

Notes on the function gsw_enthalpy_second_derivatives(SA,CT,p)

This function, `gsw_enthalpy_second_derivatives(SA,CT,p)`, evaluates three second order partial derivatives of enthalpy $h = \hat{h}(S_A, \Theta, p)$ with respect to Absolute Salinity and Conservative Temperature. This code uses the 75-term polynomial expression for specific volume is discussed in Roquet *et al.* (2015) and in appendix A.30 and appendix K of the TEOS-10 Manual (IOC *et al.* (2010)).

The appropriate thermal expansion coefficient,

$$\alpha^\ominus = - \frac{1}{\rho} \frac{\partial \rho}{\partial \Theta} \Big|_{S_A, p}, \quad (1)$$

and when evaluated from the 75-term computationally-efficient expression for specific volume, the rms error compared with the same thermal expansion coefficient evaluated directly from the TEOS-10 Gibbs function is $0.03 \times 10^{-6} \text{ K}^{-1}$ in the “oceanographic funnel”. This is to be compared with the rms error of the thermal expansion coefficient of the laboratory data to which the TEOS-10 Gibbs function was fitted of $0.73 \times 10^{-6} \text{ K}^{-1}$.

The saline contraction coefficient β^\ominus is defined as

$$\beta^\ominus = \frac{1}{\rho} \frac{\partial \rho}{\partial S_A} \Big|_{\Theta, p}, \quad (1)$$

and when evaluated from the 75-term computationally-efficient expression for specific volume. In terms of the evaluation of density gradients, the haline contraction coefficient evaluated from Eqn. (K.3) is many times more accurate than the thermal expansion coefficient. Compared with the mean value of β^\ominus , this error is small compared with the ratio of the uncertainty in the thermal expansion coefficient to its mean value, and so the error in β^\ominus is negligible.

In dynamical oceanography it is the thermal expansion and haline contraction coefficients α^\ominus and β^\ominus which are the most important aspects of the equation of state since the “thermal wind” is proportional to $\alpha^\ominus \nabla_p \Theta - \beta^\ominus \nabla_p S_A$ and the vertical static stability is given in terms of the buoyancy frequency N by $g^{-1} N^2 = \alpha^\ominus \Theta_z - \beta^\ominus (S_A)_z$. Hence for dynamical oceanography we may take the 75-term polynomial function expression for specific volume as essentially reflecting the full accuracy of TEOS-10.

This 75-term expression for specific volume is the obvious choice for use in ocean models since it is a function of the model’s temperature variable, Conservative Temperature. The highly accurate nature of the 75-term expressions means that theoretical studies, observational oceanography and ocean modeling can all be performed using the same equation of state which is conveniently expressed in terms of Conservative Temperature. This ends the need to continually transform from Conservative Temperature back to in situ temperature in order to calculate density and its derivatives. It is this 75-term expression for specific volume that is used in the GSW functions to evaluate the buoyancy frequency N and the various geostrophic streamfunctions, and will be the basis for updated algorithms for ω -surfaces (Klocker *et al.* (2010)) and Neutral Density γ^n (Jackett and McDougall (1997)).

References

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- McDougall, T.J., D.R. Jackett, D.G. Wright and R. Feistel, 2003: Accurate and computationally efficient algorithms for potential temperature and density of seawater. *J. Atmosph. Ocean. Tech.*, **20**, pp. 730-741.
- Roquet, F., G. Madec, T. J. McDougall and P. M. Barker, 2015: Accurate polynomial expressions for the density and specific volume of seawater using the TEOS-10 standard. *Ocean Modelling*, **90**, pp. 29-43. <http://dx.doi.org/10.1016/j.ocemod.2015.04.002>

Here follows appendix A.30 and appendix K of the TEOS-10 Manual (IOC *et al.* (2010)).

A.30 Computationally efficient 75-term expression for the specific volume of seawater in terms of Θ

Ocean models to date have treated their salinity and temperature variables as being Practical Salinity S_p and potential temperature θ . Ocean models that are TEOS-10 compatible need to calculate Absolute Salinity S_A and Conservative Temperature Θ (as discussed in appendices A.20 and A.21), and they need a computationally efficient expression for calculating specific volume (or density) in terms of Absolute Salinity S_A , Conservative Temperature Θ and pressure p .

