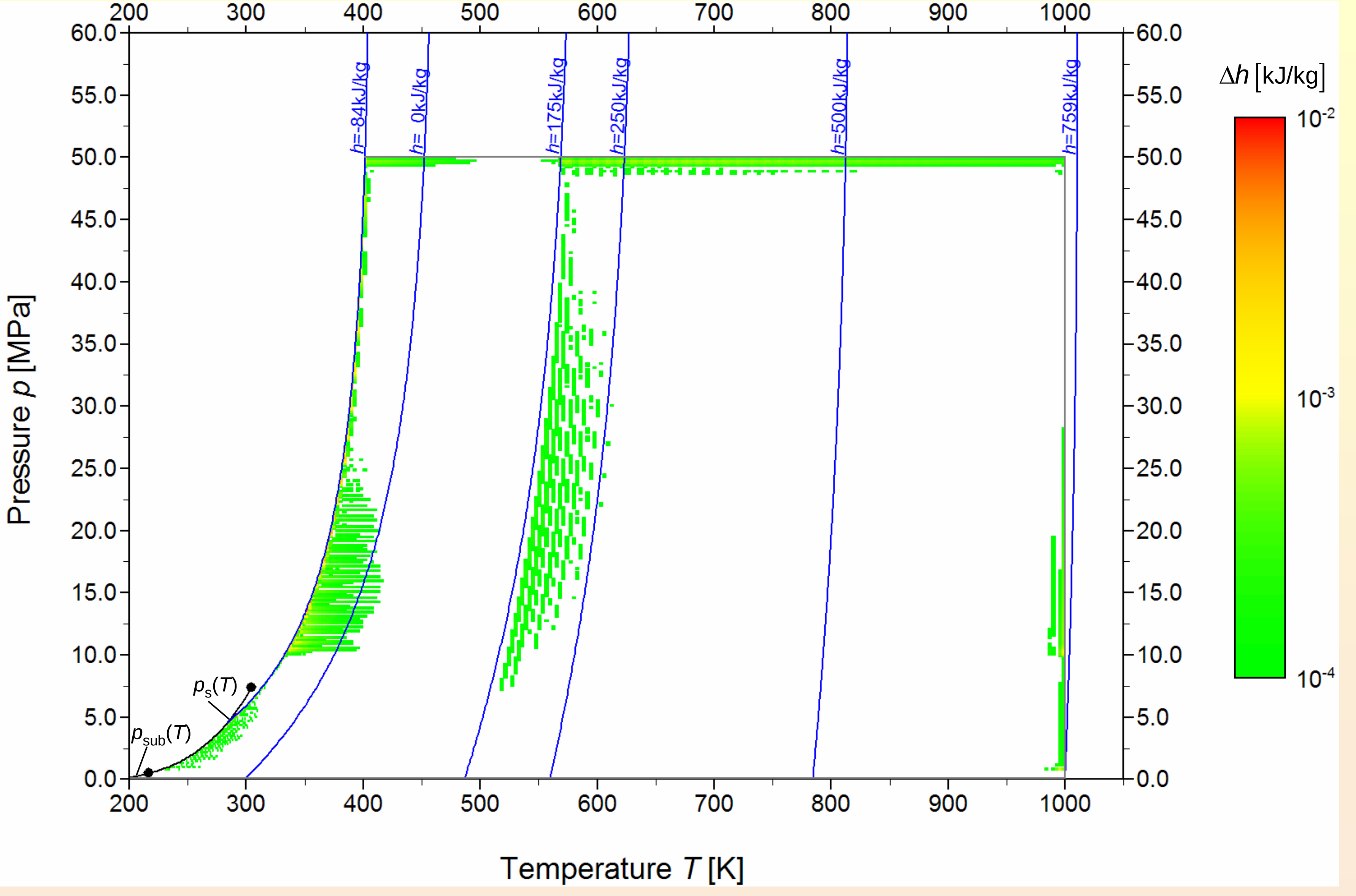
Example 1: A Set of Spline-Functions for gaseous CO_2

→ Relative deviation of $T^{SPL}(p,h)$:



Example 1: A Set of Spline-Functions for gaseous CO_2

→ Absolute deviation of $h^{INV}(p,T)$:



Computing Time Comparisons

→ Computing time has been compared with:

- EOS for scientific use of Span, R. and Wagner, W. (1996) and
- EOS for technical applications of Span, R. and Wagner, W. (2003).

