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Numerical implementation and oceanographic application of the thermodynamic potentials of liquid water, water vapour, ice, seawater and humid air – Part 1: Background and equations

R. Feistel[1], D.G. Wright[2], D.R. Jackett[3], K. Miyagawa[4], J.H. Reissmann[5], W. Wagner[6], U. Overhoff[6], C. Guder[6], A. Feistel[7] and G.M. Marion[8]

[1]Leibniz-Institut für Ostseeforschung, Seestraße 15, D-18119 Warnemünde, Germany
[2]Bedford Institute of Oceanography, Dartmouth, NS B2Y 4A2, Canada
[3]CSIRO Marine and Atmospheric Research, GPO Box 1538, Hobart, TAS 7001, Australia
[4]4-12-11-628, Nishiogu, Arakawa-ku, Tokyo 116-0011, Japan
[5]Bundesamt für Seeschifffahrt und Hydrographie, Bernhard-Nocht-Straße 78, 20359 Hamburg, Germany
[6]Ruhr-Universität Bochum, Lehrstuhl für Thermodynamik, D-44780 Bochum, Germany
[7]Technische Universität Berlin, Einsteinufer 25, D-10587 Berlin, Germany
[8]Desert Research Institute, Reno, NV, USA

In this supplement, tables with groups of thermodynamic properties are summarized, corresponding to the particular section number of the main text, as given in the table caption. The names of available library routines for the property are set in a distinct font type.
The implemented potential functions are reported in Table 1 of the paper.

Table S1: Conversion functions between molar and mass fractions of humid air, section 2.4. Here, $M_\mathrm{A} = 0.02896546$ kg mol^{-1} is the currently best value of the molar mass of dry air, and $M_\mathrm{W} = 0.018015268$ kg mol^{-1} is the molar mass of pure water. In the original dry-air formulation of Lemmon et al. (2000) and in the SIA version 1.0, the older value of M_A = 28.958 6 g mol^{-1} was used.

Quantity Library function	Formula	SI Unit	Eq.
Molar mass of humid air `air_molar_mass_si`	$M_\mathrm{AV} = \dfrac{1}{(1-A)/M_\mathrm{W} + A/M_\mathrm{A}}$	$\dfrac{\mathrm{kg}}{\mathrm{mol}}$	(S1.1)
Mass fraction of dry air `air_massfraction_air_si`	$A = \dfrac{x_\mathrm{A}}{1-(1-x_\mathrm{A})(1-M_\mathrm{W}/M_\mathrm{A})}$	$\dfrac{\mathrm{kg}}{\mathrm{kg}}$	(S1.2)
Mass fraction of vapour `air_massfraction_vap_si`	$1-A = \dfrac{1-x_\mathrm{A}}{1-x_\mathrm{A}(1-M_\mathrm{A}/M_\mathrm{W})}$	$\dfrac{\mathrm{kg}}{\mathrm{kg}}$	(S1.3)
Mole fraction of air `air_molfraction_air_si`	$x_\mathrm{A} = \dfrac{A(M_\mathrm{W}/M_\mathrm{A})}{1-A(1-M_\mathrm{W}/M_\mathrm{A})}$	$\dfrac{\mathrm{mol}}{\mathrm{mol}}$	(S1.4)
Mole fraction of vapour `air_molfraction_vap_si`	$1-x_\mathrm{A} = \dfrac{1-A}{1-A(1-M_\mathrm{W}/M_\mathrm{A})}$	$\dfrac{\mathrm{mol}}{\mathrm{mol}}$	(S1.5)

Table S2: Properties derived from the Helmholtz function $f^{\mathrm{F}}(T,\rho)$ of fluid water, section 3.1.

Quantity Library function	Formula	SI Unit	Eq.
Specific isobaric heat capacity flu_cp_si	$c_P = T\left[\frac{\left(f_{T\rho}^{\mathrm{F}}\right)^2 \rho}{2f_{\rho}^{\mathrm{F}} + \rho f_{\rho\rho}^{\mathrm{F}}} - f_{TT}^{\mathrm{F}}\right]$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S2.1)
Specific isochoric heat capacity flu_cv_si	$c_v = -T\, f_{TT}^{\mathrm{F}}$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S2.2)
Specific enthalpy flu_enthalpy_si	$h = f^{\mathrm{F}} - T f_{T}^{\mathrm{F}} + \rho f_{\rho}^{\mathrm{F}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S2.3)
Specific entropy flu_entropy_si	$\eta = -f_{T}^{\mathrm{F}}$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S2.4)
Thermal expansion coefficient flu_expansion_si	$\alpha = \frac{f_{T\rho}^{\mathrm{F}}}{2f_{\rho}^{\mathrm{F}} + \rho f_{\rho\rho}^{\mathrm{F}}}$	$\frac{1}{\mathrm{K}}$	(S2.5)
Specific Gibbs energy flu_gibbs_energy_si	$g = f^{\mathrm{F}} + \rho f_{\rho}^{\mathrm{F}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S2.6)
Specific internal energy flu_internal_energy_si	$u = f^{\mathrm{F}} - T f_{T}^{\mathrm{F}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S2.7)
Isentropic compressibility flu_kappa_s_si	$\kappa_s = \frac{f_{TT}^{\mathrm{F}} / \rho^2}{f_{TT}^{\mathrm{F}}\left(2f_{\rho}^{\mathrm{F}} + \rho f_{\rho\rho}^{\mathrm{F}}\right) - \rho\left(f_{T\rho}^{\mathrm{F}}\right)^2}$	$\frac{1}{\mathrm{Pa}}$	(S2.8)
Isothermal compressibility flu_kappa_t_si	$\kappa_T = \frac{1}{\rho^2\left(2f_{\rho}^{\mathrm{F}} + \rho f_{\rho\rho}^{\mathrm{F}}\right)}$	$\frac{1}{\mathrm{Pa}}$	(S2.9)
Adiabatic lapse rate flu_lapserate_si	$\Gamma = \frac{f_{T\rho}^{\mathrm{F}} / \rho}{\rho\left(f_{T\rho}^{\mathrm{F}}\right)^2 - f_{TT}^{\mathrm{F}}\left(2f_{\rho}^{\mathrm{F}} + \rho f_{\rho\rho}^{\mathrm{F}}\right)}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S2.10)
Absolute pressure flu_pressure_si	$P = \rho^2 f_{\rho}^{\mathrm{F}}$	Pa	(S2.11)
Sound speed flu_soundspeed_si	$c = \sqrt{\rho^2 \frac{f_{TT}^{\mathrm{F}} f_{\rho\rho}^{\mathrm{F}} - \left(f_{T\rho}^{\mathrm{F}}\right)^2}{f_{TT}^{\mathrm{F}}} + 2\rho f_{\rho}^{\mathrm{F}}}$	$\frac{\mathrm{m}}{\mathrm{s}}$	(S2.12)

Table S3. Properties derived from the Gibbs function $g^{\mathrm{Ih}}(T,P)$ of ice, section 3.2.

Quantity Library function	Formula	SI Unit	Eq.
Chemical potential ice_chempot_si	$\mu = g^{\mathrm{Ih}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S3.1)
Specific isobaric heat capacity ice_cp_si	$c_p = -T\, g_{TT}^{\mathrm{Ih}}$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S3.2)
Density ice_density_si	$\rho = \frac{1}{g_P^{\mathrm{Ih}}}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S3.3)
Specific enthalpy ice_enthalpy_si	$h = g^{\mathrm{Ih}} - T\, g_T^{\mathrm{Ih}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S3.4)
Specific entropy ice_entropy_si	$\eta = -g_T^{\mathrm{Ih}}$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S3.5)
Thermal expansion coefficient ice_expansion_si	$\alpha = \frac{g_{TP}^{\mathrm{Ih}}}{g_P^{\mathrm{Ih}}}$	$\frac{1}{\mathrm{K}}$	(S3.6)
Specific Helmholtz energy ice_helmholtz_energy_si	$f = g^{\mathrm{Ih}} - P\, g_P^{\mathrm{Ih}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S3.7)
Specific internal energy ice_internal_energy_si	$u = g^{\mathrm{Ih}} - T\, g_T^{\mathrm{Ih}} - P\, g_P^{\mathrm{Ih}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S3.8)
Isentropic compressibility ice_kappa_s_si	$\kappa_s = \frac{g_{TP}^{\mathrm{Ih}} g_{TP}^{\mathrm{Ih}} - g_{TT}^{\mathrm{Ih}} g_{PP}^{\mathrm{Ih}}}{g_P^{\mathrm{Ih}}\, g_{TT}^{\mathrm{Ih}}}$	$\frac{1}{\mathrm{Pa}}$	(S3.9)
Isothermal compressibility ice_kappa_t_si	$\kappa_T = -\frac{g_{PP}^{\mathrm{Ih}}}{g_P^{\mathrm{Ih}}}$	$\frac{1}{\mathrm{Pa}}$	(S3.10)
Adiabatic lapse rate ice_lapserate_si	$\Gamma = -\frac{g_{TP}^{\mathrm{Ih}}}{g_{TT}^{\mathrm{Ih}}}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S3.11)
Isochoric pressure coefficient ice_p_coefficient_si	$\beta = -\frac{g_{TP}^{\mathrm{Ih}}}{g_{PP}^{\mathrm{Ih}}}$	$\frac{\mathrm{Pa}}{\mathrm{K}}$	(S3.12)
Specific volume ice_specific_volume_si	$v = g_P^{\mathrm{Ih}}$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S3.13)

Table S4. Properties derived from the saline part $g^{\mathrm{S}}(S_{\mathrm{A}},T,P)$ of the Gibbs function of seawater, section 3.3.

