Proposal
Advisory Note No. 5:
Thermodynamic Properties of Seawater for Industrial Use

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1. Motivation

Initial Situation

"Release on the IAPWS Formulation 2008 for the Thermodynamic Properties of Seawater"

Gibbs free energy equation

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

Water part calculated from IAPWS-95 Helmholtz free energy equation $f^{95}(T,v)$

Saline part

$$g^{\mathrm{W}}(p,T) = f^{95}(T,v) - v \cdot \left[\frac{\partial f^{95}(T,v)}{\partial v}\right]_T$$

where v is calculated from $p = -\left[\frac{\partial f^{95}(T,v)}{\partial v}\right]_T$ by iteration

⇨ Industry is interested in calculating the water part from IAPWS-IF97 because of the consistency with other calculations, and computing speed.

Report

K. Miyagawa:
"IAPWS-IF97 for the Water Part of the EOS for Seawater" (2008).

It describes the impact when using IAPWS-IF97 instead of IAPWS-95

Main Result: IAPWS-IF97 can be used

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Discussions in SC SW and in WGs IRS and TPWS at the last IAPWS Meetings

→ What way would be the best for preparing an Industrial Formulation on Seawater Properties

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Result: An Advisory note would be fine for colleagues from the industry

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Therefore: Proposal for an Advisory Note No. 5:
Thermodynamic Properties of Seawater for Industrial Use

Remark

The "IAPWS Supplementary Release on a Computationally Efficient Thermodynamic Formulation for Liquid Water for Oceanographic Use"
is not used because of industrial purposes.

2. Thermodynamic Properties

Gibbs free energy equation for seawater

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

water part calculated from IAPWS-IF97 region 1 equation

saline part calculated from IAPWS Formulation 2008

$$g^{W} = g_1^{97}(p,T)$$

where the salinity *S* represents the mass fraction of salt in seawater

$$S = \frac{m_{\mathrm{S}}}{m_{\mathrm{W}} + m_{\mathrm{S}}}$$

The composition of salt is based on the Reference Composition scale of Standard Seawater.

All thermodynamic properties can be calculated from $g(p,T,S)$.

Property	Calculation from $g(p,T,S)$
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	$c_p(p,T,S)=-T\,g_{TT}$
Cubic isobaric expansion coefficient	$\alpha_v(p,T,S)=\dfrac{g_{pT}}{g_p}$
Isothermal compressibility	$\kappa_T(p,T,S)=-\dfrac{g_{pp}}{g_p}$
Speed of sound	$w(p,T,S)=g_p\sqrt{\dfrac{g_{TT}}{\left(g_{Tp}^2-g_{pp}\,g_{TT}\right)}}$
Chemical potential of water	$\mu_W(p,T,S)=g-S\cdot g_S$
Osmotic coefficient	$\phi(p,T,S)=-\dfrac{g^S-S\,g_S}{b\,R_m\,T}$

3. Colligate Properties

3.1 Phase Equilibrium between Seawater and Water Vapor

Phase equilibrium condition

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

chemical potential of water in seawater

Gibbs free enthalpy of water vapor, calculated from IAPWS-IF97 region 2 equation

$$g^{vap}(p,T)=g_2^{97}(p,T)$$

Calculation of the saturation (boiling) temperature

$$T_S=f(p,S)$$

At an equilibrium state, properties are calculated:

Liquid seawater (brine) phase	$g(p,T,S)$
Water vapor phase	$g_2^{97}(p,T)$

3.2 Phase Equilibrium between Seawater and Ice

Phase equilibrium condition

$$\mu_W\left(p,T,S\right) = g^{\mathrm{Ih}}\left(p,T\right)$$

chemical potential of water in seawater

Gibbs free enthalpy of ice Ih, calculated from IAPWS formulation of 2006

Calculation of the freezing temperature

$$T_m = \mathrm{f}(p,S)$$

At an equilibrium state, properties are calculated:

Liquid seawater (brine) phase	$g(p,T,S)$
Ice phase	$g^{\mathrm{Ih}}(p,T)$

3.3 Further Properties

– Triple-point temperatures and pressures
– Osmotic pressure
– Properties of sea ice

4. Range of Validity

Corresponding to the IAPWS Formulation 2008

Pressure:	0.3 kPa … 100 MPa
Temperature:	261 K … 353 K
Salinity:	0 … 0.12 kg kg^{-1}

with restrictions in certain regions according to IAPWS-2008

5. Uncertainty

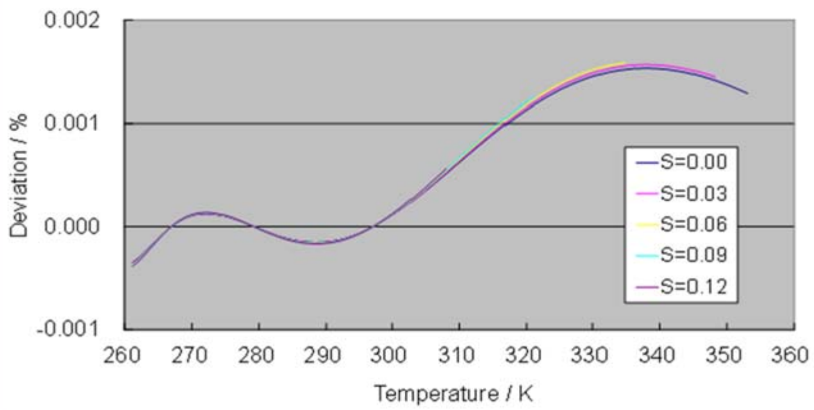
Report of K. Miyagawa, (2008) and an Update (2012)

U Uncertainty of Industrial Formulation	=	U_{08} Uncertainty of IAPWS-2008	+	Δ_{RMS} Difference between IAPWS-IF97 and IAPWS-95

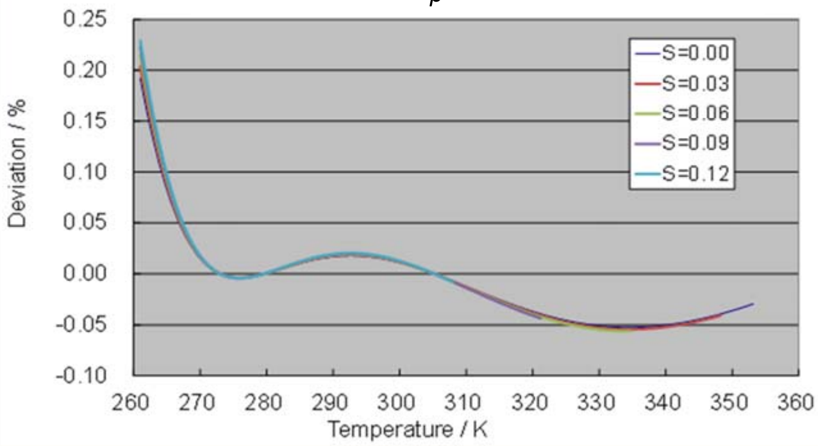
Determination of the uncertainty of a certain property