} computed with REFPROP®

→ Tested on a Pentium Xeon 3.2 GHz PC with Microsoft Windows XP ®.

Computing Time Ratio (*CTR*)

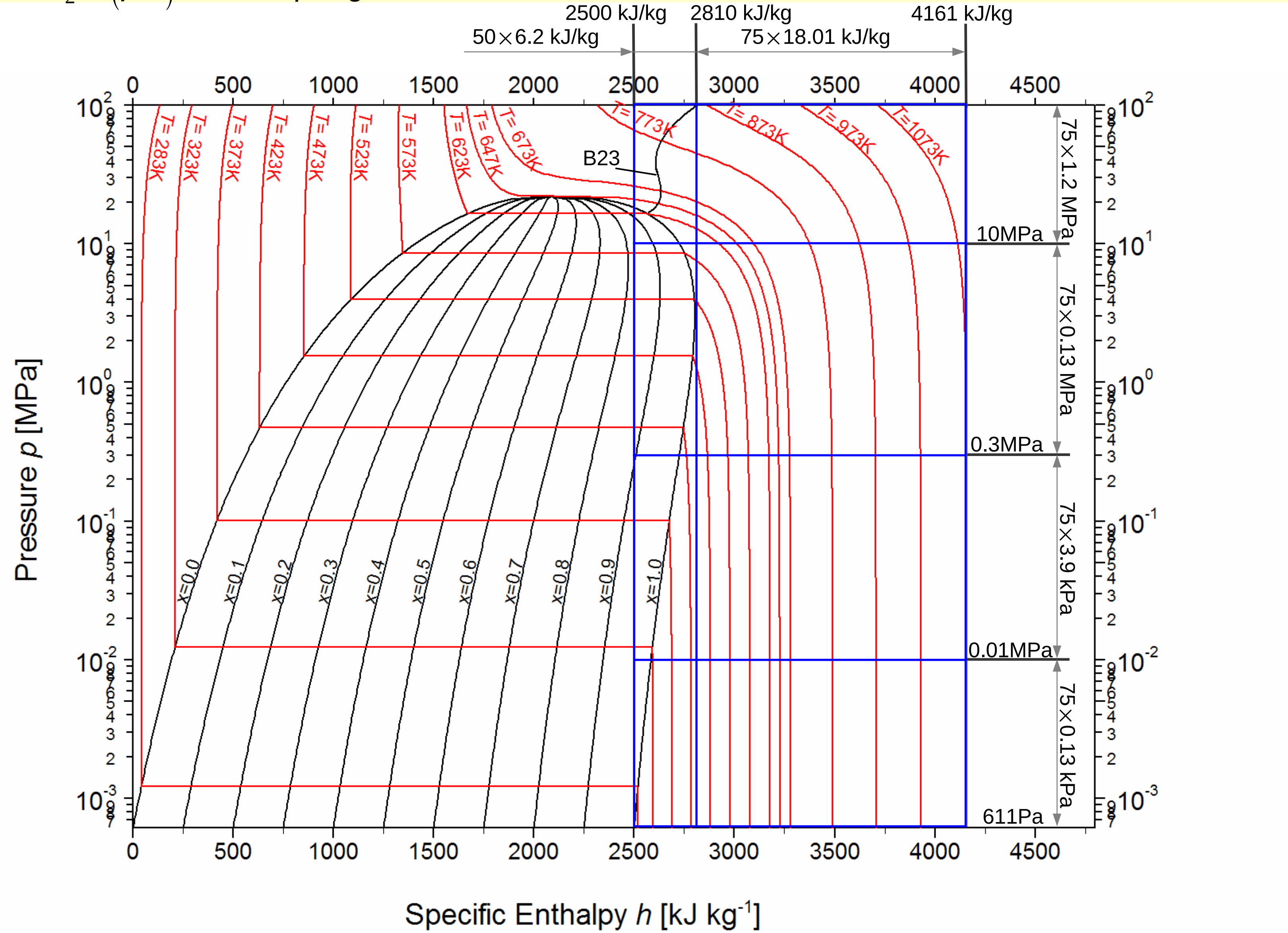
$$CTR = \frac{\text{Computing time of equation of state}}{\text{Computing time of spline function}}$$

	Spline Function		
	$T^{SPL}(p,h)$	$h^{INV}(p,T)$	$p^{INV}(h,s)$
CTR^{1996}	820	286	1250
CTR^{2003}	225	77	312

Spline-based table look-up methods are fast and accurate at the same time.