Quantity Library function	Formula	SI Unit	Eq.
Activity coefficient sal_act_coeff_si	$\ln\frac{\gamma}{\gamma^{\mathrm{id}}} = \ln(1-S_{\mathrm{A}}) - S_{\mathrm{A}} + \frac{1}{g_1(T)}\sum_{i=3}^{7} g_i(T,P)\left[S_{\mathrm{A}} + \frac{i}{2}(1-S_{\mathrm{A}})\right]S_{\mathrm{A}}^{i/2-1}$	1	(S4.1)
Activity potential sal_act_potential_si	$\psi = \ln(1-S_{\mathrm{A}}) + \frac{1}{g_1(T)}\sum_{i=3}^{7} g_i(T,P)S_{\mathrm{A}}^{i/2-1}$	1	(S4.2)
Activity of water sal_activity_w_si	$a_{\mathrm{W}} = \exp\left\{\frac{g^{\mathrm{S}} - S_{\mathrm{A}}g_S^{\mathrm{S}}}{R_{\mathrm{W}}T}\right\}$	1	(S4.3)
Saline excess chemical potential sal_chempot_h2o_si	$\mu^{\mathrm{WS}} = g^{\mathrm{S}} - S_{\mathrm{A}}g_S^{\mathrm{S}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S4.4)
Relative chemical potential sal_chempot_rel_si	$\mu = g_S^{\mathrm{S}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S4.5)
Chemical coefficient sal_chem_coeff_si	$D_{\mathrm{S}} = S_A^2 g_{SS}^{\mathrm{S}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S4.6)
Dilution coefficient sal_dilution_si	$D = S_A g_{SS}^{\mathrm{S}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S4.7)
Mixing enthalpy sal_mixenthalpy_si	$\Delta h = h^{\mathrm{S}}(w_1S_1 + w_2S_2, T, P) - w_1h^{\mathrm{S}}(S_1,T,P) - w_2h^{\mathrm{S}}(S_2,T,P)$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S4.8)
Mixing entropy sal_mixentropy_si	$\Delta\eta = -g_T^{\mathrm{S}}(w_1S_1 + w_2S_2, T, P) + w_1g_T^{\mathrm{S}}(S_1,T,P) + w_2g_T^{\mathrm{S}}(S_2,T,P)$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S4.9)
Mixing volume sal_mixvolume_si	$\Delta v = g_P^{\mathrm{S}}(w_1S_1 + w_2S_2, T, P) - w_1g_P^{\mathrm{S}}(S_1,T,P) - w_2g_P^{\mathrm{S}}(S_2,T,P)$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S4.10)
Osmotic coefficient sal_osm_coeff_si	$\phi = -\frac{(g^{\mathrm{S}} - S_{\mathrm{A}}g_S^{\mathrm{S}})(1-S_{\mathrm{A}})}{S_{\mathrm{A}}R_{\mathrm{S}}T}$	1	(S4.11)
Specific enthalpy of sea salt sal_saltenthalpy_si	$h_{\mathrm{S}} = \frac{g^{\mathrm{S}} - Tg_T^{\mathrm{S}}}{S_{\mathrm{A}}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S4.12)
Specific entropy of sea salt sal_saltentropy_si	$\eta_{\mathrm{S}} = -\frac{g_T^{\mathrm{S}}}{S_{\mathrm{A}}}$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S4.13)
Specific volume of sea salt sal_saltvolume_si	$v_{\mathrm{S}} = \frac{g_P^{\mathrm{S}}}{S_{\mathrm{A}}}$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S4.14)

Table S5. Properties of humid air derived from the Helmholtz function $f^{\mathrm{AV}}(A,T,\rho)$, Eq. (2.7), section 3.4. Subscripts on f^{AV} indicate partial derivatives with respect to the natural independent variables A, T or ρ. Note that the adiabatic lapse rate is given with respect to pressure rather than altitude and refers to subsaturated humid air, often referred to as "dry-adiabatic" in the meteorological literature. The so-called "moist-adiabatic" lapse rate is given in section 5.8.

Quantity Library function	Formula	SI Unit	Eq.
Specific isobaric heat capacity air_f_cp_si	$c_P = T\left[\dfrac{\left(f_{T\rho}^{\mathrm{AV}}\right)^2\rho}{2f_\rho^{\mathrm{AV}}+\rho f_{\rho\rho}^{\mathrm{AV}}} - f_{TT}^{\mathrm{AV}}\right]$	$\dfrac{\mathrm{J}}{\mathrm{kg\,K}}$	(S5.1)
Specific isochoric heat capacity air_f_cv_si	$c_v = -T\,f_{TT}^{\mathrm{AV}}$	$\dfrac{\mathrm{J}}{\mathrm{kg\,K}}$	(S5.2)
Specific enthalpy air_f_enthalpy_si	$h = f^{\mathrm{AV}} - T f_T^{\mathrm{AV}} + \rho f_\rho^{\mathrm{AV}}$	$\dfrac{\mathrm{J}}{\mathrm{kg}}$	(S5.3)
Specific entropy air_f_entropy_si	$\eta = -f_T^{\mathrm{AV}}$	$\dfrac{\mathrm{J}}{\mathrm{kg\,K}}$	(S5.4)
Thermal expansion coefficient air_f_expansion_si	$\alpha = \dfrac{f_{T\rho}^{\mathrm{AV}}}{2f_\rho^{\mathrm{AV}}+\rho f_{\rho\rho}^{\mathrm{AV}}}$	$\dfrac{1}{\mathrm{K}}$	(S5.5)
Specific Gibbs energy air_f_gibbs_energy_si	$g = f^{\mathrm{AV}} + \rho f_\rho^{\mathrm{AV}}$	$\dfrac{\mathrm{J}}{\mathrm{kg}}$	(S5.6)
Specific internal energy air_f_internal_energy_si	$u = f^{\mathrm{AV}} - T f_T^{\mathrm{AV}}$	$\dfrac{\mathrm{J}}{\mathrm{kg}}$	(S5.7)
Isentropic compressibility air_f_kappa_s_si	$\kappa_s = \dfrac{f_{TT}^{\mathrm{AV}}/\rho^2}{f_{TT}^{\mathrm{AV}}\left(2f_\rho^{\mathrm{AV}}+\rho f_{\rho\rho}^{\mathrm{AV}}\right)-\rho\left(f_{T\rho}^{\mathrm{AV}}\right)^2}$	$\dfrac{1}{\mathrm{Pa}}$	(S5.8)
Isothermal compressibility air_f_kappa_t_si	$\kappa_T = \dfrac{1}{\rho^2\left(2f_\rho^{\mathrm{AV}}+\rho f_{\rho\rho}^{\mathrm{AV}}\right)}$	$\dfrac{1}{\mathrm{Pa}}$	(S5.9)
Adiabatic lapse rate air_f_lapserate_si	$\Gamma = \dfrac{f_{T\rho}^{\mathrm{AV}}/\rho}{\rho\left(f_{T\rho}^{\mathrm{AV}}\right)^2 - f_{TT}^{\mathrm{AV}}\left(2f_\rho^{\mathrm{AV}}+\rho f_{\rho\rho}^{\mathrm{AV}}\right)}$	$\dfrac{\mathrm{K}}{\mathrm{Pa}}$	(S5.10)
Absolute pressure air_f_pressure_si	$P = \rho^2 f_\rho^{\mathrm{AV}}$	Pa	(S5.11)
Sound speed air_f_soundspeed_si	$c = \sqrt{\rho^2\dfrac{f_{TT}^{\mathrm{AV}}f_{\rho\rho}^{\mathrm{AV}}-\left(f_{T\rho}^{\mathrm{AV}}\right)^2}{f_{TT}^{\mathrm{AV}}}+2\rho f_\rho^{\mathrm{AV}}}$	$\dfrac{\mathrm{m}}{\mathrm{s}}$	(S5.12)

Table S6: Partial derivatives of the Gibbs function of liquid water, $g^{\mathrm{W}}(T,P)$, section 4.1, expressed as partial derivatives of the Helmholtz function, $f^{\mathrm{F}}(T,\rho)$. Subscripts indicate partial derivatives with respect to the respective variables. Here, ρ is the density of liquid pure water at given *T* and *P*. The library function vap_g_si for vapour is defined equivalently with respect to f^{F} taken at the vapour density ρ.

