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The IAPWS industrial formulation for the thermodynamic properties of seawater

Hans-Joachim Kretzschmar[a,*], Rainer Feistel[b], Wolfgang Wagner[c], Kiyoshi Miyagawa[d], Allan H. Harvey[e], Jeff R. Cooper[f], Michael Hiegemann[g], Francisco L. Blangetti[g], Konstantin A. Orlov[h], Ingo Weber[i], Anurag Singh[j], Sebastian Herrmann[a]

[a]*Zittau/Goerlitz University of Applied Sciences, Zittau, Germany, Tel. +49 3583 61 1846; email: hj.kretzschmar@hszg.de (H.-J. Kretzschmar), Tel. +49 3583 61 1817; email: s.herrmann@hszg.de (S. Herrmann)*
[b]*Baltic Sea Research Institute, Warnemuende, Germany, Tel. +49 381 5197 152; email: rainer.feistel@io-warnemuende.de*
[c]*Ruhr-University Bochum, Bochum, Germany, Tel. +49 234 32 29033; email: wagner@thermo.rub.de*
[d]*Nishiogu Arakawa-ku, Tokyo 116-0011, Japan, Tel. +81 3 3894 7039; email: miyagawa.kiyoshi@nifty.com*
[e]*National Institute of Standards and Technology, Boulder, CO, USA, Tel. +1 303 497 3555; email: allan.harvey@nist.gov*
[f]*Queen Mary, University of London, London, England, Tel. +44 20 7882 4313; email: j.r.cooper@qmul.ac.uk*
[g]*ALSTOM (Switzerland) Ltd, Baden, Switzerland, Tel. +41 56 205 2104; email: michael.hiegemann@power.alstom.com (M. Hiegemann), Tel. +41 56 205 6628; email: francisco.blangetti@power.alstom.com (F.L. Blangetti)*
[h]*Moscow Power Engineering Institute, Moscow, Russia, Tel. +7 495 362 71 71; email: orlov@twt.mpei.ru*
[i]*Siemens AG, Energy Sector, Erlangen, Germany, Tel. +49 9131 18 6603; email: ingo.iw.weber@siemens.com*
[j]*General Electric, Power and Water, Schenectady, NY, USA, Tel. +1 518 385 7274; email: anurag.singh@ge.com*

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ABSTRACT

In 2008, the International Association for the Properties of Water and Steam (IAPWS) adopted a standard formulation for the thermodynamic properties of seawater as a sum of contributions to the Gibbs free energy from pure water and from dissolved sea salt. For pure water, the IAPWS formulation for general and scientific use (IAPWS-95) was used. However, for industrial uses such as desalination and seawater power-plant cooling, it is likely to be more convenient to use the computationally simpler IAPWS formulation for industrial use (IAPWS-IF97), which is standard in the steam power industry. This paper documents this approach and gives formulas for calculating thermodynamic properties of seawater and steam (volume, enthalpy, isobaric heat capacity, etc.). The calculation of colligative properties (such as boiling and freezing points and osmotic pressure) is also described, as is the calculation of properties of two-phase states such as brine-vapor and brine-ice (sea ice). The computing speeds for these calculations are faster than those using IAPWS-95 by factors on the order of 100–200. The use of IAPWS-IF97 instead of IAPWS-95 for industrial seawater calculations is endorsed in IAPWS Advisory Note No. 5: Industrial Calculation of the Thermodynamic Properties of Seawater. This use is valid for IAPSO

*Corresponding author.

Table 1
Relations between the relevant thermodynamic properties of seawater and $g(p,T,S)$, Eq. (1), and its derivatives[a,b]

