1. Introduction

- The International Association for the Properties of Water and Steam (IAPWS) adopted the "Advisory Note No. 5: Industrial Calculation of the Thermodynamic Properties of Seawater" as an international standard at its conference in London (2013).

- The following institutions and companies were involved in the development:
  - Zittau/Goerlitz University of Applied Sciences, Germany
  - Leibniz Institute for Baltic Sea Research, Rostock, Germany
  - Ruhr University of Bochum, Germany
  - K. Miyagawa, Tokyo, Japan
  - NIST, Boulder, USA
  - Queen Mary, University of London, England
  - Alstom Power, Baden, Switzerland
  - Moscow Power Engineering Institute, Russia
  - Siemens Energy Sector, Erlangen, Germany
  - General Electric, Power & Water, Schenectady, USA
In addition, there is a scientific standard for calculating thermodynamic properties of seawater, the IAPWS-2008 Formulation.

The difference between both formulations is the calculation of the pure water part:

- **IAPWS-2008 Scientific Formulation**
  - Scientific Formulation IAPWS-95
- **IAPWS Industrial Formulation 2013**
  - Industrial Formulation IAPWS-IF97

The reasons for developing an industrial formulation were:

1. The IAPWS-95 is computationally intensive because it consists of an Helmholtz equation as a function of \((T, \rho)\) and therefore all properties have to be calculated iteratively.
   → Computing speed is important for modeling and optimizing of processes, e.g., desalination processes.

2. The IAPWS-IF97 is used by industry for calculating properties of pure steam and water.
   → When using IAPWS-IF97 for seawater, the crossover of the calculations to pure water will be consistent.

### 2. Description of the IAPWS Industrial Formulation for Seawater

#### 2.1 Fundamental Equation

Gibbs free energy equation for seawater

\[
g(p, T, S) = g^W(p, T) + g^S(p, T, S)
\]

Water part calculated from IAPWS-IF97 region 1 equation

\[
g^W = g_{197}^W(p, T)
\]

Saline part calculated from IAPWS Formulation 2008

\[
g^S = g_{08}^S(p, T, S)
\]

The salinity \(S\) represents the mass fraction of sea salt in seawater

\[
S = \frac{m_S}{m}
\]

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

All thermodynamic properties can be calculated from the fundamental equation \(g(p, T, S)\) and its derivatives for \(p, T,\) and \(S.\)
<table>
<thead>
<tr>
<th>Property</th>
<th>Calculation from $g(p,T,S)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific volume</td>
<td>$v(p,T,S) = g_p$</td>
</tr>
<tr>
<td>Specific enthalpy</td>
<td>$h(p,T,S) = g - T g_T$</td>
</tr>
<tr>
<td>Specific entropy</td>
<td>$s(p,T,S) = -g_T$</td>
</tr>
<tr>
<td>Specific isobaric heat capacity</td>
<td>$c_p(p,T,S) = -T g_{TTT}$</td>
</tr>
<tr>
<td>Cubic isobaric expansion coeff.</td>
<td>$\alpha_v(p,T,S) = \frac{g_{pT}}{g_p}$</td>
</tr>
<tr>
<td>Isothermal compressibility</td>
<td>$\kappa_T(p,T,S) = -\frac{g_{pp}}{g_p}$</td>
</tr>
<tr>
<td>Speed of sound</td>
<td>$w(p,T,S) = g_p \sqrt{\frac{g_{TT}}{(g_{pT}^2 - g_{pp} g_{TT})}}$</td>
</tr>
<tr>
<td>Chemical potential of water</td>
<td>$\mu_W(p,T,S) = g - S g_S$</td>
</tr>
<tr>
<td>Osmotic coefficient</td>
<td>$\phi(p,T,S) = -\frac{g^S - S g_S}{b R_m T}$</td>
</tr>
</tbody>
</table>
2.2 Phase Equilibrium between Seawater and Water Vapor