Expression in $g^{\mathrm{W}}(T,P)$ Library function	Equivalent in $f^{\mathrm{F}}(T,\rho)$	Unit	Eq.
P	$\rho^2 f_\rho^{\mathrm{F}}$	Pa	(S6.1)
g^{W} liq_g_si	$f^{\mathrm{F}} + \rho f_\rho^{\mathrm{F}}$	$\mathrm{J\,kg^{-1}}$	(S6.2)
g_P^{W} liq_g_si	ρ^{-1}	$\mathrm{m^3 kg^{-1}}$	(S6.3)
g_T^{W} liq_g_si	f_T^{F}	$\mathrm{J\,kg^{-1}\,K^{-1}}$	(S6.4)
g_{PP}^{W} liq_g_si	$-\dfrac{1}{\rho^3\left(2f_\rho^{\mathrm{F}} + \rho f_{\rho\rho}^{\mathrm{F}}\right)}$	$\mathrm{m^3 kg^{-1}\,Pa^{-1}}$	(S6.5)
g_{TP}^{W} liq_g_si	$\dfrac{f_{T\rho}^{\mathrm{F}}}{\rho\left(2f_\rho^{\mathrm{F}} + \rho f_{\rho\rho}^{\mathrm{F}}\right)}$	$\mathrm{m^3 kg^{-1}\,K^{-1}}$	(S6.6)
g_{TT}^{W} liq_g_si	$f_{TT}^{\mathrm{F}} - \dfrac{\rho\left(f_{T\rho}^{\mathrm{F}}\right)^2}{\left(2f_\rho^{\mathrm{F}} + \rho f_{\rho\rho}^{\mathrm{F}}\right)}$	$\mathrm{J\,kg^{-1}\,K^{-2}}$	(S6.7)

Table S7a: Thermodynamic properties derived from the Gibbs function (4.4) of seawater, $g^{\mathrm{SW}}(S_{\mathrm{A}}, T, P)$, section 4.2, and its temperature, pressure and salinity derivatives. The superscript SW on g is suppressed for simplicity.

Quantity Library function	Formula	SI Unit	Eq.
Density sea_density_si	$\rho = g_P^{-1}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S7.1)
Specific entropy sea_entropy_si	$\eta = -g_T$	$\frac{\mathrm{J}}{\mathrm{kgK}}$	(S7.2)
Specific enthalpy sea_enthalpy_si	$h = g - T g_T$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S7.3)
Specific internal energy sea_internal_energy_si	$u = g - T g_T - P g_P$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S7.4)
Specific Helmholtz energy	$f = g - P g_P$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S7.5)
Specific isobaric heat capacity sea_cp_si	$c_P = -T g_{TT}$	$\frac{\mathrm{J}}{\mathrm{kgK}}$	(S7.6)
Specific isochoric heat capacity	$c_v = T\left(g_{TP}^2 - g_{TT} g_{PP}\right) / g_{PP}$	$\frac{\mathrm{J}}{\mathrm{kgK}}$	(S7.7)
Isothermal compressibility sea_kappa_t_si	$\kappa_T = -g_{PP} / g_P$	$\frac{1}{\mathrm{Pa}}$	(S7.8)
Isentropic compressibility sea_kappa_s_si	$\kappa_s = \left(g_{TP}^2 - g_{TT} g_{PP}\right) / \left(g_P g_{TT}\right)$	$\frac{1}{\mathrm{Pa}}$	(S7.9)
Sound speed sea_soundspeed_si	$c = g_P \sqrt{g_{TT} / \left(g_{TP}^2 - g_{TT} g_{PP}\right)}$	$\frac{\mathrm{m}}{\mathrm{s}}$	(S7.10)
Adiabatic lapse rate sea_lapserate_si	$\Gamma = -g_{TP} / g_{TT}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S7.11)
Chemical potential of water sea_chempot_h2o_si	$\mu^{\mathrm{W}} = g - S_{\mathrm{A}} g_S$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S7.12)
Chemical potential of sea salt	$\mu^{\mathrm{S}} = g + \left(1 - S_{\mathrm{A}}\right) g_S$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S7.13)
Barodiffusion ratio	$k_P = P\, g_{SP} / g_{SS}$	1	(S7.14)

Table S7b: Thermodynamic properties derived from the Gibbs function (4.4) of seawater, $g^{\mathrm{SW}}(S_{\mathrm{A}},T,P)$, section 4.2, and its temperature, pressure and salinity derivatives. The superscript SW on g is suppressed for simplicity. Thermal and haline contraction coefficients with respect to potential temperature and potential enthalpy are given here in terms of the Gibbs potential for completeness. A full discussion of these quantities is given in section 4.3. The potential Gibbs energy g^{θ} is defined as $g^{\theta} \equiv g(S_{\mathrm{A}},\theta,P_{\mathrm{r}})$ where θ is absolute potential temperature in kelvins and P_{r} is the associated absolute reference pressure in pascals.

Quantity Library function	Formula	SI Unit	Eq.
Thermal expansion coefficient sea_g_expansion_t_si	$\alpha = g_{TP} / g_{P}$	$\frac{1}{\mathrm{K}}$	(S7.15)
Thermal expansion coefficient w.r.t. potential temperature	$\alpha^{\theta} = \frac{g_{TP}\, g^{\theta}_{\theta\theta}}{g_{P}\, g_{TT}}$	$\frac{1}{\mathrm{K}}$	(S7.16)
Thermal expansion coefficient w.r.t. potential enthalpy	$\alpha^{h} = -\frac{g_{TP}}{g_{P}\, g_{TT}\, \theta}$	$\frac{\mathrm{kg}}{\mathrm{J}}$	(S7.17)
Haline contraction coefficient sea_g_contraction_t_si	$\beta = -g_{SP} / g_{P}$	1	(S7.18)
Haline contraction coefficient w.r.t. potential temperature	$\beta^{\theta} = \frac{g_{TP}\left(g_{ST} - g^{\theta}_{S\theta}\right) - g_{SP}\, g_{TT}}{g_{P}\, g_{TT}}$	1	(S7.19)
Haline contraction coefficient w.r.t. potential enthalpy	$\beta^{\Theta} = \frac{g_{TP}\left(g_{ST} - g^{\theta}_{S} / \theta\right) - g_{SP}\, g_{TT}}{g_{P}\, g_{TT}}$	1	(S7.20)

Table S8: Partial derivatives of the enthalpy potential function $h^{\mathrm{SW}}(S_{\mathrm{A}},\eta,P)$ of seawater, Eq. (4.5), section 4.3, expressed as partial derivatives of the Gibbs function $g^{\mathrm{SW}}(S_{\mathrm{A}},T,P)$ of seawater, Eq. (4.4). Subscripts indicate partial derivatives with respect to the respective variables. The superscripts SW on *g* and *h* are omitted for simplicity.

Expression in $h^{\mathrm{SW}}(S_{\mathrm{A}},\eta,P)$ Library function	Equivalent in $g^{\mathrm{SW}}(S_{\mathrm{A}},T,P)$	SI Unit	Eq.
η	$-g_T$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S8.1)
h sea_h_si	$g - Tg_T$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S8.2)
h_S sea_h_si	g_S	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S8.3)
h_η sea_h_si	T	K	(S8.4)
h_P sea_h_si	g_P	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S8.5)
h_{SS} sea_h_si	$\frac{g_{SS}g_{TT}-g_{ST}^2}{g_{TT}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S8.6)
$h_{S\eta}$ sea_h_si	$-\frac{g_{ST}}{g_{TT}}$	K	(S8.7)
h_{SP} sea_h_si	$\frac{g_{SP}g_{TT}-g_{ST}g_{TP}}{g_{TT}}$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S8.8)
$h_{\eta\eta}$ sea_h_si	$-\frac{1}{g_{TT}}$	$\frac{\mathrm{kg\,K}^2}{\mathrm{J}}$	(S8.9)
$h_{\eta P}$ sea_h_si	$-\frac{g_{TP}}{g_{TT}}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S8.10)
h_{PP} sea_h_si	$\frac{g_{TT}g_{PP}-g_{TP}^2}{g_{TT}}$	$\frac{\mathrm{m}^3}{\mathrm{kg\,Pa}}$	(S8.11)

Table S9: Thermodynamic properties derived from the enthalpy $h^{\mathrm{SW}}(S_{\mathrm{A}}, \eta, P)$ of seawater, Eq. (4.5), section 4.3, and its entropy, pressure and salinity derivatives. The superscripts SW on h is suppressed for simplicity. Entropy is available from in-situ temperature using Eq. (S8.1).