Following the work of McDougall *et al.* (2003) and Jackett *et al.* (2006), the TEOS-10 specific volume \hat{v} has been approximated by a 75-term polynomial by Roquet *et al.* (2015). This polynomial is expressed in terms of the following three dimensionless salinity, temperature and pressure variables,

$$s \equiv \sqrt{\frac{S_A + 24 \text{ g kg}^{-1}}{S_{Au}}}, \quad \tau \equiv \frac{\Theta}{\Theta_u} \quad \text{and} \quad \pi \equiv \frac{p}{p_u}, \quad (\text{A.30.1})$$

in terms of the unit-related scaling constants

$$S_{Au} \equiv 40 \times 35.16504 \text{ g kg}^{-1} / 35, \quad \Theta_u \equiv 40^\circ\text{C} \quad \text{and} \quad p_u \equiv 10^4 \text{ dbar}. \quad (\text{A.30.2})$$

Their polynomial expression for the specific volume of seawater is

$$\hat{v}(S_A, \Theta, p) = v_u \sum_{i,j,k} v_{ijk} s^i \tau^j \pi^k, \quad (\text{A.30.3})$$

where $v_u \equiv 1 \text{ m}^3 \text{ kg}^{-1}$ and the non-zero dimensionless constants v_{ijk} are given in Table K.1 of appendix K. The specific volume data was fitted in a “funnel” of data points in (S_A, Θ, p) space (McDougall *et al.* (2003)) which extends to a pressure of 8000 dbar. At the sea surface the “funnel” covers the full range of temperature and salinity while for pressures greater than 6500 dbar the maximum temperature of the fitted data is 10°C and the minimum Absolute Salinity is 30 g kg^{-1} . That is, the fit has been performed over a region of parameter space which includes water that is approximately 8°C warmer and 5 g kg^{-1} fresher in the deep ocean than the seawater which exists in the present ocean.

As outlined in appendix K, this 75-term polynomial expression for v yields the thermal expansion and saline contraction coefficients, α^Θ and β^Θ , that are essentially as accurate as those derived from the full TEOS-10 Gibbs function for data in the “oceanographic funnel”. In dynamical oceanography it is these thermal expansion and haline contraction coefficients which are the most important aspects of the equation of state since the “thermal wind” is proportional to $\alpha^\Theta \nabla_p \Theta - \beta^\Theta \nabla_p S_A$ and the vertical static stability is given in terms of the buoyancy frequency N by $g^{-1} N^2 = \alpha^\Theta \Theta_z - \beta^\Theta (S_A)_z$. Hence for dynamical oceanography we may take Roquet *et al.*'s (2015) 75-term polynomial expression for specific volume as essentially reflecting the full accuracy of TEOS-10.

Appendix P describes how an expression for the enthalpy of seawater in terms of Conservative Temperature, specifically the functional form $\hat{h}(S_A, \Theta, p)$, together with an expression for entropy in the form $\hat{\eta}(S_A, \Theta)$, can be used as an alternative thermodynamic potential to the Gibbs function $g(S_A, t, p)$. The need for the functional form $\hat{h}(S_A, \Theta, p)$ also arises in section 3.32 and in Eqns. (3.26.3) and (3.29.1). The 75-term expression, Eqn. (A.30.3) for $v^{75} = \hat{v}^{75}(S_A, \Theta, p)$ can be used to find a closed expression for $\hat{h}(S_A, \Theta, p)$ by integrating $\hat{v}^{75}(S_A, \Theta, p)$ with respect to pressure (in Pa), since $\hat{h}_p = v = \rho^{-1}$ (see Eqn. (2.8.3)). Specific enthalpy calculated from $\hat{v}^{75}(S_A, \Theta, p)$ is available in the GSW Oceanographic Toolbox as the function `gsw_enthalpy(SA,CT,p)`. Using `gsw_enthalpy` to

evaluate $\hat{h}(S_A, \Theta, p)$ is 7 times faster than first evaluating the in situ temperature t (from **gsw_t_from_CT**(SA,CT,p)) and then calculating enthalpy from the full Gibbs function expression $h(S_A, t, p)$ using **gsw_enthalpy_t_exact**(SA,t,p). (These last two function calls have also been combined into the one function, **gsw_enthalpy_CT_exact**(SA,CT,p).)

Also, the enthalpy difference at the same values of S_A and Θ but at different pressures (see Eqn. (3.32.5)) is available as the function **gsw_enthalpy_diff**(SA,CT,p_shallow,p_deep).