$$u = \sqrt{u_{08}^2 + \Delta_{RMS}^2}$$

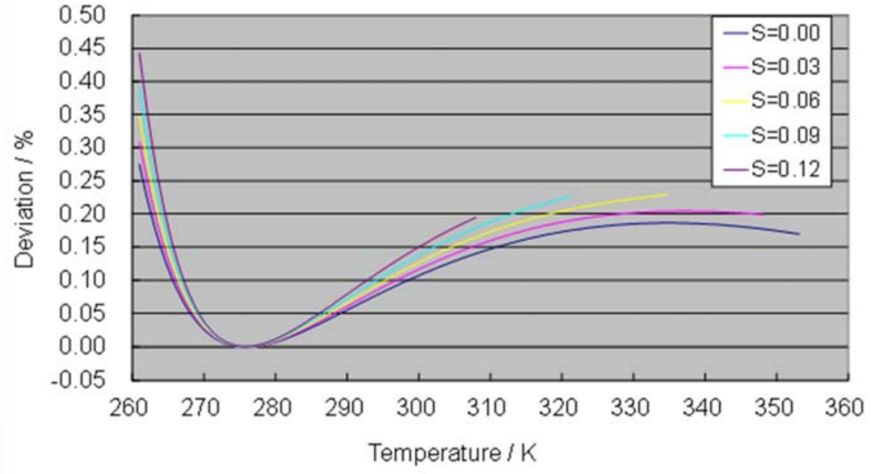
Deviation of ρ at 0.101325 MPa



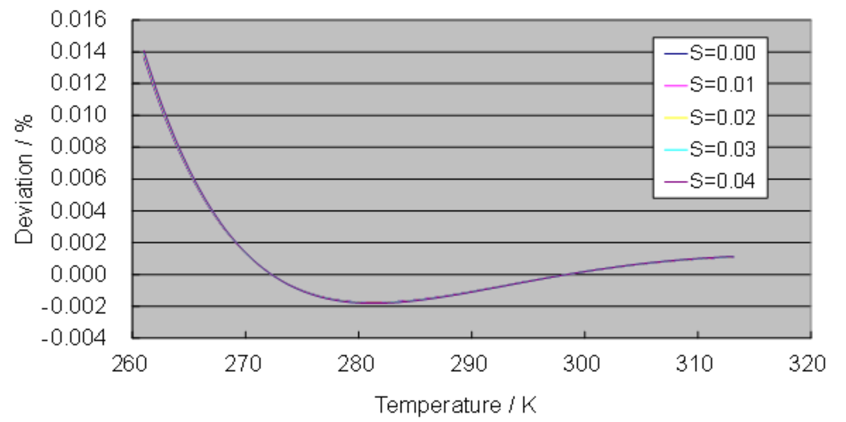
Deviation of c_p at 0.101325 MPa



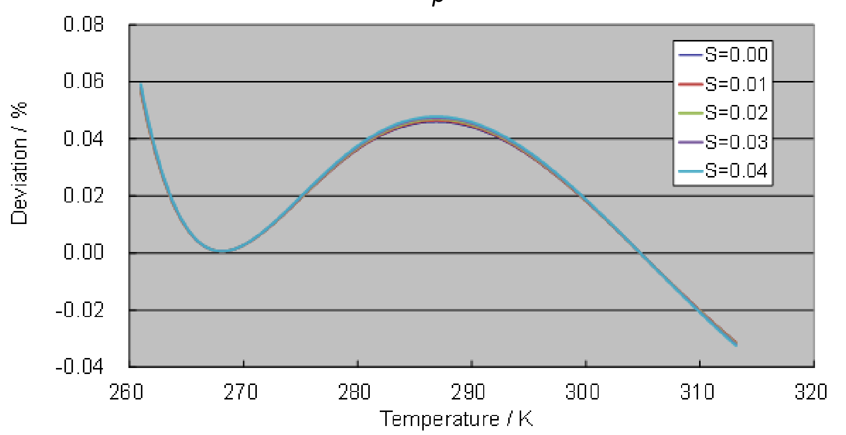
Deviation of *w* at 0.101325 MPa

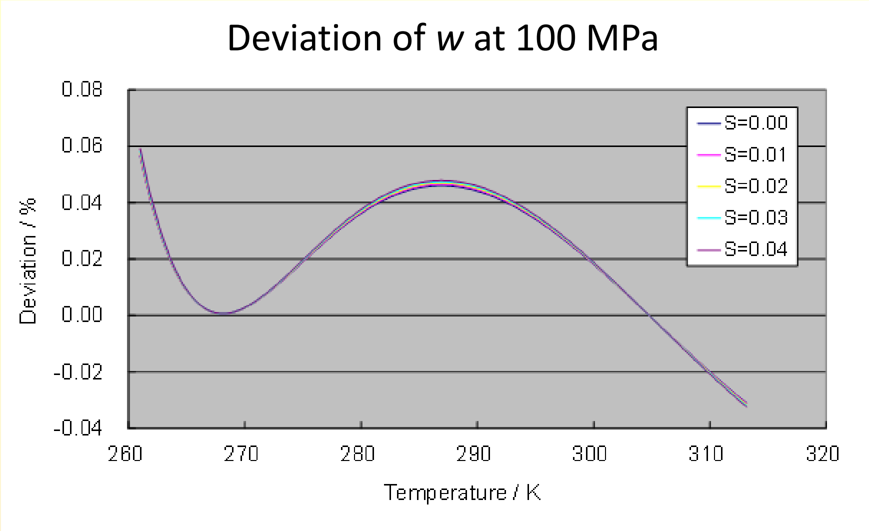


Deviation of ρ at 100 MPa



Deviation of c_p at 100 MPa





Uncertainties

Quantity	S interval kg kg^{-1}	T interval K	p interval MPa	u_{08}	Δ_{RMS}	u
$\left\|\frac{\Delta\rho}{\rho}\right\|$	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	0.1 - 10	1×10^{-5}	2.6×10^{-6}	1×10^{-5}
	0.005 - 0.04	273 - 313	10 - 100	2×10^{-5}	5.3×10^{-6}	2×10^{-5}
	0.04 - 0.12	293 - 313	0.1	3×10^{-4}	4.2×10^{-6}	3×10^{-4}
	0 - 0.04	313 - 333	0.1	4×10^{-4}	1.3×10^{-5}	4×10^{-4}
	0.04 - 0.08	313 - 333	0.1	9×10^{-4}	1.3×10^{-5}	9×10^{-4}
	0 - 0.04	333 - 353	0.1	1.4×10^{-3}	1.5×10^{-5}	1.4×10^{-3}
	0.08 - 0.12	313 - 333	0.1	3×10^{-3}	1.3×10^{-5}	3×10^{-3}
	0.04 - 0.08	333 - 353	0.1	4×10^{-3}	1.5×10^{-5}	4×10^{-3}
	0.08 - 0.12	333 - 353	0.1	1.3×10^{-2}	1.6×10^{-5}	1.3×10^{-2}
$\left\|\Delta\alpha_v\right\|$	0.01 - 0.03	267 - 274	0.7 - 33	6×10^{-7} K^{-1}	1×10^{-6} K^{-1}	1×10^{-6} K^{-1}

Uncertainties

Quantity	S interval kg kg^{-1}	T interval K	p interval MPa	u_{08}	Δ_{RMS}	u