Quantity Library function	Formula	SI Unit	Eq.
Density	$\rho = \frac{1}{h_P}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S9.1)
Temperature `sea_temperature_si`	$T = h_\eta$	K	(S9.2)
Relative chemical potential	$\mu = h_S$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S9.3)
Specific Gibbs energy	$g = h - \eta h_\eta$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S9.4)
Specific internal energy	$u = h - P h_P$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S9.5)
Specific Helmholtz energy	$f = h - \eta h_\eta - P h_P$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S9.6)
Specific isobaric heat capacity	$c_P = \frac{T}{h_{\eta\eta}}$	$\frac{\mathrm{J}}{\mathrm{kgK}}$	(S9.7)
Isentropic compressibility	$\kappa_s = -\frac{h_{PP}}{h_P}$	$\frac{1}{\mathrm{Pa}}$	(S9.8)
Sound speed	$c = \frac{h_P}{\sqrt{-h_{PP}}}$	$\frac{\mathrm{m}}{\mathrm{s}}$	(S9.9)
Adiabatic lapse rate	$\Gamma = h_{\eta P}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S9.10)

Table S10: Thermodynamic properties derived from the enthalpy $h^{\mathrm{SW}}(S_{\mathrm{A}}, \eta, P)$ of seawater, Eq. (4.5), section 4.3, and its entropy, pressure and salinity derivatives. The superscripts SW on h is suppressed for simplicity. Note that potential temperature is given here as absolute potential temperature in the basic SI unit, K, rather than °C. Entropy is available from in-situ temperature or potential temperature, $\eta(S_{\mathrm{A}}, T, P) = \eta(S_{\mathrm{A}}, \theta, P_{\mathrm{r}})$, using Eq. (S7.2) which appears in the library as sea_entropy_si (S_{A}, T, P) or sea_entropy_si (S_{A}, θ, P_r). Entropy can also be determined from in-situ enthalpy or potential enthalpy, $\eta^{\mathrm{SW}}(S_{\mathrm{A}}, h, P) = \eta^{\mathrm{SW}}(S_{\mathrm{A}}, h^{\theta}, P_{\mathrm{r}})$, using Eq. (4.35) which appears in the library as sea_eta_entropy_si (S_{A}, h, P) or sea_eta_entropy_si (S_{A}, h^{θ}, P_r). The parameter η refers to entropy as the property (S7.2) derived from the Gibbs potential g^{SW} of seawater.

Quantity Library function	Formula	SI Unit	Eq.
Potential enthalpy sea_potenthalpy_si	h^{θ}	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S10.1)
Potential temperature sea_pottemp_si	$\theta = h^{\theta}_{\eta}$	K	(S10.2)
Potential density sea_potdensity_si	$\rho^{\theta} = \frac{1}{h^{\theta}_{P}}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S10.3)
Thermal expansion coefficient sea_h_expansion_t_si	$\alpha^{T} = \frac{h_{\eta P}}{h_P h_{\eta\eta}}$	$\frac{1}{\mathrm{K}}$	(S10.4)
Thermal expansion coefficient w.r.t. potential temperature sea_h_expansion_theta_si	$\alpha^{\theta} = \frac{h_{\eta P}}{h_P h^{\theta}_{\eta\eta}}$	$\frac{1}{\mathrm{K}}$	(S10.5)
Thermal expansion coefficient w.r.t. potential enthalpy sea_h_expansion_h_si	$\alpha^{h} = \frac{h_{\eta P}}{h_P h^{\theta}_{\eta}}$	$\frac{\mathrm{kg}}{\mathrm{J}}$	(S10.6)
Isothermal haline contraction sea_h_contraction_t_si	$\beta = \frac{h_{S\eta} h_{\eta P} - h_{SP} h_{\eta\eta}}{h_P h_{\eta\eta}}$	1	(S10.7)
Haline contraction coefficient w.r.t. potential temperature Sea_h_contraction_theta_si	$\beta^{\theta} = \frac{h^{\theta}_{S\eta} h_{\eta P} - h_{SP} h^{\theta}_{\eta\eta}}{h_P h^{\theta}_{\eta\eta}}$	1	(S10.8)
Haline contraction coefficient w.r.t. potential enthalpy sea_h_contraction_h_si	$\beta^{\Theta} = \frac{h^{\theta}_{S} h_{\eta P} - h_{SP} h^{\theta}_{\eta}}{h_P h^{\theta}_{\eta}}$	1	(S10.9)

Table S11: Partial derivatives of the Gibbs function of humid air, $g^{\mathrm{AV}}(A,T,P)$, section 4.4, expressed as partial derivatives of the Helmholtz function, $f^{\mathrm{AV}}(A,T,\rho)$. Subscripts indicate partial derivatives with respect to the respective variables. Computed iteratively from Eq. (4.38), ρ is the density of humid air at given values of *A*, *T* and *P*.

Expression in $g^{\mathrm{AV}}(A,T,P)$ Library function	Equivalent in $f^{\mathrm{AV}}(A,T,\rho)$	SI Unit	Eq.
P	$\rho^2 f_\rho^{\mathrm{AV}}$	Pa	(S11.1)
g^{AV} air_g_si	$f^{\mathrm{AV}} + \rho f_\rho^{\mathrm{AV}}$	$\mathrm{J\,kg^{-1}}$	(S11.2)
g_A^{AV} air_g_si	f_A^{AV}	$\mathrm{J\,kg^{-1}}$	(S11.3)
g_P^{AV} air_g_si	ρ^{-1}	$\mathrm{m^3kg^{-1}}$	(S11.4)
g_T^{AV} air_g_si	f_T^{AV}	$\mathrm{J\,kg^{-1}\,K^{-1}}$	(S11.5)
g_{AA}^{AV} air_g_si	$f_{AA}^{\mathrm{AV}} - \dfrac{\rho\left(f_{A\rho}^{\mathrm{AV}}\right)^2}{\left(2f_\rho^{\mathrm{AV}} + \rho f_{\rho\rho}^{\mathrm{AV}}\right)}$	$\mathrm{J\,kg^{-1}}$	(S11.6)
g_{AT}^{AV} air_g_si	$f_{AT}^{\mathrm{AV}} - \dfrac{\rho f_{A\rho}^{\mathrm{AV}} f_{\rho T}^{\mathrm{AV}}}{\left(2f_\rho^{\mathrm{AV}} + \rho f_{\rho\rho}^{\mathrm{AV}}\right)}$	$\mathrm{J\,kg^{-1}\,K^{-1}}$	(S11.7)
g_{AP}^{AV} air_g_si	$\dfrac{f_{A\rho}^{\mathrm{AV}}}{\rho\left(2f_\rho^{\mathrm{AV}} + \rho f_{\rho\rho}^{\mathrm{AV}}\right)}$	$\mathrm{m^3kg^{-1}}$	(S11.8)
g_{PP}^{AV} air_g_si	$-\dfrac{1}{\rho^3\left(2f_\rho^{\mathrm{AV}} + \rho f_{\rho\rho}^{\mathrm{AV}}\right)}$	$\mathrm{m^3kg^{-1}\,Pa^{-1}}$	(S11.9)
g_{TP}^{AV} air_g_si	$\dfrac{f_{T\rho}^{\mathrm{AV}}}{\rho\left(2f_\rho^{\mathrm{AV}} + \rho f_{\rho\rho}^{\mathrm{AV}}\right)}$	$\mathrm{m^3kg^{-1}\,K^{-1}}$	(S11.10)
g_{TT}^{AV} air_g_si	$f_{TT}^{\mathrm{AV}} - \dfrac{\rho\left(f_{T\rho}^{\mathrm{AV}}\right)^2}{\left(2f_\rho^{\mathrm{AV}} + \rho f_{\rho\rho}^{\mathrm{AV}}\right)}$	$\mathrm{J\,kg^{-1}\,K^{-2}}$	(S11.11)

Table S12: Thermodynamic properties derived from the Gibbs function $g^{\mathrm{AV}}(A,T,P)$ of humid air, Eq. (4.37), section 4.4, and its temperature, pressure and air-fraction derivatives. The superscript AV on g is suppressed for simplicity. The molar mass of humid air M_{AV} is given by Eq. (2.8). R = 8.314472 J mol^{-1} K^{-1} is the molar gas constant.

Quantity Library function	Formula	SI Unit	Eq.
Density air_g_density_si	$\rho = 1/g_P$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S12.1)
Specific entropy air_g_entropy_si	$\eta = -g_T$	$\frac{\mathrm{J}}{\mathrm{kgK}}$	(S12.2)
Specific enthalpy air_g_enthalpy_si	$h = g - T g_T$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S12.3)
Partial enthalpy of vapour	$h^{\mathrm{W}} = g - T g_T - A g_A + AT g_{AT}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S12.4)
Specific internal energy air_g_internal_energy_si	$u = g - T g_T - P g_P$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S12.5)
Specific Helmholtz energy	$f = g - P g_P$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S12.6)
Specific isobaric heat capacity air_g_cp_si	$c_P = -T g_{TT}$	$\frac{\mathrm{J}}{\mathrm{kgK}}$	(S12.7)
Specific isochoric heat capacity air_g_cv_si	$c_v = T\left(g_{TP}^2 - g_{TT} g_{PP}\right)/ g_{PP}$	$\frac{\mathrm{J}}{\mathrm{kgK}}$	(S12.8)
Thermal expansion coefficient air_g_expansion_si	$\alpha = g_{TP} / g_P$	$\frac{1}{\mathrm{K}}$	(S12.9)
Isothermal compressibility air_g_kappa_t_si	$\kappa_T = -g_{PP} / g_P$	$\frac{1}{\mathrm{Pa}}$	(S12.10)
Isentropic compressibility air_g_kappa_s_si	$\kappa_s = \left(g_{TP}^2 - g_{TT} g_{PP}\right)/\left(g_P g_{TT}\right)$	$\frac{1}{\mathrm{Pa}}$	(S12.11)
Compressibility factor air_g_compressibilityfactor_si	$Z_{\mathrm{AV}} = M_{\mathrm{AV}} \frac{P g_P}{RT}$	1	(S12.12)
Sound speed air_g_soundspeed_si	$c = g_P \sqrt{g_{TT} /\left(g_{TP}^2 - g_{TT} g_{PP}\right)}$	$\frac{\mathrm{m}}{\mathrm{s}}$	(S12.13)
Adiabatic lapse rate air_g_lapserate_si	$\Gamma = -g_{TP} / g_{TT}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S12.14)
Chemical potential of vapour	$\mu^{\mathrm{W}} = g - A g_A$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S12.15)
Chemical Coefficient	$D_{\mathrm{A}} = A^2 g_{AA}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S12.16)
Air contraction coefficient air_g_contraction_si	$\beta = -g_{AP}/g_P$	1	(S12.17)

Table S13: Partial derivatives of the enthalpy potential function $h^{\mathrm{AV}}(A,\eta,P)$ of humid air, Eq. (4.40), section 4.5, expressed as partial derivatives of the Gibbs function $g^{\mathrm{AV}}(A,T,P)$ of humid air, Eq. (4.37). Subscripts indicate partial derivatives with respect to the respective variables. The superscripts AV on *g* and *h* are omitted for simplicity.