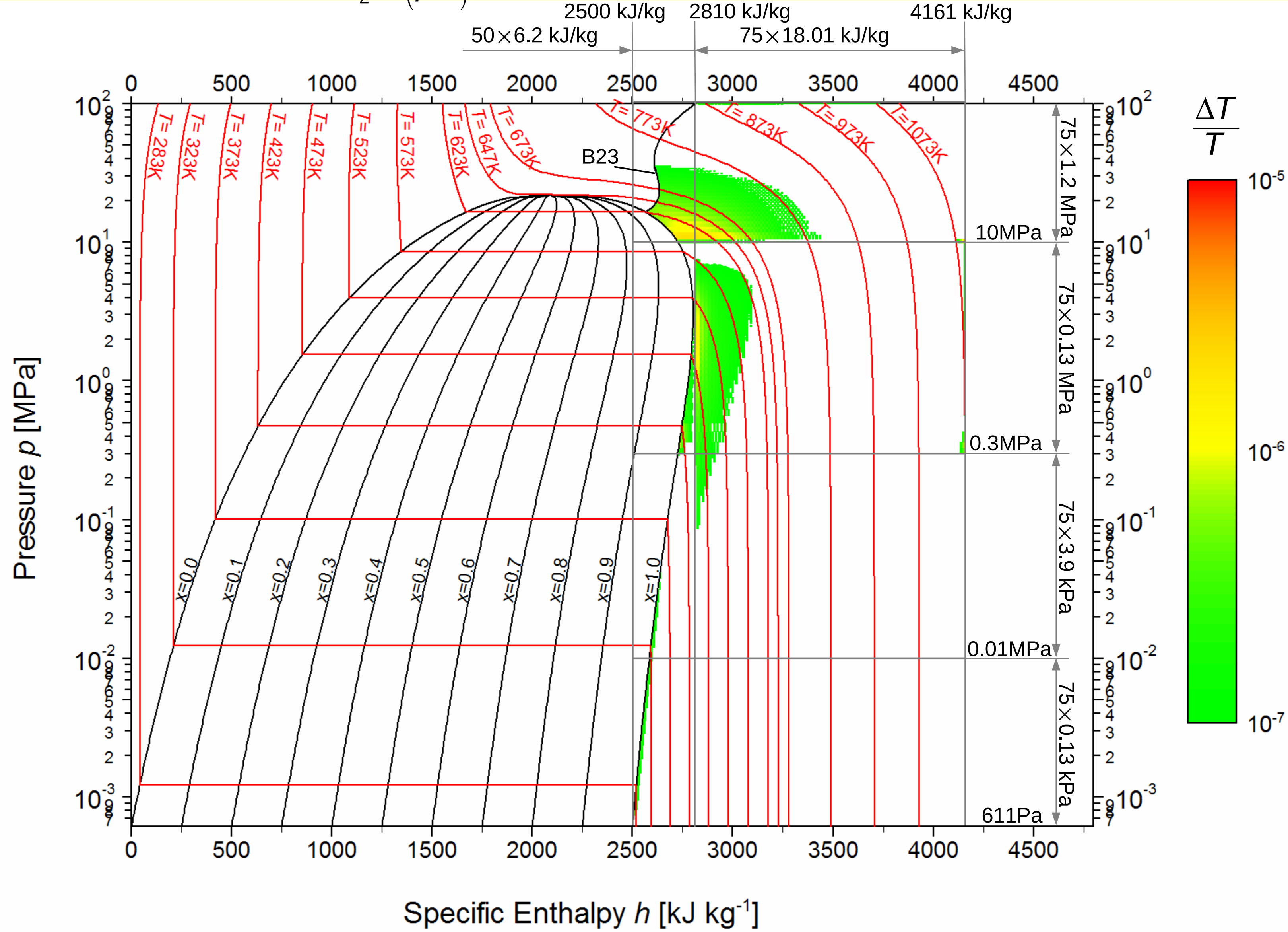
Example 2: Spline Function $T_2^{SPL}(p,h)$ and Inverse Spline Function $h_2^{INV}(p,T)$ for region 2 of IAPWS-IF97

