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The IAPWS Industrial Formulation for the Thermodynamic Properties of Seawater

for Calculating Desalination Processes

Calculating Thermodynamic Properties

Fundamental equation for the specific Gibbs energy of the IAPWS 2013 formulation for seawater [1]

$$g(p,T,S) = g^{W}(p,T) + g^{S}(p,T,S)$$

Water part from IAPWS-IF97, region 1 [2]: $g^{W} = g_1^{97}(p,T)$

Saline part from IAPWS 2008 [3]: $g^{S} = g^{08}(p,T,S)$

The saline part S indicates the mass fraction of salt in seawater: $S = m_S / m$.

The composition of sea salt is based on the "Reference Composition Scale of Standard Seawater."

All thermodynamic properties can be calculated with the fundamental equation $g(p,T,S)$ and its derivatives from p, T, and S.

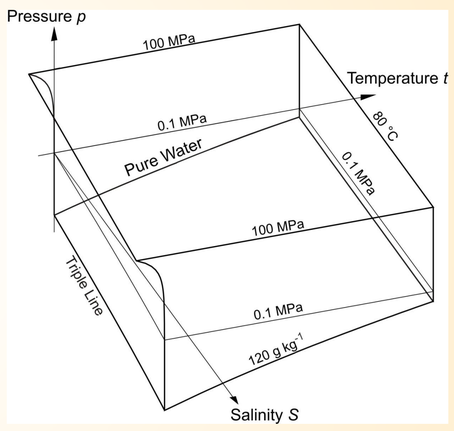
Examples for calculating the properties of seawater

Specific volume:	$v(p,T,S) = g_p$
Specific enthalpy:	$h(p,T,S) = g - T\,g_T$
Specific entropy:	$s(p,T,S) = -g_T$
Specific isobaric heat capacity:	$c_p(p,T,S) = -T\,g_{TT}$
Isobaric volume expansion coefficient:	$\alpha_v(p,T,S) = g_{pT} / g_p$
Chemical potential of water in seawater:	$\mu_W(p,T,S) = g - S\,g_S$
Osmotic pressure:	$\phi(p,T,S) = -(g^{S} - S\,g_S)/(bR_m T)$

Range of Validity

Pressure p:	0.3 kPa to 100 MPa
Celsius temperature t:	–12.15 °C to 80 °C
Kelvin Temperature T:	261 K to 353.15 K
Salinity S:	0 to 120 g kg^{-1}

With restrictions for certain regions corresponding to IAPWS 2008 [3]



Uncertainties of the Calculated Quantities

Uncertainties of the Industrial Formulation, u, largely correspond to the scientific formulation IAPWS-08 [3], u_{08}, and are adequate for industrial use:

$$u = u_{08} + \Delta_{RMS},$$

with Δ_{RMS} as a difference of the uncertainties between IAPWS 2013 and IAPWS 2008.

Quantity	S range kg kg^{-1}	T range K	p range MPa	u_{08}	Δ_{RMS}	u
$\lvert\Delta\rho/\rho\rvert$	0 - 0.04	273 - 313	0.1	4×10^{-6}	2.9×10^{-6}	5×10^{-6}
	0.04 - 0.05	288 - 303	0.1	1×10^{-5}	1.3×10^{-6}	1×10^{-5}
	0.005 - 0.04	273 - 313	10 - 100	2×10^{-5}	5.3×10^{-6}	2×10^{-5}
$\lvert\Delta\alpha_v\rvert$	0.01 - 0.03	267 - 274	0.7 - 33	6×10^{-7} K^{-1}	1×10^{-6} K^{-1}	1×10^{-6} K^{-1}
$\lvert\Delta w/w\rvert$	0.029 - 0.043	273 - 308	0.1 - 2	3×10^{-5}	8.2×10^{-4}	8.2×10^{-4}
	0.029 - 0.043	273 - 303	0.1 - 5	3×10^{-5}	6.4×10^{-4}	6.4×10^{-4}
	0.033 - 0.037	273 - 278	0.1 - 100	5×10^{-5}	1.8×10^{-4}	1.8×10^{-4}
$\lvert\Delta p^{vap}/p^{vap}\rvert$	0.02 - 0.12	293 - 353	0.002 - 0.05	1×10^{-3}	3.9×10^{-5}	1×10^{-3}
	0.018 - 0.04	298	0.003	2×10^{-4}	1.5×10^{-5}	2×10^{-4}
$\lvert\Delta T_f\rvert$	0.004 - 0.04	271 - 273	0.1	2 mK	0.014 mK	2 mK
$\lvert\Delta\phi/\phi\rvert$	0.004 - 0.04	273	0.1	2×10^{-3}	- [a]	2×10^{-3}
	0.0017 - 0.038	298	0.1	2×10^{-3}	- [a]	2×10^{-3}
$\lvert\Delta c_p^S\rvert$	0 - 0.04	273 - 313	0.1	0.5 J kg^{-1} K^{-1}	- [a]	0.5 J kg^{-1} K^{-1}
$\lvert\Delta c_p\rvert$	0 - 0.12	273 - 353	0.1	4 J kg^{-1} K^{-1}	1.3 J kg^{-1} K^{-1}	4.2 J kg^{-1} K^{-1}