Expression in $h^{\mathrm{AV}}(A,\eta,P)$ Library function	Equivalent in $g^{\mathrm{AV}}(A,T,P)$	SI Unit	Eq.
η	$-g_T$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S13.1)
h air_h_si	$g - Tg_T$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S13.2)
h_A air_h_si	g_A	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S13.3)
h_η air_h_si	T	K	(S13.4)
h_P air_h_si	g_P	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S13.5)
h_{AA} air_h_si	$\frac{g_{AA}g_{TT} - g_{AT}^2}{g_{TT}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S13.6)
$h_{A\eta}$ air_h_si	$-\frac{g_{AT}}{g_{TT}}$	K	(S13.7)
h_{AP} air_h_si	$\frac{g_{AP}g_{TT} - g_{AT}g_{TP}}{g_{TT}}$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S13.8)
$h_{\eta\eta}$ air_h_si	$-\frac{1}{g_{TT}}$	$\frac{\mathrm{kg\,K}^2}{\mathrm{J}}$	(S13.9)
$h_{\eta P}$ air_h_si	$-\frac{g_{TP}}{g_{TT}}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S13.10)
h_{PP} air_h_si	$\frac{g_{TT}g_{PP} - g_{TP}^2}{g_{TT}}$	$\frac{\mathrm{m}^3}{\mathrm{kg\,Pa}}$	(S13.11)

Table S14: Thermodynamic properties derived from the enthalpy $h^{\mathrm{AV}}(A,\eta,P)$ of humid air, Eq. (4.40), section 4.5, and its derivatives with respect to dry-air mass fraction, entropy and pressure. The superscripts AV on h and g are suppressed for simplicity. If the temperature (S14.2) is evaluated at a pressure different from that used for the computation of the entropy, T is regarded as "potential temperature", θ, referenced to this pressure. The adiabatic lapse rate is given with respect to pressure rather than altitude and refers to subsaturated humid air, often referred to as "dry-adiabatic" in the meteorological literature.

Quantity Library function	Formula	SI Unit	Eq.
Density	$\rho = \frac{1}{h_P}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S14.1)
Temperature air_temperature_si	$T = h_\eta$	K	(S14.2)
Relative chemical potential	$\mu = h_A$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S14.3)
Specific Gibbs energy	$g = h - \eta h_\eta$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S14.4)
Specific internal energy	$u = h - P h_P$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S14.5)
Specific Helmholtz energy	$f = h - \eta h_\eta - P h_P$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S14.6)
Specific isobaric heat capacity	$c_P = \frac{T}{h_{\eta\eta}}$	$\frac{\mathrm{J}}{\mathrm{kgK}}$	(S14.7)
Isentropic compressibility	$\kappa_s = -\frac{h_{PP}}{h_P}$	$\frac{1}{\mathrm{Pa}}$	(S14.8)
Sound speed	$c = \frac{h_P}{\sqrt{-h_{PP}}}$	$\frac{\mathrm{m}}{\mathrm{s}}$	(S14.9)
Adiabatic lapse rate	$\Gamma = h_{\eta P}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S14.10)

Table S15: Properties of the saturation equilibrium, section 5.1, computed from the variables $T, P,\ \rho^{\mathrm{V}}$ and ρ^{W}, the iteratively determined solution of Eqs. (5.2) - (5.4)

Quantity Library function	Formula	SI Unit	Eq.
Boiling temperature liq_vap_boilingtemperature_si liq_vap_temperature_si	T	K	(S15.1)
Chemical potential liq_vap_chempot_si	$f^{\mathrm{F}}\left(T,\rho^{\mathrm{W}}\right)+\frac{P}{\rho^{\mathrm{W}}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S15.2)
Liquid density liq_vap_density_liq_si	ρ^{W}	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S15.3)
Vapour density liq_vap_density_vap_si	ρ^{V}	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S15.4)
Evaporation enthalpy liq_vap_enthalpy_evap_si	$Tf_T^{\mathrm{F}}\left(T,\rho^{\mathrm{W}}\right)-Tf_T^{\mathrm{F}}\left(T,\rho^{\mathrm{V}}\right)$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S15.5)
Liquid enthalpy liq_vap_enthalpy_liq_si	$f^{\mathrm{F}}\left(T,\rho^{\mathrm{W}}\right)+\frac{P}{\rho^{\mathrm{W}}}-Tf_T^{\mathrm{F}}\left(T,\rho^{\mathrm{W}}\right)$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S15.6)
Vapour enthalpy liq_vap_enthalpy_vap_si	$f^{\mathrm{F}}\left(T,\rho^{\mathrm{V}}\right)+\frac{P}{\rho^{\mathrm{V}}}-Tf_T^{\mathrm{F}}\left(T,\rho^{\mathrm{V}}\right)$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S15.7)
Evaporation entropy liq_vap_entropy_evap_si	$f_T^{\mathrm{F}}\left(T,\rho^{\mathrm{W}}\right)-f_T^{\mathrm{F}}\left(T,\rho^{\mathrm{V}}\right)$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S15.8)
Liquid entropy liq_vap_entropy_liq_si	$-f_T^{\mathrm{F}}\left(T,\rho^{\mathrm{W}}\right)$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S15.9)
Vapour entropy liq_vap_entropy_vap_si	$-f_T^{\mathrm{F}}\left(T,\rho^{\mathrm{V}}\right)$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S15.10)
Vapour pressure liq_vap_vapourpressure_si liq_vap_pressure_liq_si liq_vap_pressure_vap_si	P	Pa	(S15.11)
Evaporation volume liq_vap_volume_evap_si	$\frac{1}{\rho^{\mathrm{V}}}-\frac{1}{\rho^{\mathrm{W}}}$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S15.12)
Liquid volume	$\frac{1}{\rho^{\mathrm{W}}}$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S15.13)
Vapour volume	$\frac{1}{\rho^{\mathrm{V}}}$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S15.14)

Table S16: Properties of the melting equilibrium, section 5.2, computed from the variables T, P and ρ^{W}, the iteratively determined solution of Eqs. (5.6), (5.7).

Quantity Library function	Formula	SI Unit	Eq.
Melting temperature ice_liq_meltingtemperature_si ice_liq_temperature_si	T	K	(S16.1)
Chemical potential ice_liq_chempot_si	$g^{\mathrm{Ih}}(T,P)$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S16.2)
Liquid density ice_liq_density_liq_si	ρ^{W}	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S16.3)
Ice density ice_liq_density_ice_si	$\frac{1}{g_P^{\mathrm{Ih}}(T,P)}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S16.4)
Melting enthalpy ice_liq_enthalpy_melt_si	$Tg_T^{\mathrm{Ih}}(T,P)-Tf_T^{\mathrm{F}}(T,\rho^{\mathrm{W}})$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S16.5)
Liquid enthalpy ice_liq_enthalpy_liq_si	$f^{\mathrm{F}}(T,\rho^{\mathrm{W}})+\frac{P}{\rho^{\mathrm{W}}}-Tf_T^{\mathrm{F}}(T,\rho^{\mathrm{W}})$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S16.6)
Ice enthalpy ice_liq_enthalpy_ice_si	$g^{\mathrm{Ih}}(T,P)-Tg_T^{\mathrm{Ih}}(T,P)$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S16.7)
Melting entropy ice_liq_entropy_melt_si	$g_T^{\mathrm{Ih}}(T,P)-f_T^{\mathrm{F}}(T,\rho^{\mathrm{W}})$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S16.8)
Liquid entropy ice_liq_entropy_liq_si	$-f_T^{\mathrm{F}}(T,\rho^{\mathrm{W}})$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S16.9)
Ice entropy ice_liq_entropy_ice_si	$-g_T^{\mathrm{Ih}}(T,P)$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S16.10)
Melting pressure ice_liq_meltingpressure_si ice_liq_pressure_liq_si	P	Pa	(S16.11)
Melting volume ice_liq_volume_melt_si	$\frac{1}{\rho^{\mathrm{W}}}-g_P^{\mathrm{Ih}}(T,P)$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S16.12)
Liquid volume	$\frac{1}{\rho^{\mathrm{W}}}$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S16.13)
Ice volume	$g_P^{\mathrm{Ih}}(T,P)$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S16.14)

Table S17: Properties of the sublimation equilibrium, section 5.3, computed from the variables *T*, *P* and ρ^{V}, the iteratively determined solution of Eqs. (5.9), (5.10).