Following Young (2010), the difference between h and $c_p^0 \Theta$ is called “dynamic enthalpy” and can be found using the function **gsw_dynamic_enthalpy**(SA,CT,p) in the GSW Oceanographic Toolbox.

Appendix K: Coefficients of the 75-term expression for the specific volume of seawater in terms of Θ

The TEOS-10 Gibbs function of seawater $g(S_A, t, p)$ is written as a polynomial in terms of in situ temperature t , while for ocean models, specific volume (or density) needs to be expressed as a computationally efficient expression in terms of Conservative Temperature Θ . Roquet *et al.* (2015) have published such a computationally efficient polynomial for specific volume. Their non-dimensional (root) salinity s , temperature τ , and pressure π , variables are

$$s \equiv \sqrt{\frac{S_A + 24 \text{ g kg}^{-1}}{S_{A_u}}}, \quad \tau \equiv \frac{\Theta}{\Theta_u} \quad \text{and} \quad \pi \equiv \frac{p}{p_u}, \quad (\text{K.1})$$

in terms of the unit-related scaling constants

$$S_{A_u} \equiv 40 \times 35.16504 \text{ g kg}^{-1} / 35, \quad \Theta_u \equiv 40^\circ\text{C} \quad \text{and} \quad p_u \equiv 10^4 \text{ dbar}. \quad (\text{K.2})$$

Their polynomial expression for the specific volume of seawater is

$$\hat{v}(S_A, \Theta, p) = v_u \sum_{i,j,k} v_{ijk} s^i \tau^j \pi^k, \quad (\text{K.3})$$

where $v_u \equiv 1 \text{ m}^3 \text{ kg}^{-1}$ and the non-zero dimensionless constants v_{ijk} are given in Table K.1.

Roquet *et al.* (2015) fitted the TEOS-10 values of specific volume v to S_A , Θ and p in a “funnel” of data points in (S_A, Θ, p) space. This is the same “funnel” of data points as used in McDougall *et al.* (2013); at the sea surface it covers the full range of temperature and salinity while for pressure greater than 6500 dbar, the maximum temperature of the fitted data is 10°C and the minimum Absolute Salinity is 30 g kg^{-1} . The maximum pressure of the “funnel” is 8000 dbar. Table K.1 contains the 75 coefficients of the expression (K.3) for specific volume in terms of (S_A, Θ, p) .

The rms error of this 75-term approximation to the full Gibbs function-derived TEOS-10 specific volume over the “funnel” is $0.2 \times 10^{-9} \text{ m}^3 \text{ kg}^{-1}$; this can be compared with the rms uncertainty of $4 \times 10^{-9} \text{ m}^3 \text{ kg}^{-1}$ of the underlying laboratory density data to which the TEOS-10 Gibbs function was fitted (see the first two rows of Table O.1 of appendix O). Similarly, the appropriate thermal expansion coefficient,

$$\alpha^\Theta = \frac{1}{v} \left. \frac{\partial v}{\partial \Theta} \right|_{S_A, p} = - \frac{1}{\rho} \left. \frac{\partial \rho}{\partial \Theta} \right|_{S_A, p}, \quad (\text{K.4})$$

of the 75-term equation of state is different from the same thermal expansion coefficient evaluated from the full Gibbs function-derived TEOS-10 with an rms error in the “funnel” of $0.03 \times 10^{-6} \text{ K}^{-1}$; this can be compared with the rms error of the thermal expansion coefficient of the laboratory data to which the Feistel (2008) Gibbs function was fitted of $0.73 \times 10^{-6} \text{ K}^{-1}$ (see row six of Table O.1 of appendix O). In terms of the evaluation of density gradients, the haline contraction coefficient evaluated from Eqn. (K.3) is many times more accurate than the thermal expansion coefficient. Hence we may consider the 75-term polynomial expression for specific volume, Eqn. (K.3), to be equally as accurate as the full TEOS-10 expressions for specific volume, for the thermal expansion coefficient and for the haline contraction coefficient for data that reside inside the “oceanographic funnel”.

The sound speed evaluated from the 75-term polynomial of Eqn. (K.3) has an rms error over the “funnel” of 0.025 m s^{-1} which is a little less than the rms error of the underlying sound speed data that was incorporated into the Feistel (2008) Gibbs function, being 0.035 m s^{-1} (see rows 7 to 9 of Table O.1 of appendix O). Hence, especially for the purposes of dynamical oceanography where α^Θ and β^Θ are the aspects of the equation of

state that, together with spatial gradients of S_A and Θ , drive ocean currents and affect the calculation of the buoyancy frequency, we may take the 75-term expression for specific volume, Eqn. (K.3), as essentially reflecting the full accuracy of TEOS-10.