[a] This quantity is only a function of the salinity of the fundamental equation for seawater.

Calculating the Phase Equilibrium between Seawater and Water Vapor

Criteria for the phase equilibrium

$$\mu_W(p,T,S) = g^{vap}(p,T)$$

Chemical potential of water in seawater: $\mu_W(p,T,S) = g - S\,g_S$

Free Gibbs energy of pure water vapor from IAPWS-IF97, region 2 [2]: $g^{vap}(p,T) = g_2^{97}(p,T)$

The boiling temperature can then be calculated iteratively from: $T_b = T = f(p,S)$

The specific Gibbs energy for the two-phase mixture of brine and vapor is calculated for:

- Saturated seawater liquid: $g(p,T_b,S)$,
- Pure water vapor: $g_2^{97}(p,T_b)$.

The following equation for calculating the specific enthalpy h thus results for this two-phase mixture (BV - Brine Vapor) as follows:

$$h^{BV}(p,T,S) = (1-x)\,h(p,T,S_b) + x\,h^{vap}(p,T),$$

whereas x is the vapor fraction with $x = 1 - S / S_b(p,T)$
and S_b is the salinity of the saturated seawater of the brine.

Comparing the Computing Time

- Using the "computing time ratio" CTR

$$CTR = \frac{\text{computing time for IAPWS 2008}}{\text{computing time for IAPWS 2013}}$$

- Resulting CTR values for calculating selected properties of seawater according to the table on the right

Property	CTR
Specific volume v	243
Specific enthalpy h	236
Specific entropy s	220
Specific isobaric heat capacity c_p	430
Chemical potential of water in seawater μ_W	134
Boiling temperature of seawater T_b	206
Freezing temperature of seawater T_f	32

The calculations are on average 200 times faster with the new IAPWS Industrial Standard for seawater IAPWS 2013 compared to the scientific formulation IAPWS 2008.

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- Fundamentals: IAPWS Industrial Formulation 2013 [1] and algorithms according to the Fichtner-Handbook [4]
- Range of validity extended by equations of the Fichtner-handbook up to p = 100 MPa, T = 493.15 K (t = 200 °C) and S = 200 g kg^{-1}
- Calculation of liquid seawater, two-phase mixture seawater and water vapor as well as pure water vapor
- 40 functions for calculating thermodynamic properties, transport properties, backward functions and derivatives
- Add-ons available for Excel®, MATLAB®, Mathcad®, Engineering Equation Solver® (EES), LabVIEW™, DYMOLA®, and SimulationX® (Modelica)

References

[1] IAPWS: Advisory Note No. 5: Industrial Calculation of the Thermodynamic Properties of Seawater (2013).
[2] IAPWS: Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (The Revision only Relates to the Extension of Region 5 to 50 MPa) (2007).
[3] IAPWS: Release on the IAPWS Formulation 2008 for the Thermodynamic Properties of Seawater (2008).
[4] H. E. Hömig: Fichtner-Handbook, Vulkan-Verlag, Dr. W. Classen, Essen (1978).