Quantity Library function	Formula	SI Unit	Eq.
Sublimation temperature ice_vap_sublimationtemp_si ice_vap_temperature_si	T	K	(S17.1)
Chemical potential ice_vap_chempot_si	$g^{\mathrm{Ih}}(T,P)$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S17.2)
Vapour density ice_vap_density_vap_si	ρ^{V}	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S17.3)
Ice density ice_vap_density_ice_si	$\frac{1}{g_P^{\mathrm{Ih}}(T,P)}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S17.4)
Sublimation enthalpy ice_vap_enthalpy_subl_si	$Tg_T^{\mathrm{Ih}}(T,P) - Tf_T^{\mathrm{F}}(T,\rho^{\mathrm{V}})$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S17.5)
Vapour enthalpy ice_vap_enthalpy_vap_si	$f^{\mathrm{F}}(T,\rho^{\mathrm{V}}) + \frac{P}{\rho^{\mathrm{V}}} - Tf_T^{\mathrm{F}}(T,\rho^{\mathrm{V}})$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S17.6)
Ice enthalpy ice_vap_enthalpy_ice_si	$g^{\mathrm{Ih}}(T,P) - Tg_T^{\mathrm{Ih}}(T,P)$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S17.7)
Sublimation entropy ice_vap_entropy_subl_si	$g_T^{\mathrm{Ih}}(T,P) - f_T^{\mathrm{F}}(T,\rho^{\mathrm{V}})$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S17.8)
Vapour entropy ice_vap_entropy_vap_si	$-f_T^{\mathrm{F}}(T,\rho^{\mathrm{V}})$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S17.9)
Ice entropy ice_vap_entropy_ice_si	$-g_T^{\mathrm{Ih}}(T,P)$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S17.10)
Sublimation pressure ice_vap_sublimationpressure_si ice_vap_pressure_vap_si	P	Pa	(S17.11)
Sublimation volume ice_vap_volume_subl_si	$\frac{1}{\rho^{\mathrm{V}}} - g_P^{\mathrm{Ih}}(T,P)$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S17.12)
Vapour volume	$\frac{1}{\rho^{\mathrm{V}}}$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S17.13)
Ice volume	$g_P^{\mathrm{Ih}}(T,P)$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S17.14)

Table S18: Single-phase properties of the seawater-ice equilibrium, section 5.4, and sea-ice properties, superscript SI, computed from the variables S_A, T, P and ρ^W, the iteratively determined solution of Eqs. (5.12), (5.13).

Quantity Library function	Formula	SI Unit	Eq.
Freezing temperature sea_ice_freezingtemperature_si	T	K	(S18.1)
Brine salinity sea_ice_brinesalinity_si sea_ice_salinity_si	S_A	$\frac{\mathrm{kg}}{\mathrm{kg}}$	(S18.2)
Chemical potential	$g^\mathrm{Ih}(T,P)$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S18.3)
Brine density sea_ice_density_sea_si	$\frac{1}{g_P^\mathrm{S}(S_\mathrm{A},T,P)+1/\rho^\mathrm{W}}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S18.4)
Ice density sea_ice_density_ice_si	$\frac{1}{g_P^\mathrm{Ih}(T,P)}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S18.5)
Brine enthalpy sea_ice_enthalpy_sea_si	$f^\mathrm{F}(T,\rho^\mathrm{W})+\frac{P}{\rho^\mathrm{W}}-Tf_T^\mathrm{F}(T,\rho^\mathrm{W})$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S18.6)
Ice enthalpy sea_ice_enthalpy_ice_si	$g^\mathrm{Ih}(T,P)-Tg_T^\mathrm{Ih}(T,P)$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S18.7)
Brine entropy sea_ice_entropy_sea_si	$-f_T^\mathrm{F}(T,\rho^\mathrm{W})-g_T^\mathrm{S}(S_\mathrm{A},T,P)$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S18.8)
Ice entropy sea_ice_entropy_ice_si	$-g_T^\mathrm{Ih}(T,P)$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S18.9)
Melting pressure sea_ice_meltingpressure_si	P	Pa	(S18.10)
Brine volume	$\frac{1}{\rho^\mathrm{W}}+g_P^\mathrm{S}(S_\mathrm{A},T,P)$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S18.11)
Ice volume	$g_P^\mathrm{Ih}(T,P)$	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S18.12)
Expansion coefficient of sea ice	$\alpha^\mathrm{SI}=g_{TP}^\mathrm{SI}(S_\mathrm{SI},T,P)/g_P^\mathrm{SI}(S_\mathrm{SI},T,P)$	$\frac{1}{\mathrm{K}}$	(S18.13)
Adiabatic lapse rate of sea ice	$\Gamma^\mathrm{SI}=-g_{TP}^\mathrm{SI}(S_\mathrm{SI},T,P)/g_{TT}^\mathrm{SI}(S_\mathrm{SI},T,P)$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S18.14)

Table S19: Properties of the seawater evaporation equilibrium, section 5.5, computed from the variables S_A, T, P, ρ^V and ρ^W, the iteratively determined solutions of Eqs. (5.27) - (5.29).

Quantity Library function	Formula	SI Unit	Eq.
Boiling temperature sea_vap_boilingtemperature_si sea_vap_temperature_si	T	K	(S19.1)
Brine salinity sea_vap_brinesalinity_si sea_vap_salinity_si	S_A		(S19.2)
Brine density sea_vap_density_sea_si	$\frac{1}{g_P^{Ih}(T,P)}$	$\frac{\text{kg}}{\text{m}^3}$	(S19.3)
Vapour density sea_vap_density_vap_si	ρ^V	$\frac{\text{kg}}{\text{m}^3}$	(S19.4)
Brine enthalpy sea_vap_enthalpy_sea_si	$g^{Ih}(T,P) - Tg_T^{Ih}(T,P)$	$\frac{\text{J}}{\text{kg}}$	(S19.5)
Vapour enthalpy sea_vap_enthalpy_vap_si	$f^F(T,\rho^V) + \frac{P}{\rho^V} - Tf_T^F(T,\rho^V)$	$\frac{\text{J}}{\text{kg}}$	(S19.6)
Brine entropy sea_vap_entropy_sea_si	$-g_T^{Ih}(T,P)$	$\frac{\text{J}}{\text{kg K}}$	(S19.7)
Vapour entropy sea_vap_entropy_vap_si	$-f_T^F(T,\rho^V)$	$\frac{\text{J}}{\text{kg K}}$	(S19.8)
Vapour pressure sea_vap_vapourpressure_si sea_vap_pressure_si	P	Pa	(S19.9)
Vapour volume	$\frac{1}{\rho^V}$	$\frac{\text{m}^3}{\text{kg}}$	(S19.10)
Brine volume	$g_P^{Ih}(T,P)$	$\frac{\text{m}^3}{\text{kg}}$	(S19.11)

Table S20: Derivatives of the Gibbs function $g^{\mathrm{AW}}\left(w^{\mathrm{A}},T,P\right)$, Eq. (5.58), section 5.8, of wet air expressed in terms of the Gibbs functions $g^{\mathrm{AV}}\left(A,T,P\right)$, Eq. (4.37), of humid air, and $g^{\mathrm{W}}\left(T,P\right)$, Eq. (4.2), of liquid water. The latency operator Λ_{AW} is specified in Eqs. (5.61) - (5.62). The chemical coefficient D_{A} is defined in Eq. (S12.16). The function $A(T, P)$ is the solution of Eq. (5.48).

Derivative of $g^{\mathrm{AW}}\left(w^{\mathrm{A}},T,P\right)$ Library function	Expression in $g^{\mathrm{AV}}\left(A,T,P\right)$ and $g^{\mathrm{W}}\left(T,P\right)$	Equation
g^{AW} liq_air_g_si	$\frac{w^{\mathrm{A}}}{A}g^{\mathrm{AV}}+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g^{\mathrm{W}}$	(S20.1)
$g_{w^{\mathrm{A}}}^{\mathrm{AW}}$ liq_air_g_si	$\frac{g^{\mathrm{AV}}-g^{\mathrm{W}}}{A}$	(S20.2)
g_{T}^{AW} liq_air_g_si	$\frac{w^{\mathrm{A}}}{A}g_{T}^{\mathrm{AV}}+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g_{T}^{\mathrm{W}}$	(S20.3)
g_{P}^{AW} liq_air_g_si	$\frac{w^{\mathrm{A}}}{A}g_{P}^{\mathrm{AV}}+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g_{P}^{\mathrm{W}}$	(S20.4)
$g_{w^{\mathrm{A}}w^{\mathrm{A}}}^{\mathrm{AW}}$ liq_air_g_si	0	(S20.5)
$g_{w^{\mathrm{A}}T}^{\mathrm{AW}}$ liq_air_g_si	$\frac{g_{T}^{\mathrm{AV}}-g_{T}^{\mathrm{W}}}{A}$	(S20.6)
$g_{w^{\mathrm{A}}P}^{\mathrm{AW}}$ liq_air_g_si	$\frac{g_{P}^{\mathrm{AV}}-g_{P}^{\mathrm{W}}}{A}$	(S20.7)
g_{TT}^{AW} liq_air_g_si	$\frac{w^{\mathrm{A}}}{A}\left(g_{TT}^{\mathrm{AV}}-\frac{\left(\Lambda_{\mathrm{AW}}[\eta]\right)^{2}}{D_{\mathrm{A}}}\right)+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g_{TT}^{\mathrm{W}}$	(S20.8)
g_{TP}^{AW} liq_air_g_si	$\frac{w^{\mathrm{A}}}{A}\left(g_{TP}^{\mathrm{AV}}+\frac{\Lambda_{\mathrm{AW}}[\eta]\Lambda_{\mathrm{AW}}[v]}{D_{\mathrm{A}}}\right)+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g_{TP}^{\mathrm{W}}$	(S20.9)
g_{PP}^{AW} liq_air_g_si	$\frac{w^{\mathrm{A}}}{A}\left(g_{PP}^{\mathrm{AV}}-\frac{\left(\Lambda_{\mathrm{AW}}[v]\right)^{2}}{D_{\mathrm{A}}}\right)+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g_{PP}^{\mathrm{W}}$	(S20.10)

