Proposal
Advisory Note No. 5:
Industrial Calculation of the Thermodynamic Properties of Seawater

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Contents

1. The IAPWS Formulation 2008

Initial Situation

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

Equation of State

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

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

Saline part

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

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.

2. Proposal for the Industrial Formulation
2.1 Fundamental Equation

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

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

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	$\alpha_v(p,T,S) = \frac{g_{pT}}{g_p}$
Isothermal compressibility	$\kappa_T(p,T,S) = -\frac{g_{pp}}{g_p}$
Speed of sound	$w(p,T,S) = g_p \sqrt{\frac{g_{TT}}{\left(g_{Tp}^2 - g_{pp}\,g_{TT}\right)}}$
Chemical potential of water	$\mu_{\mathrm{W}}(p,T,S) = g - S \cdot g_S$
Osmotic coefficient	$\phi(p,T,S) = -\frac{g^{\mathrm{S}} - S\,g_S}{b\,R_{\mathrm{m}}\,T}$

2.2 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 energy 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

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

2.3 Further Properties

- Phase equilibrium between seawater and ice
- Triple-point temperatures and pressures
- Osmotic pressure
- Properties of sea ice

3. 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

4. Computing Time Consumption

Estimation of Kiyoshi Miyagawa

→ Computing time ratio of a property

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

⇩

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

5. Current State of the Evaluation

Evaluation Task Group: A. Singh (Chair), F. Blangetti, K. Orlov, I. Weber

Subjects:

a) Title:
- Proposal for Boulder:
  "Thermodynamic Properties of Seawater for Industrial Use"
- Proposal for Evaluation:
  "The IAPWS Industrial Formulation for the Thermodynamic Properties of Seawater"
- Proposal of A. Harvey:
  "Industrial Calculation of the Thermodynamic Properties of Seawater"

b) Errors in Table 2:

$$g^{\mathrm{W}} = R_{\mathrm{W}} T \gamma\,, \qquad \left(\frac{\partial g^{\mathrm{W}}}{\partial p}\right)_T = \frac{R_{\mathrm{W}} T}{p} \pi \gamma_\pi\,, \qquad \left(\frac{\partial^2 g^{\mathrm{W}}}{\partial p^2}\right)_T = \frac{R_{\mathrm{W}} T}{p^2} \pi^2 \gamma_{\pi\pi}\,,$$

$$\left(\frac{\partial g^{\mathrm{W}}}{\partial T}\right)_p = R_{\mathrm{W}} \left(\gamma - \tau \gamma_\tau\right)\,, \qquad \left(\frac{\partial^2 g^{\mathrm{W}}}{\partial T^2}\right)_p = \frac{R_{\mathrm{W}}}{T} \tau^2 \gamma_{\tau\tau}\,, \qquad \left(\frac{\partial^2 g^{\mathrm{W}}}{\partial p \partial T}\right) = \frac{R_{\mathrm{W}} \pi}{p} \left(\gamma_\pi - \tau \gamma_{\pi\tau}\right)$$

c) Syntax of Several Equations:
   - Proposal of K. Orlov

d) Symbols
   Examples:
   - g^{W} for the water part of the Gibbs free energy equation
   - g^{S} for the saline part of the Gibbs free energy equation

The Industrial Formulation for Seawater can be adopted by IAPWS at the Annual Meeting in Greenwich this year.