The use of Eqn. (K.3) to evaluate $\hat{v}(S_A, \Theta, p)$ or $\hat{\rho}(S_A, \Theta, p)$ from **gsw_specvol**(SA,CT,p) or **gsw_rho**(SA,CT,p) is approximately five times faster than first evaluating the *in situ* temperature t (from **gsw_t_from_CT**(SA,CT,p)) and then calculating *in situ* specific volume or density from the full Gibbs function expression $v(S_A, t, p)$ or $\rho(S_A, t, p)$ via **gsw_specvol_t_exact**(SA,t,p) or **gsw_rho_t_exact**(SA,t,p). (These two function calls have been combined into **gsw_specvol_CT_exact**(SA,CT,P) and **gsw_rho_CT_exact**(SA,CT,P).)

Table K.1. Coefficients of the 75-term polynomial of Roquet *et al.* (2015).

i	j	k	v_{ijk}	i	j	k	v_{ijk}	i	j	k	v_{ijk}
0	0	0	1.0769995862e-3	0	5	0	-8.0539615540e-7	1	0	2	-5.8484432984e-7
1	0	0	-3.1038981976e-4	1	5	0	-3.3052758900e-7	2	0	2	-4.8122251597e-6
2	0	0	6.6928067038e-4	0	6	0	2.0543094268e-7	3	0	2	4.9263106998e-6
3	0	0	-8.5047933937e-4	0	0	1	-6.0799143809e-5	4	0	2	-1.7811974727e-6
4	0	0	5.8086069943e-4	1	0	1	2.4262468747e-5	0	1	2	-1.1736386731e-6
5	0	0	-2.1092370507e-4	2	0	1	-3.4792460974e-5	1	1	2	-5.5699154557e-6
6	0	0	3.1932457305e-5	3	0	1	3.7470777305e-5	2	1	2	5.4620748834e-6
0	1	0	-1.5649734675e-5	4	0	1	-1.7322218612e-5	3	1	2	-1.3544185627e-6
1	1	0	3.5009599764e-5	5	0	1	3.0927427253e-6	0	2	2	2.1305028740e-6
2	1	0	-4.3592678561e-5	0	1	1	1.8505765429e-5	1	2	2	3.9137387080e-7
3	1	0	3.4532461828e-5	1	1	1	-9.5677088156e-6	2	2	2	-6.5731104067e-7
4	1	0	-1.1959409788e-5	2	1	1	1.1100834765e-5	0	3	2	-4.6132540037e-7
5	1	0	1.3864594581e-6	3	1	1	-9.8447117844e-6	1	3	2	7.7618888092e-9
0	2	0	2.7762106484e-5	4	1	1	2.5909225260e-6	0	4	2	-6.3352916514e-8
1	2	0	-3.7435842344e-5	0	2	1	-1.1716606853e-5	0	0	3	-1.1309361437e-6
2	2	0	3.5907822760e-5	1	2	1	-2.3678308361e-7	1	0	3	3.6310188515e-7
3	2	0	-1.8698584187e-5	2	2	1	2.9283346295e-6	2	0	3	1.6746303780e-8
4	2	0	3.8595339244e-6	3	2	1	-4.8826139200e-7	0	1	3	-3.6527006553e-7
0	3	0	-1.6521159259e-5	0	3	1	7.9279656173e-6	1	1	3	-2.7295696237e-7
1	3	0	2.4141479483e-5	1	3	1	-3.4558773655e-6	0	2	3	2.8695905159e-7
2	3	0	-1.4353633048e-5	2	3	1	3.1655306078e-7	0	0	4	1.0531153080e-7
3	3	0	2.2863324556e-6	0	4	1	-3.4102187482e-6	1	0	4	-1.1147125423e-7
0	4	0	6.9111322702e-6	1	4	1	1.2956717783e-6	0	1	4	3.1454099902e-7
1	4	0	-8.7595873154e-6	0	5	1	5.0736766814e-7	0	0	5	-1.2647261286e-8
2	4	0	4.3703680598e-6	0	0	2	9.9856169219e-6	0	0	6	1.9613503930e-9