Table S21: Selected properties of wet air computed from the Gibbs function (5.58), $g^{\mathrm{AW}}\left(w^{\mathrm{A}}, T, P\right)$, section 5.8, and its partial derivatives, Table S20. The superscript AW is suppressed here for simplicity. The latency operator Λ_{AW} is specified in Eqs. (5.61) - (5.62). The function $A = A^{\mathrm{sat}}(T, P)$ is the solution of Eq. (5.48). The lapse rate of wet air is often regarded as the "moist-adiabatic" lapse rate in the meteorological literature.

Quantity Library function	Formula	SI Unit	Eq.
Specific isobaric heat capacity liq_air_g_cp_si	$c_P = -T g_{TT}$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S21.1)
Density liq_air_g_density_si	$\rho = 1/g_P$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S21.2)
Specific entropy liq_air_g_entropy_si	$\eta = -g_T$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S21.3)
Specific enthalpy liq_air_g_enthalpy_si	$h = g - T g_T$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S21.4)
Evaporation enthalpy liq_air_enthalpy_evap_si	$L_P^{\mathrm{AW}} = T\Lambda_{\mathrm{AW}}[\eta]$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S21.5)
Thermal expansion coefficient liq_air_g_expansion_si	$\alpha = g_{TP}/g_P$	$\frac{1}{\mathrm{K}}$	(S21.6)
Isothermal compressibility liq_air_g_kappa_t_si	$\kappa_T = -g_{PP}/g_P$	$\frac{1}{\mathrm{Pa}}$	(S21.7)
Adiabatic lapse rate liq_air_g_lapserate_si	$\Gamma = -g_{TP}/g_{TT}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S21.8)
Air mass fraction liq_air_massfraction_air_si	$A = A^{\mathrm{sat}}(T, P)$	1	(S21.9)
Liquid mass fraction liq_air_liquidfraction_si	$w^{\mathrm{W}} = 1 - w^{\mathrm{A}}/A$	1	(S21.10)
Vapour mass fraction liq_air_vapourfraction_si	$w^{\mathrm{V}} = (1/A - 1)w^{\mathrm{A}}$	1	(S21.11)

Table S22: Partial derivatives of the enthalpy potential function $h^{\mathrm{AW}}\left(w^{\mathrm{A}},\eta,P\right)$ of wet air, Eq. (5.63), section 5.8, expressed as partial derivatives of the Gibbs function $g^{\mathrm{AW}}\left(w^{\mathrm{A}},T,P\right)$ of wet air, Eq. (5.58). Subscripts indicate partial derivatives with respect to the respective variables. The superscripts AW on *g* and *h* are omitted for simplicity. Because of minor practical relevance, derivatives with respect to w^{A} are omitted.

Expression in $h^{\mathrm{AW}}\left(w^{\mathrm{A}},\eta,P\right)$ Library function	Equivalent in $g^{\mathrm{AW}}\left(w^{\mathrm{A}},T,P\right)$	SI Unit	Eq.
η	$-g_T$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S22.1)
h liq_air_h_si	$g-Tg_T$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S22.2)
h_η liq_air_h_si	T	K	(S22.3)
h_P liq_air_h_si	g_P	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S22.4)
$h_{\eta\eta}$ liq_air_h_si	$-\frac{1}{g_{TT}}$	$\frac{\mathrm{kg\,K}^2}{\mathrm{J}}$	(S22.5)
$h_{\eta P}$ liq_air_h_si	$-\frac{g_{TP}}{g_{TT}}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S22.6)
h_{PP} liq_air_h_si	$\frac{g_{TT}g_{PP}-g_{TP}^2}{g_{TT}}$	$\frac{\mathrm{m}^3}{\mathrm{kg\,Pa}}$	(S22.7)

Table S23: Selected properties of wet air computed from the enthalpy (5.63), $h^{\mathrm{AW}}\left(w^{\mathrm{A}},\eta,P\right)$, section 5.8, and its partial derivatives, Table S22. The superscript AW is suppressed here for simplicity. The lapse rate of wet air is often regarded as the “moist-adiabatic” lapse rate in the meteorological literature.

Quantity Library function	Formula	SI Unit	Eq.
Density liq_air_h_density_si	$\rho=\frac{1}{h_P}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S23.1)
Temperature liq_air_h_temperature_si	$T=h_\eta$	K	(S23.2)
Specific isobaric heat capacity liq_air_h_cp_si	$c_P=\frac{T}{h_{\eta\eta}}$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S23.3)
Isentropic compressibility liq_air_h_kappa_s_si	$\kappa_s=-\frac{h_{PP}}{h_P}$	$\frac{1}{\mathrm{Pa}}$	(S23.4)
Adiabatic lapse rate liq_air_h_lapserate_si	$\Gamma=h_{\eta P}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S23.5)

Table S24: Derivatives of the Gibbs function $g^{\mathrm{AI}}\left(w^{\mathrm{A}},T,P\right)$, Eq. (5.73), section 5.9, of ice air expressed in terms of the Gibbs functions $g^{\mathrm{AV}}\left(A,T,P\right)$, Eq. (4.37), of humid air, and $g^{\mathrm{Ih}}\left(T,P\right)$, of ice Ih, section 2.2. The latency operator Λ_{AI} is specified in Eqs. (5.76) - (5.77). The chemical coefficient D_{A} is defined in Eq. (S12.16). The function $A(T, P)$ is the solution of Eq. (5.70).

Derivative of $g^{\mathrm{AW}}\left(w^{\mathrm{A}},T,P\right)$ Library function	Expression in $g^{\mathrm{AV}}\left(A,T,P\right)$ and $g^{\mathrm{Ih}}\left(T,P\right)$	Equation
g^{AI} ice_air_g_si	$\frac{w^{\mathrm{A}}}{A}g^{\mathrm{AV}}+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g^{\mathrm{Ih}}$	(S24.1)
$g^{\mathrm{AI}}_{w^{\mathrm{A}}}$ ice_air_g_si	$\frac{g^{\mathrm{AV}}-g^{\mathrm{Ih}}}{A}$	(S24.2)
g^{AI}_{T} ice_air_g_si	$\frac{w^{\mathrm{A}}}{A}g^{\mathrm{AV}}_{T}+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g^{\mathrm{Ih}}_{T}$	(S24.3)
g^{AI}_{P} ice_air_g_si	$\frac{w^{\mathrm{A}}}{A}g^{\mathrm{AV}}_{P}+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g^{\mathrm{Ih}}_{P}$	(S24.4)
$g^{\mathrm{AI}}_{w^{\mathrm{A}}w^{\mathrm{A}}}$ ice_air_g_si	0	(S24.5)
$g^{\mathrm{AI}}_{w^{\mathrm{A}}T}$ ice_air_g_si	$\frac{g^{\mathrm{AV}}_{T}-g^{\mathrm{Ih}}_{T}}{A}$	(S24.6)
$g^{\mathrm{AI}}_{w^{\mathrm{A}}P}$ ice_air_g_si	$\frac{g^{\mathrm{AV}}_{P}-g^{\mathrm{Ih}}_{P}}{A}$	(S24.7)
g^{AI}_{TT} ice_air_g_si	$\frac{w^{\mathrm{A}}}{A}\left(g^{\mathrm{AV}}_{TT}-\frac{\left(\Lambda_{\mathrm{AI}}[\eta]\right)^2}{D_{\mathrm{A}}}\right)+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g^{\mathrm{Ih}}_{TT}$	(S24.8)
g^{AI}_{TP} ice_air_g_si	$\frac{w^{\mathrm{A}}}{A}\left(g^{\mathrm{AV}}_{TP}+\frac{\Lambda_{\mathrm{AI}}[\eta]\Lambda_{\mathrm{AI}}[v]}{D_{\mathrm{A}}}\right)+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g^{\mathrm{Ih}}_{TP}$	(S24.9)
g^{AI}_{PP} ice_air_g_si	$\frac{w^{\mathrm{A}}}{A}\left(g^{\mathrm{AV}}_{PP}-\frac{\left(\Lambda_{\mathrm{AI}}[v]\right)^2}{D_{\mathrm{A}}}\right)+\left(1-\frac{w^{\mathrm{A}}}{A}\right)g^{\mathrm{Ih}}_{PP}$	(S24.10)

Table S25: Selected properties of ice air computed from the Gibbs function (5.73), $g^{\mathrm{AI}}\left(w^{\mathrm{A}}, T, P\right)$, section 5.9, and its partial derivatives, Table S24. The superscript AI is suppressed here for simplicity. The latency operator Λ_{AI} is specified in Eqs. (5.76) - (5.77). The function $A = A^{\mathrm{sat}}(T, P)$ is the solution of Eq. (5.70). The lapse rate of ice air is often regarded as the "moist-adiabatic" lapse rate in the meteorological literature.