Phase equilibrium condition

\[ \mu_N(p, T, S) = g^{vap}(p, T) \]

Chemical potential of water in seawater

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

\[ g^{vap}(p, T) = g^{97}_2(p, T) \]

Calculation of the boiling temperature by iteration

\[ T_b = T = f(p, S) \]

Brine-vapor properties are calculated as follows:

- Liquid seawater (brine) phase \( g(p, T_b, S) \)
- Vapor phase \( g^{97}_2(p, T_b) \)

2.3 Further Properties

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

3. Range of Validity

Corresponding to the IAPWS 2008 Formulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>0.3 kPa … 100 MPa</td>
</tr>
<tr>
<td>Temperature</td>
<td>261 K … 353 K</td>
</tr>
<tr>
<td>Salinity</td>
<td>0 … 120 g / kg</td>
</tr>
</tbody>
</table>

with restrictions in certain regions according to IAPWS-2008
4. Uncertainty of the Industrial Formulation

The uncertainty of the Industrial Formulation IAPWS 2013 is comparable to that of the Scientific Formulation IAPWS 2008 and is sufficient for industrial use.
5. Computing Time Consumption

Comparison of the Computing time consumption by using the "Computing Time Ratio":

$$CTR = \frac{\text{computing time of IAPWS-2008}}{\text{computing time of the Industrial Formulation 2013}}$$

<table>
<thead>
<tr>
<th>Property</th>
<th>CTR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific volume</td>
<td>243</td>
</tr>
<tr>
<td>Specific enthalpy</td>
<td>236</td>
</tr>
<tr>
<td>Specific entropy</td>
<td>220</td>
</tr>
<tr>
<td>Specific isobaric heat capacity</td>
<td>430</td>
</tr>
<tr>
<td>Chemical potential of water in seawater</td>
<td>134</td>
</tr>
<tr>
<td>Boiling temperature of seawater</td>
<td>206</td>
</tr>
<tr>
<td>Freezing temperature of seawater</td>
<td>32</td>
</tr>
</tbody>
</table>

The IAPWS Industrial Formulation 2013 for seawater is in average 200 times faster than the scientific Formulation IAPWS-2008

6. Property Library LibSeaWa for Seawater

Used Algorithms:
- IAPWS Industrial Formulation 2013
- Fichtner Handbook of Hömig (1978) for extending the range of state and for calculating transport properties

Range of Validity:
- Pressure: 0.0023 … 100 MPa
- Temperature: 273 … 493 K
- Salinity: 0 … 200 g / kg

Ranges of State:
- Liquid seawater
- Brine vapor (mixture of saturated seawater and vapor)
- Vapor (pure water)

Property Functions:
- Thermodynamic properties
- Transport properties
- Backward functions
- Thermodynamic derivatives

(40 functions)

Interface Programs:
- FluidEXL for Excel®
- FluidLAB for MATLAB®
- FluidMAT for Mathcad®
- FluidEES for Engineering Equation Solver (EES)®
- FluidVIEW for LabVIEW™
- FluidDYM for DYMOLA and SimulationX (Modelica)®
7. Summary

➢ There is a new international standard for calculating the thermodynamic properties of seawater for modeling processes using seawater, e.g., desalination processes: "IAPWS Advisory Note No. 5: Industrial Calculation of the Thermodynamic Properties of Seawater" (IAPWS 2013).

Available at: www.iapws.org, under "Releases and Guidelines"

➢ The paper "The IAPWS Industrial Formulation for the Thermodynamic Properties of Seawater" has been published: Desalination and Water Treatment 55, 1177-1199 (2015).

➢ For calculating seawater properties, the property library LibSeaWa can be used in Excel, MATLAB, Mathcad, EES, LabVIEW, DYMOLA and SimulationX.

More information at: www.thermodynamics-zittau.de, under "Property Libraries"

This presentation is available at: www.thermodynamics-zittau.de, under "News"