$\left\lvert\frac{\Delta w}{w}\right\rvert$	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}
$\left\lvert\frac{\Delta p^{vap}}{p^{vap}}\right\rvert$	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
$\lvert\Delta T_b\rvert$	0.006 - 0.07	333 - 353	0.02 - 0.05	2 mK	1.2 mK	2.3 mK
$\left\lvert\frac{\Delta\phi}{\phi}\right\rvert$	0.004 - 0.04	273	0.1	2×10^{-3}	- [e]	2×10^{-3}
	0.0017 - 0.038	298	0.1	2×10^{-3}	- [e]	2×10^{-3}
	0.01 - 0.12	273 - 278	0.1	3×10^{-3}	- [e]	3×10^{-3}
$\lvert\Delta c_p^S\rvert$	0 - 0.04	273 - 313	0.1	0.5 J kg^{-1} K^{-1}	- [e]	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}

[e] The quantity is only dependent on the saline part of Eq. (1).

6. Computing Time Consumption

Estimation of Kiyoshi Miyagawa

→ Computing time ratio of a property

$$\mathrm{CTR} = \frac{\text{computing time of IAPWS-2008}}{\text{computing time of this Industrial Formulation}} \cong 67$$

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The industrial formulation for seawater is in average 67 times faster than IAPWS-2008

7. Summary

The Draft Advisory Note No. 5 :

Thermodynamic Properties of Seawater for Industrial Use

is completed.

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If SC SW and WGs TPWS and IRS, agree
an Evaluation Task Group can be appointed.