→ $T_2^{SPL}(p,h)$ and the *p-h* grid:



Example 2: Spline Function $T_2^{\mathrm{SPL}}(p,h)$ and Inverse Spline Function $h_2^{\mathrm{INV}}(p,T)$ for region 2 of IAPWS-IF97

→ Relative deviation of $T_2^{\mathrm{SPL}}(p,h)$:



Computing Time Comparisons

- Computing time of $T_2^{\mathrm{SPL}}(p,h)$ has been compared with $T_2^{\mathrm{97BW}}(p,h)$.
- Computing time of $h_2^{\mathrm{INV}}(p,T)$ has been compared with $h_2^{\mathrm{IF97}}(p,T)$.
- Tested on a Pentium Xeon 3.2 GHz PC with Microsoft Windows XP ®.

Computing Time Ratio (*CTR*)

$$CTR = \frac{\text{Computing time of backward eq.}}{\text{Computing time of spline function}}$$

$$CTR = \frac{\text{Computing time of equation of state}}{\text{Computing time of spline function}}$$

	Spline Function	
	$T_2^{\mathrm{SPL}}(p,h)$	$h_2^{\mathrm{INV}}(p,T)$
CTR	2	1.2

Spline based table look-up methods can be faster than a backward equation.

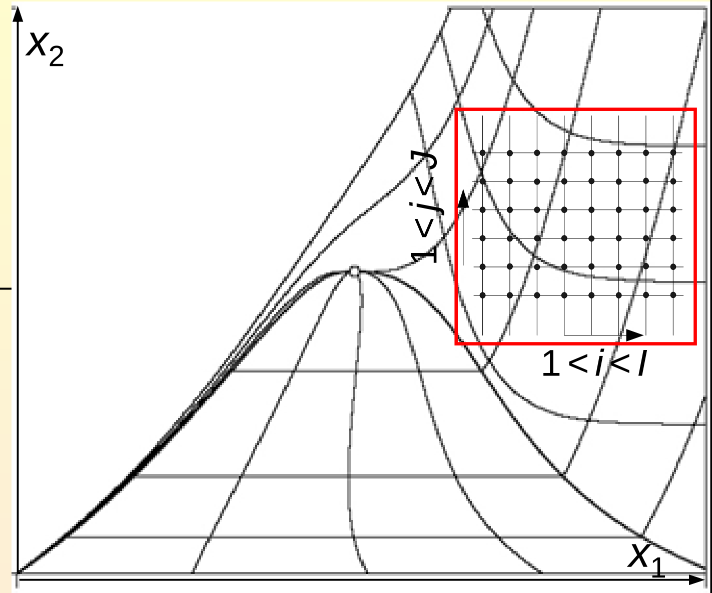
Software-Tool for Generating Spline-Based Property Libraries

Essential for the application of spline-based table look-up methods.

FluidGrid – Spline-Based Calculation of Thermodynamic Properties

INPUT

- Choice of an equation of state (pre-defined or external)
- Choice of a function
- Definition of required range of validity
- Definition of required accuracy



- Grid-optimization for desired range of validity and desired accuracy
- Calculation of all spline-coefficients
- Verification
- Estimation of CTR (computing time ratio)

OUTPUT

- Applicable source code including data grid and spline polynomials

A flexible software tool for generating spline-based property libraries is being developed.

Summary

- Spline functions are able to represent thermodynamic properties continuously.
- High accuracy and low computing times can be achieved at the same time.
- Example CO_2:
  - $T^{SPL}(p,h)$ is over 200 times faster than the iteration from the EOS $T^{EOS}(p,h)$.
  - The inverse spline function $h^{INV}(p,T)$ is over 70 times faster than the iteration from the EOS $h^{EOS}(p,T)$ and completely numerically consistent to $T^{SPL}(p,h)$.
- Example steam:
  - $T_2^{SPL}(p,h)$ is 2 times faster than the corresponding backward equation $T_2^{97BW}(p,h)$.
  - The inverse spline function $h_2^{INV}(p,T)$ is completely numerically consistent to $T_2^{SPL}(p,h)$.

Outlook

- An algorithm for grid optimization is being developed.
- The algorithm will be extended for mixtures.
- Software for automatic generation of spline functions is being developed.

Thank you for paying attention.