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Thermodynamic Properties and Derivatives Calculable from the New IAPWS Industrial Formulation for Water and Steam

Contents

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1 Introduction

► Thermodynamic properties and derivatives such as

- Relative pressure coefficient $\alpha_p = p^{-1}\left(\frac{\partial p}{\partial T}\right)_v$
- Isothermal throttling coefficient $\delta_T = \left(\frac{\partial h}{\partial p}\right)_T$
- Isobaric cubic expansion coefficient $\alpha_v = v^{-1}\left(\frac{\partial v}{\partial T}\right)_p$
- Isothermal compressibility $\kappa_T = -v^{-1}\left(\frac{\partial v}{\partial p}\right)_T$
- Isothermal stress coefficient $\beta_p = -p^{-1}\left(\frac{\partial p}{\partial v}\right)_T$
- Joule-Thomson coefficient $\beta_p = -p^{-1}\left(\frac{\partial p}{\partial v}\right)_T$

and other derivatives: $\left(\frac{\partial h}{\partial p}\right)_v, \left(\frac{\partial u}{\partial p}\right)_v, \left(\frac{\partial s}{\partial p}\right)_v, \left(\frac{\partial T}{\partial p}\right)_s, \left(\frac{\partial v}{\partial h}\right)_p, \left(\frac{\partial v}{\partial s}\right)_p, \ldots$

are required for:

- CFD and *non-stationary* simulations of energy conversion processes
- Solving equation systems of stationary heat cycle simulations.

► IAPWS Advisory Note No. 3 Thermodynamic Derivatives from IAPWS Formulations (2007, Rev. 2018) describes how these or other thermodynamic quantities and derivatives can be calculated using the fundamental equations of IAPWS-95, IAPWS-IF97 and other IAPWS formulations.

► The SBTL method intended for the new IAPWS Industrial Formulation currently includes spline functions for the following thermodynamic properties:

p, T, v, h, s, c_p, c_v, and isentropic speed of sound w.

Direct calculable quantities using these properties are:

Internal energy $u = h - pv$, Helmholtz free energy $f = u - Ts$,

Gibbs free enthalpy $g = h - Ts$, and isentropic exponent $\kappa = \dfrac{w^2}{pv}$

But: All thermodynamic properties and derivatives should be determined from the new IAPWS Industrial Formulation.

Problem: The derivatives of the bi-quadratic SBTL polynomials are not sufficiently accurate.

Solution: SBTL functions are required for those quantities from which all thermodynamic properties and derivatives can be determined.

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For which quantities are SBTL functions required?

2 Required SBTL Functions for Determining any Thermodynamic Property or Derivative

► Common expression for forming any partial derivative $\left(\frac{\partial z}{\partial x}\right)_y$ from derivatives of *x*, *y*, *z* over *p* and *T* according IAPWS Advisory Note No. 3

$$\boxed{\left(\frac{\partial z}{\partial x}\right)_y = \frac{\left(\frac{\partial z}{\partial p}\right)_T \cdot \left(\frac{\partial y}{\partial T}\right)_p - \left(\frac{\partial z}{\partial T}\right)_p \cdot \left(\frac{\partial y}{\partial p}\right)_T}{\left(\frac{\partial x}{\partial p}\right)_T \cdot \left(\frac{\partial y}{\partial T}\right)_p - \left(\frac{\partial x}{\partial T}\right)_p \cdot \left(\frac{\partial y}{\partial p}\right)_T}} \quad \text{(a)}$$

where

x, y, z can represent one of the thermodynamic properties: *p*, *T*, *v*, *h*, *u*, *s*, *f*, or *g*

► Determination of these derivatives

$$\left(\frac{\partial z}{\partial x}\right)_y = \frac{\left(\frac{\partial z}{\partial p}\right)_T \cdot \left(\frac{\partial y}{\partial T}\right)_p - \left(\frac{\partial z}{\partial T}\right)_p \cdot \left(\frac{\partial y}{\partial p}\right)_T}{\left(\frac{\partial x}{\partial p}\right)_T \cdot \left(\frac{\partial y}{\partial T}\right)_p - \left(\frac{\partial x}{\partial T}\right)_p \cdot \left(\frac{\partial y}{\partial p}\right)_T} \qquad \text{(a)}$$