Property	Relation
Specific volume v	$v(p,T,S) = g_p$
Density $\rho = v^{-1}$	$\rho(p,T,S) = \frac{1}{g_p}$
Specific internal energy u	$u(p,T,S) = g - p\,g_p - T\,g_T$
Specific enthalpy $h = u + pv$	$h(p,T,S) = g - T\,g_T$
Specific entropy s	$s(p,T,S) = -g_T$
Specific isobaric heat capacity $c_p = c_p = (\partial h/\partial T)_p$	$c_p(p,T,S) = -T\,g_{TT}$
Specific isochoric heat capacity $c_v = (\partial u/\partial T)_v$	$c_v(p,T,S) = T\left(\frac{g_{pT}^2}{g_{pp}} - g_{TT}\right)$
Cubic isobaric expansion coefficient $\alpha_v = v^{-1}(\partial v/\partial T)_p$	$\alpha_v(p,T,S) = \frac{g_{pT}}{g_p}$
Isothermal compressibility $\kappa_T = -v^{-1}(\partial v/\partial p)_T$	$\kappa_T(p,T,S) = -\frac{g_{pp}}{g_p}$
Speed of sound $w = v\sqrt{-(\partial p/\partial v)_s}$	$w(p,T,S) = g_p\sqrt{\frac{g_{TT}}{(g_{pT}^2 - g_{pp}g_{TT})}}$
Isentropic exponent $\kappa = -vp^{-1}(\partial p/\partial v)_s$	$\kappa(p,T,S) = \frac{1}{p}\frac{g_p g_{TT}}{(g_{pT}^2 - g_{pp}g_{TT})}$
Relative chemical potential $\mu = (\partial g/\partial S)_{p,T}$	$\mu(p,T,S) = g_S$
Chemical potential of water $\mu_W = g - S\,\mu$	$\mu_W(p,T,S) = g - S\,g_S$
Chemical potential of sea salt $\mu_S = \mu + \mu_W$	$\mu_S(p,T,S) = g + (1-S)g_S$
Osmotic coefficient $\phi = (g^W - \mu_W)b^{-1}R_m^{-1}T^{-1}$	$\phi(p,T,S) = -\frac{(g^S - S\,g_S)}{b\,R_m\,T}$
Haline contraction coefficient $\beta = \rho^{-1}(\partial\rho/\partial S)_{p,T}$	$\beta(p,T,S) = -\frac{g_{pS}}{g_p}$

[a] $g_p = \left(\frac{\partial g}{\partial p}\right)_{T,S} = \left(\frac{\partial g^W}{\partial p}\right)_T + \left(\frac{\partial g^S}{\partial p}\right)_{T,S}$, $g_{pp} = \left(\frac{\partial^2 g}{\partial p^2}\right)_{T,S} = \left(\frac{\partial^2 g^W}{\partial p^2}\right)_T + \left(\frac{\partial^2 g^S}{\partial p^2}\right)_{T,S}$, $g_T = \left(\frac{\partial g}{\partial T}\right)_{p,S} = \left(\frac{\partial g^W}{\partial T}\right)_p + \left(\frac{\partial g^S}{\partial T}\right)_{p,S}$, $g_{TT} = \left(\frac{\partial^2 g}{\partial T^2}\right)_{p,S} = \left(\frac{\partial^2 g^W}{\partial T^2}\right)_p + \left(\frac{\partial^2 g^S}{\partial T^2}\right)_{p,S}$, $g_{pT} = \left(\frac{\partial^2 g}{\partial p\partial T}\right)_S = \left(\frac{\partial^2 g^W}{\partial p\partial T}\right) + \left(\frac{\partial^2 g^S}{\partial p\partial T}\right)_S$, $g_S = \left(\frac{\partial g}{\partial S}\right)_{p,T} = \left(\frac{\partial g^S}{\partial S}\right)_{p,T}$, $g_{pS} = \left(\frac{\partial^2 g}{\partial p\partial S}\right)_T = \left(\frac{\partial^2 g^S}{\partial p\partial S}\right)_T$.

[b] The value of the molar gas constant $R_m = 8.314\ 472$ kJ kmol^{-1} K^{-1} was taken from CODATA 2006 [18] and is used in the 2008 IAPWS formulation for seawater.

Numerical check values for the water contribution computed from $g^W(p,T)$, Eq. (4), and its derivatives, for the seawater properties computed from the Gibbs function $g(p,T,S)$, Eq. (1), and its derivatives as well as for selected seawater properties of Table 1 at given points (p,T,S) are given in Table A1.

2.3. Saline contribution

The saline contribution of Eq. (1) is calculated from the Gibbs free energy equation of the IAPWS formulation for seawater properties [1].

$$\frac{g^S(p,T,S)}{g^*} = \sum_{k=0}^{5}\sum_{j=0}^{6}\left(n_{1jk}\xi^2\ln\xi + \sum_{i=2}^{7} n_{ijk}\xi^i\right)(\theta-\theta_0)^j(\pi-\pi_0)^k \tag{5}$$

where the reduced pressure is $\pi = p/p^*$, the reduced atmospheric pressure is $\pi_0 = p_0/p^*$, the reduced temperature is $\theta = T/T^*$, the reduced Celsius zero-point temperature is $\theta_0 = T_0/T^*$, and the square root of the reduced salinity is $\xi = \sqrt{S/S^*}$. The values of the