Quantity Library function	Formula	SI Unit	Eq.
Specific isobaric heat capacity ice_air_g_cp_si	$c_P = -T g_{TT}$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S25.1)
Density ice_air_g_density_si	$\rho = 1/g_P$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S25.2)
Specific entropy ice_air_g_entropy_si	$\eta = -g_T$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S25.3)
Specific enthalpy ice_air_g_enthalpy_si	$h = g - T g_T$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S25.4)
Sublimation enthalpy ice_air_enthalpy_subl_si	$L_P^{\mathrm{AI}} = T\Lambda_{\mathrm{AI}}[\eta]$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S25.5)
Sublimation pressure ice_air_sublimationpressure_si	$P^{\mathrm{subl}} = \left(1 - x_A^{\mathrm{AV}}\right)P$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S25.6)
Thermal expansion coefficient ice_air_g_expansion_si	$\alpha = g_{TP}/g_P$	$\frac{1}{\mathrm{K}}$	(S25.7)
Isothermal compressibility ice_air_g_kappa_t_si	$\kappa_T = -g_{PP}/g_P$	$\frac{1}{\mathrm{Pa}}$	(S25.8)
Adiabatic lapse rate ice_air_g_lapserate_si	$\Gamma = -g_{TP}/g_{TT}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S25.9)
Air mass fraction ice_air_massfraction_air_si	$A = A^{\mathrm{sat}}(T, P)$	1	(S25.10)
Solid mass fraction ice_air_solidfraction_si	$w^{\mathrm{Ih}} = 1 - w^{\mathrm{A}}/A$	1	(S25.11)
Vapour mass fraction ice_air_vapourfraction_si	$w^{\mathrm{V}} = (1/A - 1)w^{\mathrm{A}}$	1	(S25.12)

Table S26: Partial derivatives of the enthalpy potential function $h^{\mathrm{AI}}\left(w^{\mathrm{A}},\eta,P\right)$ of ice air, Eq. (5.78), section 5.9, expressed as partial derivatives of the Gibbs function $g^{\mathrm{AI}}\left(w^{\mathrm{A}},T,P\right)$ of ice air, Eq. (5.73). Subscripts indicate partial derivatives with respect to the respective variables. The superscripts AI on *g* and *h* are omitted for simplicity. Because of minor practical relevance, derivatives with respect to w^{A} are omitted.

Expression in $h^{\mathrm{AI}}\left(w^{\mathrm{A}},\eta,P\right)$ Library function	Equivalent in $g^{\mathrm{AI}}\left(w^{\mathrm{A}},T,P\right)$	SI Unit	Eq.
η	$-g_T$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S26.1)
h ice_air_h_si	$g-Tg_T$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S26.2)
h_η ice_air_h_si	T	K	(S26.3)
h_P ice_air_h_si	g_P	$\frac{\mathrm{m}^3}{\mathrm{kg}}$	(S26.4)
$h_{\eta\eta}$ ice_air_h_si	$-\frac{1}{g_{TT}}$	$\frac{\mathrm{kg\,K}^2}{\mathrm{J}}$	(S26.5)
$h_{\eta P}$ ice_air_h_si	$-\frac{g_{TP}}{g_{TT}}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S26.6)
h_{PP} ice_air_h_si	$\frac{g_{TT}g_{PP}-g_{TP}^2}{g_{TT}}$	$\frac{\mathrm{m}^3}{\mathrm{kg\,Pa}}$	(S26.7)

Table S27: Selected properties of ice air computed from the enthalpy, $h^{\mathrm{AI}}\left(w^{\mathrm{A}},\eta,P\right)$, Eq. (5.78), section 5.9, and its partial derivatives, Table S26. The superscript AI is suppressed here for simplicity. The lapse rate of ice air is sometimes regarded as the "moist-adiabatic" lapse rate in the meteorological literature.

Quantity Library function	Formula	SI Unit	Eq.
Density ice_air_h_density_si	$\rho=\frac{1}{h_P}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S27.1)
Temperature ice_air_h_temperature_si	$T=h_\eta$	K	(S27.2)
Specific isobaric heat capacity ice_air_h_cp_si	$c_P=\frac{T}{h_{\eta\eta}}$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S27.3)
Isentropic compressibility ice_air_h_kappa_s_si	$\kappa_s=-\frac{h_{PP}}{h_P}$	$\frac{1}{\mathrm{Pa}}$	(S27.4)
Adiabatic lapse rate ice_air_h_lapserate_si	$\Gamma=h_{\eta P}$	$\frac{\mathrm{K}}{\mathrm{Pa}}$	(S27.5)

Table S28: Properties of wet ice air, section 5.10, computed from A, T, P, w^{A} and w as a solution of Eqs. (A60) - (A65)

Quantity Library function	Formula	SI Unit	Equation
Air fraction of humid air liq_ice_air_airfraction_si	A	$\frac{\mathrm{kg}}{\mathrm{kg}}$	(S28.1)
Air fraction of wet ice air liq_ice_air_dryairfraction_si	w^{A}	$\frac{\mathrm{kg}}{\mathrm{kg}}$	(S28.2)
Liquid fraction of wet ice air liq_ice_air_liquidfraction_si	$w^{\mathrm{W}} = w\left(1-\frac{w^{\mathrm{A}}}{A}\right)$	$\frac{\mathrm{kg}}{\mathrm{kg}}$	(S28.3)
Solid fraction of wet ice air liq_ice_air_solidfraction_si	$w^{\mathrm{Ih}} = (1-w)\left(1-\frac{w^{\mathrm{A}}}{A}\right)$	$\frac{\mathrm{kg}}{\mathrm{kg}}$	(S28.4)
Vapour fraction of wet ice air liq_ice_air_vapourfraction_si	$w^{\mathrm{V}} = w^{\mathrm{A}}\left(\frac{1}{A}-1\right)$	$\frac{\mathrm{kg}}{\mathrm{kg}}$	(S28.5)
Density liq_ice_air_density_si	$\rho = \left(w^{\mathrm{A}}/A\right)\rho^{\mathrm{AV}} + w^{\mathrm{W}}\rho^{\mathrm{W}} + w^{\mathrm{Ih}}\rho^{\mathrm{Ih}}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S28.6)
Specific enthalpy liq_ice_air_enthalpy_si	$h = \left(w^{\mathrm{A}}/A\right)h^{\mathrm{AV}} + w^{\mathrm{W}}h^{\mathrm{W}} + w^{\mathrm{Ih}}h^{\mathrm{Ih}}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S28.7)
Specific entropy liq_ice_air_entropy_si	$\eta = \left(w^{\mathrm{A}}/A\right)\eta^{\mathrm{AV}} + w^{\mathrm{W}}\eta^{\mathrm{W}} + w^{\mathrm{Ih}}\eta^{\mathrm{Ih}}$	$\frac{\mathrm{J}}{\mathrm{kg\,K}}$	(S28.8)
Pressure liq_ice_air_pressure_si	P	Pa	(S28.9)
Isentropic freezing level liq_ice_air_ifl_si	P at $w = 1$	Pa	(S28.10)
Isentropic melting level liq_ice_air_iml_si	P at $w = 0$	Pa	(S28.11)
Temperature liq_ice_air_temperature_si	T	K	(S28.12)

Table S29: Properties of sea air, section 5.11, computed from S_A, A, T, P, ρ^W and ρ^AV as a solution of Eqs. (5.88) - (5.92)

Quantity Library function	Formula	SI Unit	Equation
Air fraction of humid air sea_air_massfraction_air_si	$A = A^\mathrm{cond}\left(S_\mathrm{A}, T, P\right)$	$\frac{\mathrm{kg}}{\mathrm{kg}}$	(S29.1)
Condensation temperature sea_air_condense_temp_si	T	K	(S29.2)
Density of humid air sea_air_density_air_si	ρ^AV	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S29.3)
Vapour density sea_air_density_vap_si	$\rho^\mathrm{V} = \left(1 - A\right)\rho^\mathrm{AV}$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$	(S29.4)
Latent Heat sea_air_enthalpy_evap_si	$L_P^\mathrm{SA} = h^\mathrm{AV} - A h_A^\mathrm{AV} - h^\mathrm{SW} + S_\mathrm{A} h_S^\mathrm{SW}$	$\frac{\mathrm{J}}{\mathrm{kg}}$	(S29.5)
Specific entropy of humid air sea_air_entropy_air_si	$\eta^\mathrm{AV} = -g_T^\mathrm{AV}$	$\frac{\mathrm{J}}{\mathrm{kg\ K}}$	(S29.6)