$x,\ y,\ z$	$\left(\frac{\partial x}{\partial T}\right)_p, \left(\frac{\partial y}{\partial T}\right)_p, \left(\frac{\partial z}{\partial T}\right)_p$	$\left(\frac{\partial x}{\partial p}\right)_T, \left(\frac{\partial y}{\partial p}\right)_T, \left(\frac{\partial z}{\partial p}\right)_T$
p	0	1
T	1	0
v	$v\,\alpha_v$	$-v\,\kappa_T$
u	$c_p - p\,v\,\alpha_v$	$v\left(p\,\kappa_T - T\,\alpha_v\right)$
h	c_p	$v\left(1 - T\,\alpha_v\right)$
s	$\frac{c_p}{T}$	$-v\,\alpha_v$
g	$-s$	v
f	$-p\,v\,\alpha_v - s$	$p\,v\,\kappa_T$

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SBTL functions of (p,h) and of (v,u) for determining any thermodynamic property or derivative are required for:

p, T, v, s, c_p, α_v, κ_T

3 Example: Determination of the Derivative $\left(\frac{\partial u}{\partial p}\right)_v$ using SBTL Functions

Common Formula

$$\left(\frac{\partial z}{\partial x}\right)_y = \frac{\left(\frac{\partial z}{\partial p}\right)_T \cdot \left(\frac{\partial y}{\partial T}\right)_p - \left(\frac{\partial z}{\partial T}\right)_p \cdot \left(\frac{\partial y}{\partial p}\right)_T}{\left(\frac{\partial x}{\partial p}\right)_T \cdot \left(\frac{\partial y}{\partial T}\right)_p - \left(\frac{\partial x}{\partial T}\right)_p \cdot \left(\frac{\partial y}{\partial p}\right)_T} \quad \text{(a)}$$

Comparison of $\left(\frac{\partial z}{\partial x}\right)_y$ with $\left(\frac{\partial u}{\partial p}\right)_v$ $\Rightarrow$ $z = u$, $x = p$, $y = v$

Substitute into Eq. (a)

$$\left(\frac{\partial u}{\partial p}\right)_v = \frac{\left(\frac{\partial u}{\partial p}\right)_T \cdot \left(\frac{\partial v}{\partial T}\right)_p - \left(\frac{\partial u}{\partial T}\right)_p \cdot \left(\frac{\partial v}{\partial p}\right)_T}{\left(\frac{\partial p}{\partial p}\right)_T \cdot \left(\frac{\partial v}{\partial T}\right)_p - \left(\frac{\partial p}{\partial T}\right)_p \cdot \left(\frac{\partial v}{\partial p}\right)_T} \quad \text{(b)}$$

$$\left(\frac{\partial u}{\partial p}\right)_v = \frac{\left(\frac{\partial u}{\partial p}\right)_T \cdot \left(\frac{\partial v}{\partial T}\right)_p - \left(\frac{\partial u}{\partial T}\right)_p \cdot \left(\frac{\partial v}{\partial p}\right)_T}{\left(\frac{\partial p}{\partial p}\right)_T \cdot \left(\frac{\partial v}{\partial T}\right)_p - \left(\frac{\partial p}{\partial T}\right)_p \cdot \left(\frac{\partial v}{\partial p}\right)_T} \qquad \text{(b)}$$

Derivatives

$\underline{x}\ \underline{y}\ z$	$\left(\frac{\partial}{\partial T}\right)_p$	$\left(\frac{\partial}{\partial p}\right)_T$
p	0	1
T	-	-
v	$v\,\alpha_v$	$-v\,\kappa_T$
u	$c_p - p\,v\,\alpha_v$	$v\,(p\,\kappa_T - T\,\alpha_v)$
h	-	-
s	-	-
g	-	-
f	-	-

$$\left(\frac{\partial p}{\partial T}\right)_p = 0$$

$$\left(\frac{\partial p}{\partial p}\right)_T = 1$$

$$\left(\frac{\partial v}{\partial T}\right)_p = v\,\alpha_v$$

$$\left(\frac{\partial v}{\partial p}\right)_T = -v\,\kappa_T$$

$$\left(\frac{\partial u}{\partial p}\right)_T = v\,(p\,\kappa_T - T\,\alpha_v)$$

$$\left(\frac{\partial u}{\partial T}\right)_p = c_p - p\,v\,\alpha_v$$

⇨ Insertion into Eq. (b)

Result

$$\left(\frac{\partial u}{\partial p}\right)_v = \frac{c_p\,\kappa_T}{\alpha_v} - v\,T\,\alpha_v$$

4 Summary

► To calculate any thermodynamic property and derivative from the new Industrial Formulation, SBTL functions are required for the following quantities

- Pressure p
- Temperature T
- Specific volume v
- Specific entropy s
- Specific isobaric heat capacity c_p
- Isobaric cubic expansion coefficient α_V
- Isothermal compressibility κ_T

► The procedure, how to calculate any thermodynamic property or derivative using these SBTL functions, could be described

either

in the IAPWS Release of the new Industrial Formulation

or

in a revised version of IAPWS Advisory Note No. 3